A Bayesian nonparametric approach to ecological risk assessment

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Abstract We revisit a classical method for ecological risk assessment, the Species Sensitivity Distribution (SSD) approach, in a Bayesian nonparametric framework. SSD is a mandatory diagnostic required by environmental regulatory bodies from the European Union, the United States, Australia, China etc. Yet, it is subject to much scientific criticism, notably concerning a historically debated parametric assumption for modelling species variability. Tackling the problem using nonparametric mixture models, it is possible to shed this parametric assumption and build a statistically sounder basis for SSD. We use Normalized Random Measures with Independent Increments (NRMI) as the mixing measure because they offer a greater flexibility than the Dirichlet process. Indeed, NRMI can induce a prior on the number of components in the mixture model that is less informative than the Dirichlet process. This feature is consistent with the fact that SSD practitioners do not usually have a strong prior belief on the number of components. In this short paper, we illustrate the advantage of the nonparametric SSD over the classical normal SSD and a kernel density estimate SSD on several real datasets. We summarise the results of the complete study in Kon Kam King et al. (2016), where the method is generalised to censored data and a systematic comparison on simulated data is also presented, along with a study of the clustering induced by the mixture model to examine patterns in species sensitivity.

Keywords: Bayesian Nonparametrics, Ecotoxicology, HC_5, Mixture models, Normalized random measures, Species Sensitivity Distribution.

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1 Introduction

Assessing the response of a community of species to an environmental stress is critical for ecological risk assessment. Methods for this purpose vary in levels of complexity and realism. Species Sensitivity Distribution (SSD) represents an intermediate tier, more refined than rudimentary assessment factors (Posthuma et al., 2002) but practical enough for routine use by environmental managers and regulators in most developed countries (Australia, Canada, China, EU, South Africa, USA...). The SSD approach is intended to provide, for a given contaminant, a description of the tolerance of all species possibly exposed using information collected on a sample of those species. This information consists of Critical Effect Concentrations (CECs), a concentration specific to a species which marks a limit over which the species suffers a critical level of effect. This is for instance the concentration at which 50% of the tested organisms died (Lethal Concentration 50% (LC_{50})), or the concentration which inhibited growth or reproduction by 50% compared to the control experiment (Effect Concentration 50% (EC_{50})). Each CEC is the summary of long and costly bioassay experiments for a single species, so they are rarely available in large number. Typical sample sizes range from 10 to 15 (ECHA, 2008).

To describe the tolerance of all species to be protected, the distribution of the CECs is then estimated from the sample. In practice, a parametric distributional assumption is often adopted (Forbes and Calow, 2002): the CECs are assumed to follow a log-normal (Aldenberg and Jaworska, 2000), log-logistic (Kooijman, 1987), triangular (Van Straalen, 2002; Zhao and Chen, 2016) or BurrIII (Shao, 2000) distribution.

Once the response of the community is characterised by the distribution, the goal of risk assessment is to define a safe concentration protecting all or most of the species. In the case of distributions without a lower threshold strictly above 0, a cut-off value is often chosen as the safe concentration. Typically, this is the Hazardous Concentration for 5% of the Species (HC_5), which is the 5th percentile of the distribution. Reasonings behind this choice include: that the lowest bound of the confidence interval around the 5th percentile will be used instead of the estimate, that a safety factor will be subsequently applied to that value and that ecosystems have a certain resilience to perturbations.

The lack of justification for the choice of any given parametric distribution has sparked several research directions. Some authors (Xu et al., 2015; He et al., 2014; Jagoe and Newman, 1997; Van Straalen, 2002; Xing et al., 2014; Zhao and Chen, 2016) have sought to find the best parametric distribution by model comparison using goodness-of-fit measures. The general understanding is that no single distribution seems to provide a superior fit and that the answer is dataset dependent (Forbes and Calow, 2002). Therefore, the log-normal distribution has become the customary choice, notably because it readily provides confidence intervals on the HC_5, and because model com-

parison and goodness of fit tests have relatively low power on small datasets, precluding the emergence of a definite answer to the question. Another research direction consisted in seeking to avoid any reference to a distribution, using so-called nonparametric or distribution-free approaches. Those efforts included using the empirical distribution function (Suter II et al., 1999; Jones et al., 1999), methods based on ranks (Van Der Hoeven, 2001; Chen, 2004), bootstrap resampling (Jagoe and Newman, 1997; Wang et al., 2008) or nonparametric kernel density estimation (Wang et al., 2015). All these approaches have in common that they require large sample sizes to be effectively applicable. Finally, authors have considered the possibility that the distribution of the CECs might not be a single distribution but rather a mixture of distributions (Zajdlik et al., 2009), datasets being an assemblage of several log-normally distributed subgroups (Kefford et al., 2012; Craig, 2013). This is more realistic from an ecological point of view because several factors influence the tolerance of a species to a contaminant such as the taxonomic group or the mode of action, and contaminant such as pesticides might even target specific species groups. Therefore, there is strong evidence in favour of the presence of groups of CECs, although the CECs within a group might remain log-normally distributed.

Ignorance of the group structure is a strong motivation for a nonparametric approach. However, the method must remain applicable to small datasets, which suggests trying to improve on the existing frequentist nonparametric methods. Bayesian nonparametric mixture models offer an interesting solution for both large and small datasets, because the complexity of the mixture model adapts to the size of the dataset. It offers a good compromise between a simplistic one-component parametric model and a kernel density method which in a certain sense lacks flexibility and might cause overfitting. Moreover, the low amount of information available in small datasets to estimate the groups parameters can be complemented via the prior, as some a priori degree of information is generally available from other species or contaminants (Awkerman et al., 2008; Craig, 2013; Craig et al., 2012). This paper summarises the results of the complete study in Kon Kam King et al. (2016).

The rest of the article is organised as follows. In Section 2 we present the Bayesian nonparametric (BNP) model and existing frequentist models for SSD and explain how to obtain a density estimate. Then in Section 3 we compare the different methods on a real dataset, illustrating the benefits of the BNP SSD. We conclude with a final discussion in Section 4.

2 Models for SSD

Given that concentrations vary on a wide range, it is common practice to work on log-transformed concentrations. Consider a sample of n log-concentrations denoted by $\boldsymbol{X} = (X_1, \ldots, X_n)$. We propose to carry out density estimation for the SSD based on sample $\boldsymbol{X}$ by use of nonparametric mixtures. Bayesian

nonparametric mixtures were introduced in Lo (1984) with Dirichlet process mixtures (DPM). Generalizations of the DPM correspond to allowing the mixing distribution to be any discrete nonparametric prior. A large class of such prior distributions is obtained by normalizing increasing additive processes (Sato, 1999). The normalization step, under suitable conditions, gives rise to so-called normalized measures with independent increments (NRMI) as defined by Regazzini et al. (2003), see also Barrios et al. (2013) for a recent review. An NRMI mixture model is defined hierarchically as:

$$\begin{aligned} X_i|\mu_i,\sigma &\overset{\text{ind}}{\sim} k(\cdot|\mu_i,\sigma), \quad \mu_i|\tilde{P} \overset{\text{i.i.d.}}{\sim} \tilde{P}, \quad i=1,\dots,n, \\ \tilde{P} &\sim \text{NRMI}, \quad \sigma \sim \text{Ga}(a_\sigma, b_\sigma). \end{aligned} \tag{1}$$

where k is a kernel, which we assume parametrized by some $\theta = (\mu,\sigma) \in \mathbb{R}\times\mathbb{R}_+$, and $\tilde{P}$ is a random probability on $\mathbb{R}$ whose distribution is an NRMI. In our model, all clusters have a common variance. This is easier to fit on a small dataset, because information about the variance is pooled across clusters. Similar mixture SSD models described in Craig (2013) also assume common variance. As described in the Introduction, concentrations are commonly fitted with a log-normal distribution. Our aim is to move from this parametric model to the nonparametric one in (1). In order to allow comparisons to be made, we stick to the normal specification for k on the log-concentrations $\boldsymbol{X}$ by letting: $k(x|\mu,\sigma) = \mathcal{N}(x|\mu,\sigma)$. Under this framework, density estimation is carried out by evaluating the posterior predictive density along the lines of Barrios et al. (2013):

$$\hat{f}(x|\tilde{P},\boldsymbol{X}) = \iint k(x|\mu,\sigma)\mathrm{d}\pi(\sigma)\mathrm{d}\tilde{P}(\mu) \tag{2}$$

for any x in $\mathbb{R}$, where π denotes the posterior distribution of σ.

To specify the prior, we choose as mixing random measure the normalized stable process (Kingman, 1975) with:

i a stability parameter $\gamma = 0.4$, which controls the flatness of the prior on the number of clusters. The parameter γ can take values in $(0,1)$. Taking the limit $\gamma \to 0$ reduces the model to a Dirichlet process, larger values of γ lead to less informative priors on the number of clusters. The parameter γ was chosen as a good compromise between model flexibility and numerical stability. The total mass parameter is, without loss of generality, set equal to 1.

ii a base measure (which corresponds to the mean of the random probability measure) $P_0(\cdot) = \mathcal{N}(\cdot\,|\,\varphi_1,\varphi_2)$ with mean φ_1 and standard deviation φ_2, hyperparameters fixed a priori to specify a certain knowledge in the degree of smoothness

iii a common variance for all the clusters with a vaguely informative prior distribution $Ga(0.5,0.5)$.

Recent years have witnessed the appearance of a wealth of softwares dedicated to implement Bayesian nonparametric models and sample from their posterior. To cite a few, the R package DPpackage (Jara et al., 2011), is a rather comprehensive bundle of functions for Bayesian nonparametric models, while Bayesian Regression (Karabatsos, 2016) is a software for Bayesian nonparametric regression. For posterior sampling, we use the R package BNPdensity and the function MixNRMI1 which implements BNP density models under a general specification of normalized random measures based on the generalised gamma processes (see Barrios et al., 2013). The package is available from the Comprehensive R Archive Network (CRAN).

To illustrate the interest of the Bayesian nonparametric SSD, we compare our proposed BNP model to two commonly used frequentist models: the normal distribution (Aldenberg and Jaworska, 2000) and the nonparametric Kernel Density Estimate (KDE) recently proposed by Wang et al. (2015). For both frequentist approaches, the data is assumed to be iid. Density estimates take on respectively the following form ($\hat{\mu}$ and $\hat{\sigma}$ are MLE)

$$\hat{f}_{\mathcal{N}}(x) = \mathcal{N}(x \,|\, \hat{\mu}, \hat{\sigma}) \quad \text{and} \quad \hat{f}_{KDE}(x) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{N}(x \,|\, X_i, 1.06\hat{\sigma} n^{-\frac{1}{5}}). \tag{3}$$

2.1 Model comparison and cross-validation

For the purpose of comparing the predictive performance of the model, we resort to Leave-One-Out (LOO) cross-validation. We compute the LOOs for each of the methods as $\forall i, \mathrm{LOO}_i = \hat{f}(X_i \,|\, \boldsymbol{X}_{-i})$ where $\hat{f}(x \,|\, \boldsymbol{X}_{-i})$ is the density for one of the three methods estimated from $\boldsymbol{X}$ with X_i left out. The LOOs for the BNP model correspond to the conditional predictive ordinates (CPOs) statistics which are commonly used in applications, see Gelfand (1996). A CPO statistic is defined for each log-concentration X_i as follows:

$$\mathrm{CPO}_i = \hat{f}(X_i|\boldsymbol{X}_{-i}) = \int k(X_i|\theta)\mathrm{d}\pi(\theta|\boldsymbol{X}_{-i}) \tag{4}$$

where $\boldsymbol{X}_{-i}$ denotes the all sample $\boldsymbol{X}$ but X_i, $\mathrm{d}\pi(\theta|\boldsymbol{X}_{-i})$ is the posterior distribution associated to $\boldsymbol{X}_{-i}$ and $\hat{f}$ is the (cross-validated) posterior predictive distribution of Equation (2). As shown by Barrios et al. (2013), CPOs can be easily approximated by Monte Carlo as

$$\widehat{\mathrm{CPO}_i} = \left(\frac{1}{T}\sum_{t=1}^{T} \frac{1}{k(X_i|\theta^{(t)})} \right)^{-1} \tag{5}$$

where $\{\theta^{(t)}, t = 1, 2, \ldots, T\}$ is an MCMC sample from the posterior distribution.

2.2 Quantile estimation and HC_5

The quantity of interest for ecological risk assessment is the HC_5, which corresponds to the 5th percentile of the SSD distribution. We choose as an estimator the median of the posterior distribution of the 5th percentile, while the 95% credible bands are formed by the 2.5% and 97.5% quantiles of the posterior distribution of the 5th percentile. The 5th percentile of the KDE is obtained by numerical inversion of the cumulative distribution function, and the confidence intervals using nonparametric bootstrap. The 5th percentile of the normal SSD and its confidence intervals are obtained following the classical method of Aldenberg and Jaworska (2000).

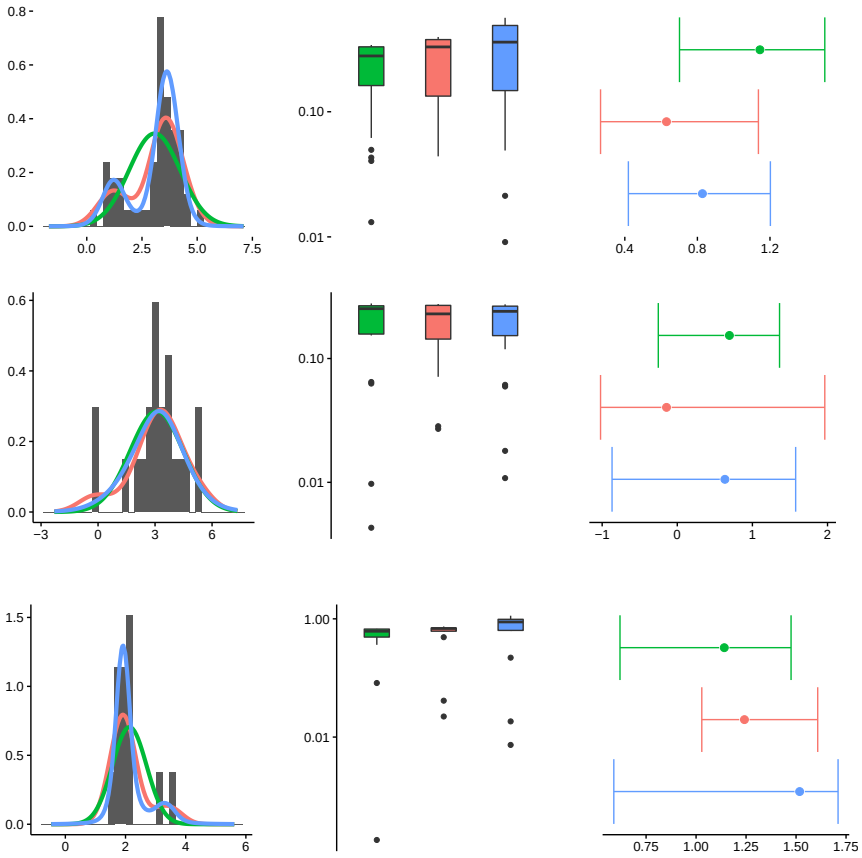
3 Application to real data

We applied this model to a selection of contaminants extracted from a large database collected by the National Institute for Public Health and the Environment (RIVM). This database was prepared, studied and published by Hickey et al. (2012). We only considered non censored data, left or right censored data were discarded, while interval censored data were replaced by the centre of the interval. Kon Kam King et al. (2016) will describe how the method can be adapted to include censored data. Using a continuous distribution for the CECs implies that the model does not support ties (or, in other words, observing ties has zero probability). However, ties may appear in the dataset due to the rounding of concentrations. Hence, we used a small jittering of the data.

We selected three example datasets which feature three typical sample sizes: a relatively large `carbaryl` dataset (CAS: 63-25-2, insecticide, 55 species), a medium-sized `temephos` dataset (CAS: 3383-96-8, mosquito larvicide, 21 species), and a small `captan` dataset (CAS: 133-06-2, fungicide, 13 species). Datasets for new contaminants are always small, the minimum requirement set by the European Chemical Agency being 10 species. The datasets can be visualised on the histograms of Figure 1 (left panel).

These datasets illustrate different features of the three approaches: when there is a clear multimodality in the data, the BNP SSD is more flexible than the fixed bandwidth KDE SSD (Figure 1, `carbaryl` and `captan`). When the data do not exhibit strong multimodality, as for `temephos`, the BNP reduces to the normal SSD model, whereas the KDE remains by construction a mixture of many normal components.

One might think to increase the flexibility of the KDE by simply decreasing the bandwidth. However, that would also decrease the robustness of the method. On the middle panel of Figure 1, the LOOs give an indication of the robustness to over-fitting of the three methods. For `carbaryl` and `captan`, they show that the superior flexibility of the BNP SSD compared to the KDE SSD does not come at the expense of robustness, because the median CPO



(a) Density (b) LOO and CPO (c) log HC_5

Fig. 1: The top panel represents large-size `carbaryl` dataset, the middle panel represents the medium-sized `temephos` dataset, the bottom panel represents small-sized `captan` dataset. Fits of the Normal (in green), KDE (in red) and BNP (in blue) models. Concentrations are log transformed.
Left: Histogram and density estimates.
Centre: Boxplot for the LOOs (for Normal and KDE) and the CPO (for BNP) on logarithmic scale. The horizontal line corresponds to the median. The box hinges extend to the inner quartiles. The whiskers extend to cover points up to one and a half times the inter-quartile distance away from the hinges. For both frequentist methods, the n LOOs are obtained by fitting the model n times, while an analytical expression is available for the BNP method (Equation 5).
Right: log HC_5 and associated confidence/credible intervals (for Normal, KDE and BNP).

of the BNP SSD is higher than the other two. In the case of `temephos`, the median LOO likelihood estimate of the normal model is very similar to the median CPO for the BNP SSD, sign that there is little over-fitting. This generally illustrates the fact that model complexity in a BNP model scales with the amount and structure of the data. On the right panel of Figure 1, the credible intervals of the HC_5 for the BNP SSD are generally larger than the confidence interval of the normal SSD, which is coherent with the model uncertainty of the nonparametric approach.

4 Discussion

The BNP SSD seems to perform well when the dataset deviates from a normal distribution. Its great flexibility is an asset to describe the variability of the data, while it does not seem prone to over-fitting. It can be thought of as an intermediate model between the normal SSD with a single component on the one hand, and the KDE which counts as many components as there are species on the other hand. We chose to base the BNP SSD on NRMI rather than on the more common Dirichlet Process, because it is more robust in case of misspecification of the number of clusters (Lijoi et al., 2007; Barrios et al., 2013). The BNP SSD provides several benefits for risk assessment: it is an effective and robust standard model which adapts to many datasets. Moreover, it readily provides credible intervals. While it is always possible to obtain confidence intervals for a frequentist method using bootstrap, it can be difficult to stabilise the interval for small datasets even with a large number of bootstrap samples. As such, the BNP SSD represents a safe tool to remove one of the arbitrary parametric assumptions of SSD (Forbes and Calow, 2002).

The extended paper supporting the BNP SSD (Kon Kam King et al., 2016) will include a comparison of methods on simulated data, an extension to the case of censored data and an emphasis on the potential benefits of the approach from a biological point of view.

Acknowledgements The authors would like to thank two anonymous reviewers for suggesting several clarifications to the article. J. Arbel was a postdoc at Bocconi University and Collegio Carlo Alberto, Italy, when this article was submitted. J. Arbel and I. Prünster are supported by the European Research Council (ERC) through StG "N-BNP" 306406.

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