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## ► To cite this version:

Julyan Arbel, Guillaume Kon Kam King, Antonio Lijoi, Luis E. Nieto-Barajas, Igor Prünster. BNPdensity: Bayesian nonparametric mixture modelling in R. Australian and New Zealand Journal of Statistics, 2021, 63 (3), pp.542-564. 10.1111/anzs.12342 . hal-03433254

**HAL Id: hal-03433254**

**<https://hal.inrae.fr/hal-03433254>**

Submitted on 17 Nov 2021

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# BNPdensity: Bayesian nonparametric mixture modeling in R

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## Summary

Robust statistical data modelling under potential model mis-specification often requires leaving the parametric world for the nonparametric. In the latter, parameters are infinite dimensional objects such as functions, probability distributions or infinite vectors. In the Bayesian nonparametric approach, prior distributions are designed for these parameters, which provide a handle to manage the complexity of nonparametric models in practice. However, most modern Bayesian nonparametric models seem often out of reach to practitioners, as inference algorithms need careful design to deal with the infinite number of parameters. The aim of this work is to facilitate the journey by providing computational tools for Bayesian nonparametric inference. The article describes a set of functions available in the R package *BNPdensity* in order to carry out density estimation with an infinite mixture model, including all types of censored data. The package provides access to a large class of such models based on normalized random measures, which represent a generalization of the popular Dirichlet process mixture. One striking advantage of this generalization is that it offers much more robust priors on the number of clusters than the Dirichlet. Another crucial advantage is the complete flexibility in specifying the prior for the scale and location parameters of the clusters, because conjugacy is not required. Inference is performed using a theoretically grounded approximate sampling methodology known as the Ferguson & Klass algorithm. The package also offers several goodness of fit diagnostics such as QQ-plots, including a cross-validation criterion, the conditional predictive ordinate. The proposed methodology is illustrated on a classical ecological risk assessment method called the Species Sensitivity Distribution (SSD) problem, showcasing the benefits of the Bayesian nonparametric framework.

**Key words:** Bayesian nonparametric inference; density estimation; Ferguson and Klass algorithm; infinite mixture models; random probability measures; R

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**Acknowledgment.** We would like to thank a Referee for several interesting suggestions and Matti Vihola for useful advice on adaptive MCMC. J. Arbel is partially supported by Grenoble Alpes Data Institute (ANR-15-IDEX-02). A. Lijoi and I. Prünster are partially supported by MIUR, PRIN Project 2015SSNS29B.

## 1. Introduction

R (RCoreTeam 2019) is often cited by Bayesian statisticians as their favorite programming language due to the many packages that provide tools for Bayesian inference. The general program for Bayesian inference BUGS (Gilks, Thomas & Spiegelhalter 1993) has been available for a couple of decades, with interfaces in R. Since then, additional software has been developed to make that language more accessible to the users, for instance OpenBUGS (Thomas et al. 2006), JAGS (Plummer 2003), and Stan (Stan Development Team & Stan Development Team 2019). All three can be accessed directly from R by respectively using R2OpenBUGS/R2WinBUGS (Sturtz, Ligges & Gelman 2005), rjags (Plummer 2019), runjags (Denwood 2016), and rstan (Stan Development Team 2018). Programs for specific fields of Bayesian statistics have appeared in recent years, for instance bspmma (Burr 2012) for meta-analysis using Dirichlet Process Mixture (DPM) models, DPpackage (Jara 2007; Jara et al. 2011), a bundle of functions for Bayesian nonparametric models, BNPmix (Canale, Corradin & Nipoti 2019), a set of functions for density estimation with Dirichlet process and Pitman–Yor mixing measures via marginal algorithms, PReMiuM (Liverani et al. 2015) for profile regression using the Dirichlet process, Biips (Todeschini, Caron & Fuentes 2014) for Bayesian inference via particle filtering, Bayesian Regression (Karabatsos 2017) for Bayesian nonparametric regression. Packages mcclust (Scrucca et al. 2016), mcclust.ext (Wade & Ghahramani 2018) and GreedyEPL (Rastelli & Friel 2018) provide point estimation and credible sets for Bayesian cluster analysis. The interested reader may refer to the CRAN Task View on Bayesian Inference for an extensive list of R packages dedicated to Bayesian statistics (see Section 4 for a more detailed discussion of R packages for Bayesian density estimation).

Robust statistical data modeling under potential model mis-specification often requires relaxing parametric assumptions for nonparametric assumptions. In Bayesian Nonparametrics (BNP), parameters are infinite dimensional objects such as functions, probability distributions or infinite vectors. Prior distributions are designed for these parameters, which provide a handle to manage the complexity of nonparametric models in practice. However, the applicability of BNP models, for data analysis, depends on the availability of user-friendly software. This is because BNP models typically require complex representations, which may not be immediately accessible to non-experts. This work focuses on inference of densities with mixture models (Frühwirth-Schnatter, Celeux & Robert 2018). The purpose of the present paper is to introduce and describe an extensive revamping of the BNPdensity package, originally presented in Barrios et al. (2013). The package is programmed in R, and is available from the Comprehensive R Archive Network (CRAN) at <https://CRAN.R-project.org/package=BNPdensity>. To the best of our

43 knowledge, `BNPdensity` is the first R package which implements BNP density models  
44 including all types of censored data (left-, right- and interval-censored data), under a general  
45 specification of BNP priors called normalised generalised gamma processes (Lijoi, Mena  
46 & Prünster 2007b; Barrios et al. 2013). The improvements to the package cover various  
47 aspects. Notably, careful profiling and re-writing of some critical parts of the code, along  
48 with the use of the R bytecode compiler, yielded a 4-fold decrease of the running time  
49 of the algorithm. Drawing on the flexibility of the algorithm to use non-conjugate prior,  
50 we also implemented a range of popular new priors on the scale parameter of the clusters  
51 such as the half-Cauchy (Gelman 2006; Chung et al. 2015), the truncated Gaussian and the  
52 uniform distributions. We also revised the truncation method in the algorithm, intended to  
53 deal with the infinite dimensional random measures in the BNP model, to include recent  
54 contributions by Arbel & Prünster (2017). These provide a better and principled control of  
55 the truncation approximation. Moreover, we extended `BNPdensity` to include all types of  
56 censored data (right-, left- or interval-censored data). To leverage on the clustering properties  
57 of BNP mixture models, we interfaced `BNPdensity` with other packages to estimate the  
58 optimal clustering from posterior samples and provided cluster visualisation tools. We also  
59 implemented functions to compute prior distributions on the number of mixture components,  
60 for various processes, to better inform prior specification. Finally, we added several new  
61 functions for graphical model checking, assessing Markov chain Monte Carlo (MCMC)  
62 convergence and parallel computation.

63 The paper is organised as follows. We start with a concise overview of Bayesian  
64 nonparametric mixture models for density estimation in Section 2, along with our strategy  
65 for posterior inference and a description of the recent improvements to `BNPdensity`. We then  
66 describe the package and its general syntax in Section 3, including some simple examples, and  
67 provide in Section 4 a comprehensive comparison of the features and functionalities offered  
68 in three R packages dedicated to BNP density estimation, namely: `BNPdensity`, `BNPmix`,  
69 and `DPpackage`. We then conclude with a case study in Section 5.

70

## 2. Bayesian nonparametric density estimation

71 This section aims at providing a concise review of the statistical model used in the  
72 `BNPdensity` package. As the name suggests, the focus of the package is density estimation  
73 based on BNP priors, including all types of censored data. The density model used is a  
74 mixture model (Frühwirth-Schnatter, Celeux & Robert 2018), where the mixing measure is a  
75 BNP prior, thus leading to an infinite mixture model.

76 The most widely used BNP mixture model for density estimation is the Dirichlet Process  
 77 Mixture (DPM) model due to Lo (1984). Generalisations of the DPM correspond to allowing  
 78 the mixing distribution to be any discrete nonparametric prior. A large class of such prior  
 79 distributions is obtained by normalising increasing additive processes (Sato 1999). The  
 80 normalisation step, under suitable conditions, gives rise to so-called Normalised Random  
 81 Measures with Independent Increments (NRMI) as introduced in Regazzini, Lijoi & Prünster  
 82 (2003). See also Barrios et al. (2013).

83 We focus on a class of NRMI that are obtained by normalising the increments of a  
 84 generalised gamma process (Brix 1999) proposed in Lijoi, Mena & Prünster (2007a), which  
 85 enjoy analytical tractability and include many well-known priors as special cases. Generalised  
 86 gamma processes are discrete random measures  $\tilde{\rho}$  of the form

$$\tilde{\rho} = \sum_{i=1}^{\infty} J_i \delta_{\theta_i}, \quad (1)$$

87 where the weights  $J_i$  do not sum to one, while the location parameters  $\theta_i$  are sampled iid  
 88 from a measure  $P_0$ , a probability distribution on the parameter space  $\Theta$ . In what follows,  $P_0$   
 89 is considered as diffuse.  $(J_i, \theta_i)$  are the points of a Poisson process with mean intensity:

$$\nu(dv, d\theta) = \frac{e^{-\kappa v}}{\Gamma(1-\gamma)v^{1+\gamma}} dv \alpha P_0(d\theta), \quad (2)$$

90 which depends on parameters  $\kappa \geq 0$  and  $\gamma \in [0, 1)$  such that  $(\kappa, \gamma) \neq (0, 0)$ . The measure  
 91  $\nu$  in (2) characterises  $\tilde{\rho}$  and is often referred to as the Lévy intensity. The base  
 92 measure is  $\alpha P_0$ , where  $\alpha > 0$ . The corresponding generalised gamma NRMI, obtained by  
 93 normalising the generalised gamma process as  $\tilde{P}(\cdot) := \tilde{\rho}(\cdot)/\tilde{\rho}(\mathbb{X})$  will be denoted as  $\tilde{P} \sim$   
 94  $\text{NGG}(\alpha, \kappa, \gamma; P_0)$ . This class of priors contains as special cases the Dirichlet process which is  
 95 a  $\text{NGG}(\alpha, 1, 0; P_0)$  process, the normalised inverse Gaussian (N-IG) process (Lijoi, Mena &  
 96 Prünster 2005), which corresponds to a  $\text{NGG}(1, \kappa, 1/2; P_0)$  process, and the N-stable process  
 97 (Kingman 1975) which arises as  $\text{NGG}(1, 0, \gamma; P_0)$ .

98 We now describe the mixture model in more detail. We consider a density kernel  $k(\cdot | \theta)$   
 99 mixed with respect to  $\tilde{P} \sim \text{NGG}(\alpha, \kappa, \gamma; P_0)$  thus obtaining the random mixture density

$$\tilde{f}(x) = \int_{\Theta} k(x | \theta) \tilde{P}(d\theta). \quad (3)$$

100 This can equivalently be written in a hierarchical form as

$$\begin{aligned} X_i &| \theta_i \stackrel{\text{iid}}{\sim} k(\cdot | \theta_i), \quad i = 1, \dots, n, \\ \theta_i &| \tilde{P} \stackrel{\text{iid}}{\sim} \tilde{P}, \quad i = 1, \dots, n, \\ \tilde{P} &\sim \text{NGG}(\alpha, \kappa, \gamma; P_0). \end{aligned} \quad (4)$$

101 Details on possible choices for the kernel  $k$  and the base measure  $P_0$  are provided in Section 3,  
102 while in Section 4 we argue that conjugacy is not required in this setting.

103 We denote by  $f_0$  the density with respect to the Lebesgue measure of the NGG base  
104 measure  $P_0$  on  $\Theta$ . When  $P_0$  depends on a further hyperparameter  $\phi$ , we use the notation  
105  $f_0(\cdot | \phi)$ . Using the `MixNRM12` function corresponds to the specification of a nonparametric  
106 model for the location and scale parameters of the mixture where the mixture parameter  $\theta$   
107 takes the form of the vector  $(\mu, \sigma)$ . In order to distinguish the hyperparameters for location  
108 and scale, we will use the notation  $f_0(\mu, \sigma | \phi) = f_0^1(\mu | \sigma, \phi) f_0^2(\sigma | \phi)$ . In applications a  
109 priori independence between  $\mu$  and  $\sigma$  is commonly assumed, and this is indeed a natural  
110 assumption for the illustration in Section 5.

111 The most popular uses of mixtures with discrete random probability measures, such as  
112 the one displayed in (4), relate to density estimation and data clustering. The former can be  
113 addressed by evaluating the posterior expectation of the random density  $\tilde{f}$  defined in (3),  
114 given a sample  $\mathbf{X} = (X_1, \dots, X_n)^\top$ ,

$$\hat{f}_n(x) = \mathbb{E}(\tilde{f}(x) | \mathbf{X}) \quad (5)$$

115 for any  $x$  in  $\mathbb{X}$ . As for the latter, if  $R_n$  is the number of distinct latent values  $\theta_1^*, \dots, \theta_{R_n}^*$  out  
116 of a sample of size  $n$ , one can deduce a partition of the observations such that any two  $X_i$   
117 and  $X_j$  belong to the same cluster if the corresponding latent variables  $\theta_i$  and  $\theta_j$  coincide.  
118 Then, it is interesting to determine an estimate  $\hat{R}_n$  of the number of clusters into which the  
119 data are grouped, along with the clustering structure. For details on clustering estimation in  
120 our setting, see Section 2.3.

121 In the next subsection, we show how to solve all estimation problems with a posterior  
122 sampling algorithm.

## 123 2.1. Posterior sampling via a conditional Gibbs sampler

124 According to the terminology of Papaspiliopoulos & Roberts (2008), posterior sampling  
125 methods for BNP mixture models can be divided into two classes: marginal and conditional  
126 methods. Marginal methods, such as Escobar & West (1995); MacEachern & Müller (1998);

127 Neal (2000), integrate out the the infinite-dimensional component (1) of the hierarchical  
 128 model and sample from the marginal distribution of the remaining variables. Conditional  
 129 methods work directly on (4) and must solve the problem of sampling the trajectories of an  
 130 infinite-dimensional random element. However, they allow inference on the latent random  
 131 measure  $\tilde{P}$ , for instance on the jump sizes. An example of conditional method, which nicely  
 132 fits our framework, can be the Ferguson and Klass algorithm. Unlike marginal samplers, it  
 133 allows for estimating non-linear functionals of the underlying posterior distribution, such as  
 134 credible intervals. Here we sketch the conditional algorithm implemented in BNPdensity  
 135 which allows to draw posterior simulations from mixtures based on a general NRM (a very  
 136 thorough description of the algorithm can be found in Barrios et al. 2013). It works equally  
 137 well regardless of whether the kernel  $k$  and  $P_0$  form a conjugate pair and readily yields  
 138 credible intervals. The algorithm is an implementation of the posterior characterisation of  
 139 NRM provided in James, Lijoi & Prünster (2009).

For  $n$  observations  $\mathbf{X} = (X_1, \dots, X_n)^\top$  in  $\mathbb{X} = \mathbb{R}$ , we consider the random distribution  
 function induced by  $\tilde{\rho}$ ,

$$\tilde{M} := \left\{ \tilde{M}(s) = (\tilde{\rho}((-\infty, s_1]), \dots, \tilde{\rho}((-\infty, s_n]))^\top, \quad s = (s_1, \dots, s_n)^\top \in \mathbb{R}^n \right\}.$$

140 For the implementation of the Gibbs sampling scheme, we use the distributions of  $[\tilde{M} \mid \mathbf{X}, \boldsymbol{\theta}]$   
 141 and  $[\boldsymbol{\theta} \mid \mathbf{X}, \tilde{M}]$ . Due to conditional independence properties, the conditional distribution  
 142 of  $\tilde{M}$ , given  $\mathbf{X}$  and  $\boldsymbol{\theta}$ , does not depend on  $\mathbf{X}$ , that is,  $[\tilde{M} \mid \mathbf{X}, \boldsymbol{\theta}] = [\tilde{M} \mid \boldsymbol{\theta}]$ . Thanks to  
 143 Theorem 1 in Barrios et al. (2013) (originating in James, Lijoi & Prünster 2009), the posterior  
 144 distribution function  $[\tilde{M} \mid \boldsymbol{\theta}]$  can be characterised as a mixture in terms of a latent variable  
 145  $U$ , that is through the distributions  $[\tilde{M} \mid U, \boldsymbol{\theta}]$  and  $[U \mid \boldsymbol{\theta}]$ . Thus, the Gibbs sampler uses the  
 146 following conditional distributions:

- 147 1.  $[U \mid \boldsymbol{\theta}]$ : sampling the latent variable  $U$  conditionally on the latent parameters  $\boldsymbol{\theta}$ , where  
 148  $U$  follows the distribution:

$$f_{U|\mathbf{X}}(u) \propto u^{n-1} (u + \kappa)^{r\gamma - n} \exp \left\{ -\frac{a}{\gamma} (u + \kappa)^\gamma \right\}. \quad (6)$$

149 Sampling  $U$  is performed via a Metropolis–Hastings (M-H) step with a gamma  
 150 proposal distribution  $\text{ga}(\delta, \delta/u^{[t]})$  centered at the previous  $U$  value  $u^{[t]}$  with a  
 151 tuning parameter  $\delta$  controlling the coefficient of variation. An adaptive version of  
 152 the M-H algorithm (Roberts & Rosenthal 2009) without the tuning parameter is also  
 153 implemented in the package, and proposed with the option `adaptive=TRUE`. It uses  
 154 a log-transformation of the random variable  $U$ . Note that the target density (6) not

155 being log-concave, ergodicity cannot be proven as in [Roberts & Rosenthal \(2009\)](#).  
 156 Nevertheless, the adaptive version appears to offer superior performance in practice.

157 2.  $[\tilde{M} \mid U, \boldsymbol{\theta}]$ : simulating the infinite dimensional process conditionally on the parameters  
 158 and the latent variable  $U$ . This is performed using the [Ferguson & Klass \(1972\)](#)  
 159 algorithm. According to Theorem 1 in [Barrios et al. \(2013\)](#), the conditional  
 160 distribution of  $\tilde{M}$  is composed of two parts, a part without fixed points of discontinuity  
 161  $\tilde{M}^*$  which can be expressed as an infinite sum of random jumps occurring at  
 162 random locations and a part with fixed points of discontinuity, or in other words:  
 163  $\tilde{M}(\mathbf{s}) = \tilde{M}^*(\mathbf{s}) + \sum_{j=1}^{R_n} J_j \mathbb{I}_{(-\infty, \mathbf{s}]}(\boldsymbol{\theta}_j^*)$  where the  $\boldsymbol{\theta}_j^*$ ,  $j = 1, \dots, R_n$  denote the  $R_n$   
 164 distinct parameters among  $\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_n$  and where  $(-\infty, \mathbf{s}] = \{\mathbf{x} \in \mathbb{R}^n : x_i \leq s_i, i =$   
 165  $1, \dots, n\}$ . In the infinite sum:

$$\tilde{M}^*(\mathbf{s}) = \sum_{j=1}^{\infty} J_j \mathbb{I}_{(-\infty, \mathbf{s}]}(\boldsymbol{\vartheta}_j), \quad (7)$$

166 the  $J_j$ s are obtained by inverting the relation  $\xi_j = N(J_j)$ , where  $\xi_1, \xi_2, \dots$  are jump  
 167 times of a standard Poisson process of unit rate, that is  $\xi_1, \xi_2 - \xi_1, \dots \stackrel{\text{iid}}{\sim} \text{ga}(1, 1)$ , with  
 168

$$N(v) = \frac{a}{\Gamma(1 - \gamma)} \int_v^{\infty} e^{-(\kappa+u)x} x^{-(1+\gamma)} dx, \quad (8)$$

169 while the jumps  $\boldsymbol{\vartheta}_j = (\boldsymbol{\vartheta}_j^{(1)}, \dots, \boldsymbol{\vartheta}_j^{(n)})^\top$  are sampled from the base measure  $P_0$ . The  
 170 jumps  $J_j^*$  at the fixed locations  $\boldsymbol{\theta}_j^*$  are gamma distributed:

$$f_j^*(v) = \frac{(\kappa + u)^{n_j - \gamma}}{\Gamma(n_j - \gamma)} v^{n_j - \gamma - 1} e^{-(\kappa+u)v}, \quad (9)$$

171 where  $n_j$  are the multiplicities, i.e. the number of  $\boldsymbol{\theta}_j$  equal to  $\boldsymbol{\theta}_j^*$ . A fundamental  
 172 merit of Ferguson and Klass' representation, compared to similar algorithms, is the  
 173 fact that the random heights  $J_i$  are obtained in a descending order. Therefore, one can  
 174 truncate the series in (7) at a certain finite index  $Q$  to be decided via a moment-matching  
 175 criterion (see Section 2.2). This also guarantees that the highest jumps are not left out.

176 3.  $[\boldsymbol{\theta} \mid \mathbf{X}, \tilde{M}]$ : resampling the latent cluster parameters given the data and the random  
 177 measure. The support of the conditional distribution of  $\boldsymbol{\theta}_i$  are the locations of the  
 178 jumps of  $\tilde{M}$ ,  $\{\bar{J}_j\}_{j=1}^{\infty} = \{J_1^*, \dots, J_{R_n}^*, J_1, \dots\}$  with associated jumps  $\{\bar{\boldsymbol{\vartheta}}_j\}_{j=1}^{\infty} =$   
 179  $\{\boldsymbol{\theta}_1^*, \dots, \boldsymbol{\theta}_{R_n}^*, \boldsymbol{\vartheta}_1, \dots\}$ ,

$$f_{\boldsymbol{\theta}_i \mid X_i, \tilde{M}}(\mathbf{s}) \propto \sum_j k(X_i \mid \mathbf{s}) \bar{J}_j \delta_{\bar{\boldsymbol{\vartheta}}_j}(\mathbf{s}). \quad (10)$$



180 Simulating from this conditional distribution when an approximation with a finite  
 181 number of jumps has been determined is straightforward: one just needs to evaluate  
 182 the right-hand side of the expression above and normalise.

183 4. Updating the hyperparameters of  $P_0$ . We only put a prior on the hyperparameters for the  
 184 location parameters, found to have a higher impact. Assuming a priori independence  
 185 between location and scale parameters of the clusters, the conditional posterior  
 186 distribution on the hyperparameters given the data and the rest of the parameters only  
 187 depends on the distinct location parameters. A simple way to proceed is thus to consider  
 188 a prior conjugate to the base measure.

189 We also include a resampling of the unique values of the cluster parameters via a M-H  
 190 step to avoid the ‘sticky clusters effect’, as suggested in [Bush & MacEachern \(1996\)](#).

191 We devote the next section to explaining the moment-matching criterion used for  
 192 truncation in the second conditional, which is a recent addition to the package `BNPdensity`.

## 193 2.2. Moment-matching criterion

194 Normalised Generalised Gamma (NGG) priors are infinite dimensional objects that are  
 195 obtained by normalising a generalised gamma process. Concrete implementation of NGG  
 196 priors requires to truncate the random series (1) at some level denoted  $Q$ , which results in  
 197 some truncation error. Previous implementation of the package used to appeal to a relative  
 198 error index, that we will denote  $e_Q = \sum_{i>Q} J_i \delta_{\theta_i}$ , based on the jumps themselves. We  
 199 improve on this approach, by implementing the methodology proposed by [Arbel & Prünster](#)  
 200 (2017) which relies on a moment-based evaluation of the error, denoted by  $\ell_M$ . One of the  
 201 main contributions of [Arbel & Prünster \(2017\)](#) is to warn that relying on the relative error  
 202 index  $e_M$  can lead to overly optimistic conclusions in terms of approximation, especially for  
 203 large values of the discount parameter  $\gamma$ .

204 To be more specific, consider  $K$  moments of the total mass of the CRM  $\tilde{\rho}(\mathbb{X}) =$   
 205  $\sum_{i=1}^{\infty} J_i$ , denoted by  $\mathbf{m}_K = (m_1, \dots, m_K)^\top$ . Such moments have a simple expression in  
 206 terms of the cumulants, which are themselves available in closed form, see for instance Table  
 207 1 in [Arbel & Prünster \(2017\)](#). Thus, these exact moments can be computed and compared  
 208 with their empirical counterparts obtained with the Ferguson & Klass algorithm ([Ferguson &](#)  
 209 [Klass 1972](#)).

210 In order to make this methodology applicable, one needs to propose the truncation level  
 211  $Q(\ell)$  required to achieve a given approximation  $\ell$ . Such map  $Q(\ell)$  only depends on the NGG  
 212 parameters and can be computed once-for-all and distributed with the package. For reference,  
 213 see the moment matching error  $\ell(Q)$  and the map  $Q(\ell)$  respectively displayed in Figures 1

214 and 2 of [Arbel & Prünster \(2017\)](#). Ferguson and Klass posterior sampling based on such a  
 215 prescribed number of jumps  $Q(\ell)$  is computationally more efficient than having to iteratively  
 216 compute the relative error  $e_Q$  as done in the previous package version.

### 217 **2.3. Clustering estimation**

218 We focus here on the problem of estimating a data clustering from the Bayesian posterior  
 219 inference conducted so far. This is a long standing problem in Bayesian statistics (see for  
 220 instance [Dahl 2006](#); [Lau & Green 2007](#)). Enumerating all partitions is practically not feasible,  
 221 which typically requires resorting to approximations.

Many ad-hoc procedures have been devised in the literature. However, as noted by [Dahl \(2006\)](#), it seems counter-intuitive to apply an ad-hoc clustering method on top of a model which itself produces clusterings. We adopt instead a fully Bayesian route by undertaking clustering on decision-theoretic grounds. We consider a loss function  $L$  and propose a Bayesian point estimator  $\hat{c}$  for a clustering obtained as an argument which minimises the posterior expected loss given data  $\mathbf{X}$

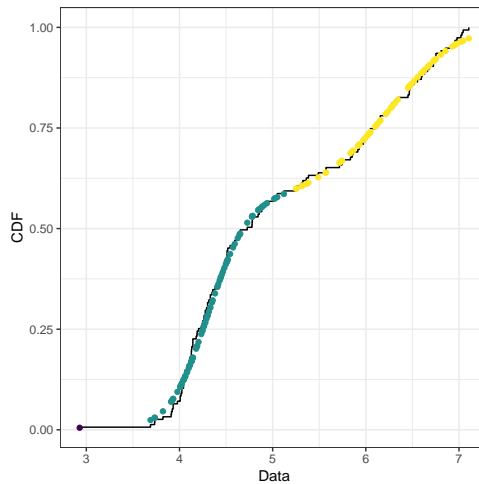
$$\hat{c} = \arg \min_{c'} \sum_c L(c', c) \pi(c | \mathbf{X}), \quad (11)$$

222 where  $\pi(c | \mathbf{X})$  is the posterior distribution of clustering  $c$ . Often considered in the literature,  
 223 the posterior mode is an example of such a Bayesian estimator, based on the very crude 0-1  
 224 loss function. When  $n$  is large, an MCMC sample from the posterior generally hardly visits  
 225 twice the same clustering, thus rendering the empirical mode of the MCMC output very  
 226 sensitive to the initialisation of the chain and of very limited validity in practice. Manifestly,  
 227 many other loss functions can be considered and expected to perform better than the 0-1  
 228 loss. One particular choice of a loss function stands out from these in best estimating the  
 229 number of groups in a clustering. It is called the variation of information, denoted by  $\mathcal{VI}$ ,  
 230 which is a loss function firmly established in information theory ([Meila 2007](#); [Wade &](#)  
 231 [Ghahramani 2018](#)). The variation of information between two clusterings is defined as the  
 232 sum of their information (their Shannon entropies) minus twice the information they share.  
 233 Simulations indicate that the variation of information is a sensible choice: when other losses  
 234 such as the Binder loss ([Binder 1978](#)) typically tend to overestimate the number of clusters,  
 235 the variation of information instead seems to consistently recover it (see for instance the  
 236 simulated examples, and more specifically Figures 6 to 8, of [Wade & Ghahramani 2018](#)).

237 An asset of the approach presented in [Wade & Ghahramani \(2018\)](#) is that it rests on a  
 238 greedy search algorithm to determine the minimum loss clustering of (11). Starting from the  
 239 MCMC output, this greedy approach explores the space of partitions and is not restricted

240 to those visited by the MCMC chain to find the optimum. We include the possibility to  
 241 estimate the optimal clustering using both the  $\mathcal{VZ}$  loss and Binder's loss, along with other loss  
 242 functions, within `BNPdensity` by adding an optional dependence to `GreedyEPL`. Note that  
 243 clustering estimation is also available for censored data, although graphical representation is  
 244 more tricky (see also the legend to Figure 8).

```
245 data(acidity)
    out <- MixNRMI2(acidity)
    clustering = compute_optimal_clustering(out)
    plot_clustering_and_CDF(out, clustering)
```



246

Figure 1. Visualisation of the clustering induced by the BNP mixture model, for the `acidity` dataset. The solid line represents the empirical Cumulative Distribution Function (CDF), dots represent data points. The abscissa of each point is its value, the ordinate is the value of the estimated CDF at that point. Each colour denotes the cluster estimated by minimising the  $\mathcal{VZ}$  loss function.

247

248

### 3. Package description

The implementation of `BNPdensity` package is available from the Comprehensive R Archive Network (CRAN) at <https://CRAN.R-project.org/package=BNPdensity>. Fitting a model with `BNPdensity` starts with calling one of the two functions, `MixNRMI1` or `MixNRMI2`, or their versions for censored data. The function `MixNRMI1` fits a semiparametric mixture model where all components have a common scale parameter  $\sigma$  with an independent parametric prior,  $\sigma \sim P_\sigma$ , while `MixNRMI2` is devoted to fully

nonparametric mixtures of *location and scale parameters*:

$$\begin{aligned} X_i \mid \theta_i, \sigma_i &\stackrel{\text{ind}}{\sim} k(\cdot \mid \theta_i, \sigma_i), \quad i = 1, \dots, n, \\ (\theta_i, \sigma_i) \mid \tilde{P} &\stackrel{\text{iid}}{\sim} \tilde{P}, \quad i = 1, \dots, n, \\ \tilde{P} &\sim \text{NGG}(\alpha, \kappa, \gamma; P_0). \end{aligned}$$

249 Data and prior parameters are passed to the model function as arguments. The  
 250 `MixNRMIX` functions also take a number of arguments to choose the BNP model, the mixture  
 251 kernels, a variety of priors and tuning parameters for the Markov chain Monte Carlo sampling  
 252 algorithm. The main arguments of the model functions are presented below.

- 253 • `distr.k`: Integer number identifying the **mixture kernel**  $k$ . Five kernels  
 254 parameterised by their location and scale are implemented: a Gaussian or double  
 255 exponential kernel for real data, a gamma or lognormal kernel for positive data and  
 256 a beta kernel for data on the unit interval. The flexibility of this choice is afforded by  
 257 the specific algorithm used in `BNPdensity`.
- 258 • `distr.py0`: Integer number identifying the base measure  $P_0$  on the location  
 259 parameters. Three choices are available, which are constrained by the conjugate  
 260 prior we place on the hyperparameters of  $P_0$ : Gaussian, gamma and beta. Additional  
 261 arguments can be used to tune the shape of the base measure.
- 262 • `distr.py0, distr.pz0`: Integer number identifying the base measure  $P_0$  on  
 263 scale parameters. For the semiparametric model (`MixNRMIX1`), this argument is not  
 264 provided and the base measure is a gamma distribution on the common scale parameter.  
 265 Traditionally, there is sufficient information in the data to estimate the common scale  
 266 parameter and inference is not very sensitive to the shape of the base measure. For  
 267 the fully nonparametric model, the base measure on the scale parameters can be a  
 268 gamma, lognormal, half Cauchy, half normal, half Student-t, uniform or truncated  
 269 normal distribution. Additional arguments can be used to tune the shape of the base  
 270 measure.
- 271 • `(Alpha, Kappa, Gama)`: Mixing measure parameters identifying a **Normalised**  
 272 **generalised gamma** process, see the Lévy intensity (2) with parameters  $(\alpha, \kappa, \gamma)$  for  
 273 more details.
- 274 • The rest of the parameters provide handles to tune the MCMC algorithm.

275 Functions to fit a model return an object with `print`, `summary` and `plot` methods, as  
 276 follows (the latter plot is represented in Figure 2):

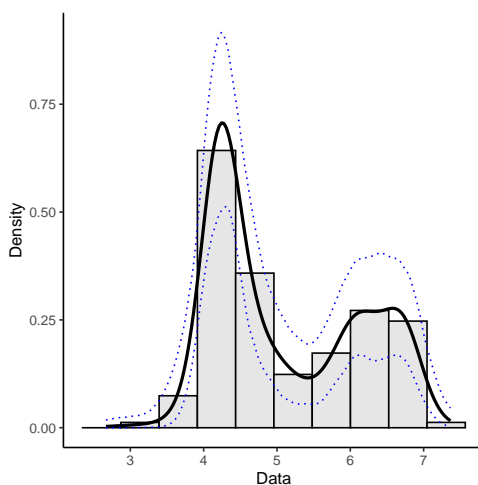


Figure 2. Density estimate (solid black line), 95% credible interval (blue dotted line) and histogram of the `acidity` data fitted with a semiparametric model. Figure obtained using the command `plot(out)`.

```

data(acidity)
out <- MixNRMI1(acidity)
## MCMC iteration 500 of 1500
## MCMC iteration 1000 of 1500
## MCMC iteration 1500 of 1500
## >>> Total processing time (sec.):
##   user  system elapsed
##  49.166   0.083   49.255

summary(out)
## Density estimation using a Normalized stable process,
## with stability parameter Gamma = 0.4
##
## A semiparametric normal mixture model was used.
##
## There were 155 data points.
##
## The MCMC algorithm was run for 1500 iterations with 10%
##
## To obtain information on the estimated number of clusters,
## please use summary(object, number_of_clusters = TRUE).

```

277

278

#### 4. Package comparison

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In this section, we discuss in detail the features and functionalities offered in three R packages addressing BNP density estimation, namely: `BNPdensity`, `BNPmix` (Canale, Corradin & Nipoti 2019), and `DPpackage` (Jara et al. 2011) (`DPpackage` was removed from the CRAN repository, but former versions are available at <https://cran.r-project.org/web/packages/BNPdensity/index.html>).

283 [r-project.org/src/contrib/Archive/DPpackage/](https://r-project.org/src/contrib/Archive/DPpackage/)). Since the focus of the  
284 present paper is mixture modeling and density estimation, note that other packages relying on  
285 BNP approaches but tackling other questions such as regression (PReMiuM, [Liverani et al.](#)  
286 [2015](#), Bayesian Regression, [Karabatsos 2017](#)), or meta-analysis (bspmma, [Burr 2012](#))  
287 are not discussed here. Likewise, non Bayesian approaches are deliberately set aside. Table 1  
288 summarises the comparative study of this section.

#### 289 4.1. Inference algorithm

290 Efficient posterior computation for BNP mixture models relies on two types of  
291 approaches: marginal or conditional. Marginal methods incorporate analytic integration of  
292 infinite dimensional parts of the parameter, which is the case of DPpackage and BNPmix.  
293 Instead, BNPdensity relies on a conditional sampler that directly samples trajectories of the  
294 processes. More specifically, the Ferguson & Klass algorithm is employed (see Section 2.1),  
295 with the crucial merit of ensuring that largest weights in the series representation are not left  
296 out. This is to be compared to the stick-breaking representation where the weights sequence  
297 is decreasing only stochastically (that is, in expectation).

#### 298 4.2. Mixing measure

299 As described in Section 2, BNP mixture modeling and density estimation require to  
300 specify some mixing measure. We start here by comparing the mixing measures available in  
301 the three packages.

302 BNPmix provides a set of functions for density estimation with Dirichlet process  
303 and Pitman–Yor mixing measures via marginal algorithms. DPpackage is a more general  
304 purpose package than both BNPdensity and BNPmix, including functions for regression  
305 models, generalised linear mixed models, and generalised additive models, on top of the  
306 density model. However, the implementation is primarily tailored to the Dirichlet process  
307 mixing measure. A natural extension to the Dirichlet and Pitman–Yor processes are Gibbs-  
308 type priors ([De Blasi et al. 2015](#)). NRMI are a larger class of priors than Gibbs-type priors,  
309 and their intersection is the NGG priors considered in BNPdensity, as established in [Lijoi,](#)  
310 [Prünster & Walker \(2008\)](#). Being an extremely general class of priors, Gibbs-type processes  
311 are beyond reach for a general treatment in a software, however both BNPdensity and  
312 BNPmix packages cover its most commonly used sub-classes. Pitman–Yor process is not  
313 implemented in BNPdensity as it is not an NRMI; yet, a dependence to BNPmix is made in  
314 BNPdensity, in such a way that users interested in comparing their results with Pitman–  
315 Yor can also use the dedicated functions `MixPY1` (semiparametric) and `MixPY2` (fully

316 nonparametric) that call `BNPmix` `PYdensity` function. The mixing measures covered by  
 317 the three packages and their mutual relationships are illustrated in Figure 3.

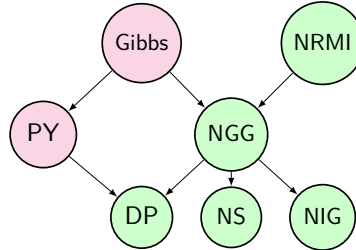


Figure 3. BNP priors mentioned in this section. An arrow indicates that the target is a special case or a limit case of its origin. Gibbs: Gibbs-type process. NRMI: normalised random measures with independent increments. NGG: normalised generalised gamma process. PY: Pitman–Yor process. NIG: normalised inverse Gaussian process. NS: normalised stable process. DP: Dirichlet process. In green: covered by `BNPdensity` package.

318

### 319 4.3. Prior characteristics

#### 320 4.3.1. Non-conjugacy

321 Mixture models present the difficulty that the likelihood goes to infinity for infinitely  
 322 small clusters located exactly on one observed data point. This may induce numerical  
 323 problems and instabilities, and such tiny clusters are almost invariably undesirable in practical  
 324 applications. A reasonable solution in the Bayesian framework is to use a prior distribution  
 325 on scale parameters with little mass on very small values, i.e. a gamma distribution with  
 326 shape parameter larger than 1 or a truncated distribution. We might also want to provide a  
 327 different kind of information on cluster scales: for instance, for a dataset whose variance has  
 328 been scaled to 1, there is no reason to find clusters with a variance much larger than one. This  
 329 would suggest using a prior with an upper bound, or with light tails for large values. Finally,  
 330 flexibility in the choice of the kernel  $k$  is a clear asset when modelling real data, to choose a  
 331 reasonable error model. These three examples suggest that we might need a certain flexibility  
 332 in the specification of the prior distribution on scale parameters or in the choice of the kernel.

333 The inference algorithm used in `BNPdensity` and presented in Section 2.1 does not  
 334 rely on conjugacy between the base measure and the kernel of the mixture, as do standard  
 335 algorithms for sampling from a Dirichlet mixture process such as that presented in Escobar

336 & West (1995). In contrast, `DPpackage` and `BNPmix` are limited to using conjugate couples  
 337 of base measure and the mixture kernel.

338 Not being bounded to conjugacy allows us first to use any relevant kernel for the mixture.  
 339 Moreover, even in the case of the normal kernel, this removes the dependence imposed in  
 340 the conjugate case between the location of the clusters and their variances. More precisely,  
 341 this allows a full flexibility on specifying priors based on external knowledge, and proves  
 342 particularly useful concerning the scale parameters of the kernels. Indeed, half-Cauchy or  
 343 half-Gaussian priors for hierarchical variance parameters have recently become popular  
 344 Gelman (2006); Chung et al. (2015). The illustration on Species Sensitivity Distribution  
 345 (SSD) (Section 5), where the data is scaled, offers such an example where both an upper  
 346 bound and lower bound on the cluster variances are useful.

### 347 4.3.2. Prior distribution on number of components

348 Prior elicitation is a delicate task in Bayesian modeling. `BNPdensity` provides some  
 349 guidelines on how to choose parameters (`Alpha`, `Kappa`, `Gama`) with two functions,  
 350 one for computing the prior expected number of components, and one for plotting this prior  
 351 distribution. Comparable functionalities are offered in `BNPmix` and `DPpackage`.

352 The (`Alpha`, `Kappa`, `Gama`) parametrisation allows to easily compare several well  
 353 known priors. We already mentioned that the Dirichlet process can be obtained by setting  
 354 `Gama = 0`, the normalised inverse Gaussian process by setting `Alpha = 1`, `Gama =`  
 355 `1/2` and the normalised stable process by setting `Alpha = 1`, `Kappa = 0`. The stable  
 356 process is a convenient model because its parameter  $\gamma$  has a simple interpretation: it can be  
 357 used to tune how informative the prior on the number of components is. Small values of `Gama`  
 358 bring the process closer to a Dirichlet process, where the prior on the number of components  
 359 is a relatively peaked distribution around  $\alpha \log n$ . In contrast, the larger the value of `Gama`  
 360 is, the flatter the distribution is. More guidelines on how to choose the parameters may be  
 361 found in Lijoi, Mena & Prünster (2007b), notably by considering the expected prior number  
 362 of components. The expected prior number of components for normalised generalised gamma  
 363 processes is not trivial to compute due to numerical instabilities, but we provide functions to  
 364 compute prior distribution on the number of clusters for the normalised stable process and  
 365 for the Dirichlet process. These functions require installing the packages `gmp` and `Rmpfr` for  
 366 Multiple Precision Arithmetic, both available on CRAN.

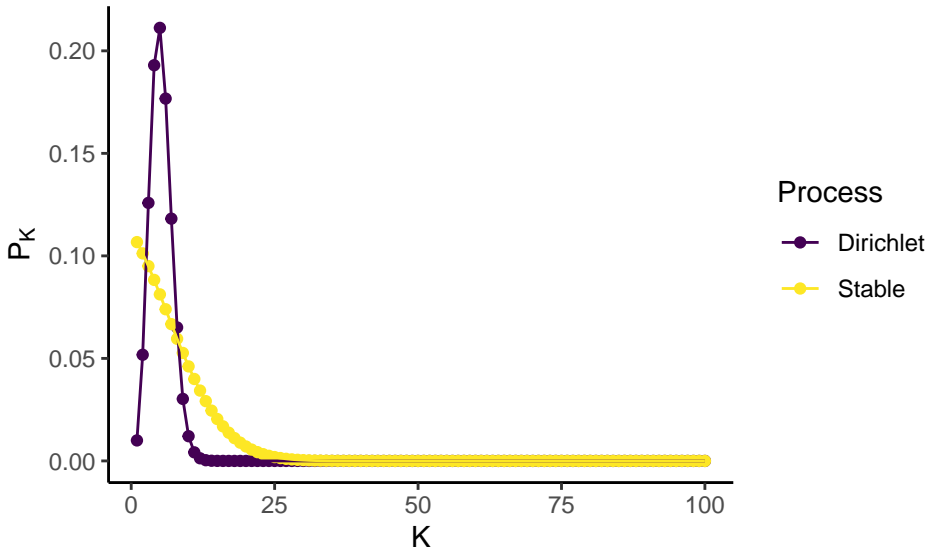
```
Rmpfr::asNumeric(expected_number_of_components_stable(n = 100, Gama = 0.4))
## [1] 7.102731

expected_number_of_components_Dirichlet(n = 100, Alpha = 1.)
## [1] 5.187378
```



367 We also provide a way to visualise the prior distribution on the number of components:

```
plot_prior_number_of_components(100, 0.4)
## Computing the prior probability on the number of clusters for the Dirichlet process
## Computing the prior probability on the number of clusters for the Stable process
```



368

369 Figure 4. Prior distribution on the number of clusters with 100 data points, for the stable process with  $\gamma = 0.4$  and for the Dirichlet process with  $\alpha = 1$ .

#### 370 4.4. Censored data

371 BNPdensity can deal with left, right and interval-censored data by using the functions  
 372 `MixNRM1lcens` and `MixNRM1rcens`. The same holds true for `DPpackage`, while  
 373 `BNPmix` does not handle censored data at all.

374 Censored data usually emerge from imperfections of the measurement process, such as  
 375 detection limits (high or low) or saturation, low measurement precision, or binning of the  
 376 data. Improper treatment of censored data is clearly a source of bias (Helsel 2005): in the  
 377 case of right-censored data due to a detection limit for high values, for instance, data are not  
 378 censored at random and discarding them or substituting them deteriorates the dataset.

379 We deal with censored data by using a version of the likelihood (Helsel 2005) adapted to  
 380 censored data. More specifically, denote by  $F_k$  the cumulative distribution function of the  
 381 kernel  $k$ . The heart of the method is then to replace  $k(x | \theta)$  by  $F_k(x | \theta)$  for a left-censored  
 382 observation, by  $1 - F_k(x | \theta)$  for a right-censored observation, and by  $F_k(x_r | \theta) - F_k(x_l |$   
 383  $\theta)$  for an interval-censored observation  $[x_l, x_r]$ .

## 384 4.5. Visualisation and programming

### 385 4.5.1. Convergence checking and model evaluation

386 BNPdensity offers several tools for assessing MCMC convergence and performing model  
 387 checking and comparison. Notably, we provide a conversion function `as.mcmc` to interface  
 388 the package with the `coda` package for analysing output and carrying out diagnostics on  
 389 MCMC. We are not aware of such tools for `BNPmix` or `DPpackage`.

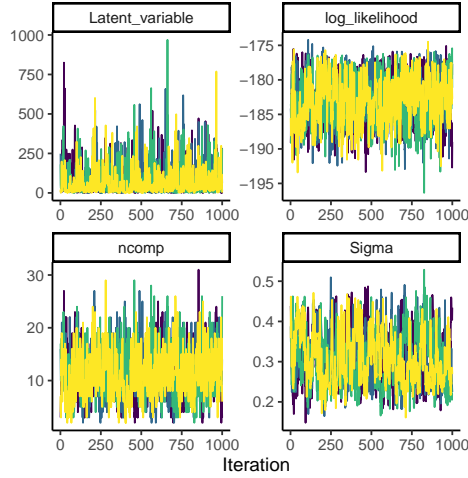
390 This is done by running multiple chains starting from different initial conditions, potentially  
 391 in parallel, and converting them into an `mcmc` object that can be processed by `coda`. A simple  
 392 solution for running multiple chains does not seem available for `BNPmix` and `DPpackage`.

393 One conceptual detail for assessing convergence is that, due to the nonparametric nature  
 394 of the model, the number of parameters which could potentially be monitored to measure  
 395 auto-correlation of the chains or effective sample size varies. The location parameters of the  
 396 clusters, for instance, vary at each iteration, and even the labels of the clusters vary, which  
 397 makes it tricky to follow. However, it is possible to monitor the log-likelihood of the data  
 398 along the iterations, the value of the latent variable  $u$ , the number of components and for the  
 399 semi-parametric model, the value of the common scale parameter. The following code shows  
 400 how to compute the potential scale reduction factor (Gelman & Rubin 1992):

```
library(coda)
data(acidity)
fit = multMixNRM1(acidity, extras = TRUE, Nit = 20000)
mcmc_list = as.mcmc(fit)
gelman.diag(mcmc_list)
```

```
## Potential scale reduction factors:
##
##           Point est. Upper C.I.
## ncomp           1.02      1.06
## Sigma           1.02      1.07
## Latent_variable  1.02      1.05
## log_likelihood   1.01      1.04
##
## Multivariate psrf
##
## 1.03
```

401 A trace plot for the chains may also be obtained by calling `traceplot(fit)`; see Figure 5.



402

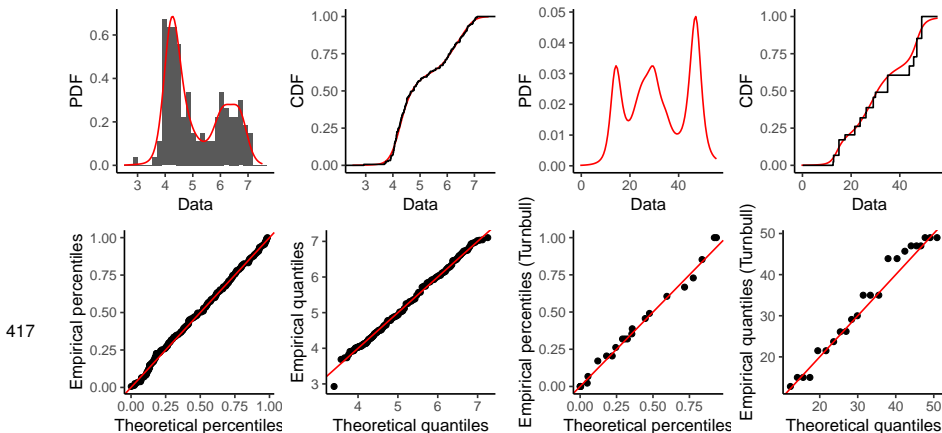
403

Figure 5. Trace plot of four chains in the MCMC for a semi-parametric model.

Table 1. Comparison of R packages performing BNP density estimation: `BNPdensity`, `BNPmix`, and `DPpackage`. (a) See discussion in Section 4.2. (b) The `DPpackage` `LDPDdoublyint` function, for *Linear Dependent Poisson Dirichlet Process Mixture Models for the Analysis of Doubly-Interval-Censored Data* could in principle be used for Pitman–Yor process mixture density estimation, although the interface (and the name) suggests it is not intended for this.

		BNPdensity	BNPmix	DPpackage
4.1 Inference algorithm	Conditional	yes	no	no
	Marginal	no	yes	yes
4.2 Mixing measure	Dirichlet process (DP)	yes	yes	yes
	Norm. inverse Gaussian (NIG)	yes	no	no
	Norm. stable (NS)	yes	no	no
	Norm. gener. gamma (NGG)	yes	no	no
	Pitman–Yor (PY)	no <sup>(a)</sup>	yes	no <sup>(b)</sup>
4.3 Prior characteristics	Non Gaussian kernels allowed	yes	no	no
	Functions for prior elicitation	yes	yes	yes
4.4 Data	All types of censored data	yes	no	yes
4.5 Vis. & Programming	MCMC conv. assessm.	yes	no	no
	Graphical model checking	yes	no	no
	Clustering vis. tools	yes	no	no
	Parallel computing	yes	no	no

404 We also provide tools for assessing goodness of fit. Graphical assessment can be performed  
 405 comparing various representations of the estimated distributions against representations  
 406 of the empirical distribution (Figure 6). Such plots may be obtained from a fitted  
 407 object using the command `GOFplots(fit, qq_plot = TRUE)`. The density plot  
 408 provides a familiar representation of the Nonparametric distribution, while the CDF plot  
 409 is probably the most classical visualisation of goodness of fit. The percentile-percentile  
 410 plot focuses on the goodness of fit in the center of the distribution, while the quantile-  
 411 quantile plot focuses on the goodness of fit in the tails of the distribution. The density,  
 412 CDF, percentile and quantiles used in the plots are the expected posterior quantities,  
 413 computed from the MCMC sample. Computation of the theoretical quantiles is a fairly  
 414 expensive operation because it requires numerically inverting the CDF. We choose not to  
 415 compute the quantile-quantile plot by default, and when we do, the computation is done  
 416 on a thinned MCMC chain with an argument provided to control the level of thinning.



417 Figure 6. Graphical goodness of fit plots for censored (right) and non censored data (left). The top row is the mean density estimate with a histogram for the non censored data. The middle row is the estimated CDF with the empirical CDF for non censored data, and with the Turnbull estimate of the CDF for censored data. The bottom row are percentile-percentile plots where the empirical percentiles are computed from the empirical CDF for the non censored data, and from the Turnbull estimate for the censored data.

418 We also provide tools for model comparison based on expected predictive density. The  
 419 conditional predictive ordinate (CPO) is the expected predictive density of a data point given  
 420 the prior and all other data points, so it is the leave-one-out expected predictive density of  
 421 the model (Gelman et al. 2014), a typical cross-validation criterion. As such, it is a measure  
 422 of predictive power with a penalisation for over-fitting. A Monte Carlo approximation of the  
 423 CPO is easily available and can be used to compare a semi-parametric model to the fully  
 424 nonparametric model for instance:

```

set.seed(0)
normal_mixture <- MixNRMI2(acidity, distr.k = 1, Nit = 15000)
dbl_exponential_mixture <- MixNRMI1(acidity, distr.k = 4, Nit = 15000)
c(median(normal_mixture$cpo), median(dbl_exponential_mixture$cpo))

```

```
## [1] 0.279 0.271
```

Model	Mean CPO	Median CPO
Nonparametric normal mixture	0.362	0.279
Semi parametric double exponential mixture	0.357	0.271

#### 4.5.2. Clustering visualisation tools

As described in Section 2.3, BNPdensity provides functions for clustering estimation, `compute_optimal_clustering`, and visual representation, `plot_clustering_and_CDF`. See also Figure 1 and Figure 8 for illustrations. We are not aware of such clustering tools for BNPmix or DPpackage.

### 5. Case study: Species Sensitivity Distribution

We present an application of nonparametric density estimation for environmental data. Assessing the response of a community of species to an environmental stress is of critical importance for ecological risk assessment. Methods for this purpose vary in levels of complexity and realism. SSD represents an intermediate tier, more refined than rudimentary assessment factors (Posthuma, Suter II & Trass 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 a single species-specific value, which marks a limit over which the species suffers adverse effects. This value is very often censored (Kon Kam King et al. 2014), because measuring it is both costly and difficult (bioassay experiments). The tolerance of all species possibly exposed is described by a distribution, fitted on the sample of species (Aldenberg & Jaworska 2000). The quantity of interest for ecological risk assessment is the Hazardous Concentration for 5% of the Species (HC<sub>5</sub>), which corresponds to the 5th percentile of the SSD distribution. 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 & Newman 1997; Van Straalen 2002; Xing et al. 2014; Zhao & 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 & Calow 2002). Therefore, the log-normal distribution has become the

453 customary choice, notably because it readily provides confidence intervals on the  $HC_5$ , and  
454 because model comparison and goodness of fit tests have relatively low power on small  
455 datasets, precluding the emergence of a definite answer to the question.

456 The availability of a package such as `BNPdensity` allows to move beyond this customary  
457 assumption very easily. NRMIs offer a flexible nonparametric mixture model, which can  
458 accommodate distributions very different from a normal distribution. [Barrios et al. \(2013\)](#)  
459 and [Kon Kam King, Arbel & Prünster \(2017\)](#) show that NRMIs have better performance than  
460 Dirichlet process mixtures, kernel density estimates (the recent approach proposed by [Wang](#)  
461 [et al. \(2015\)](#)) or simple one-component normal models. Moreover, there are good reasons to  
462 believe that the distribution of species sensibility should at least allow for multimodality.  
463 Indeed, many stressors target specifically certain species groups, such as insecticides for  
464 insects, while they are developed with the aim of leaving other species group unaffected.  
465 Therefore, it is expected that there should at the very least be a group of sensitive species and  
466 a group of less sensitive species. This is why [Zajdlik, Dixon & Stephenson \(2009\)](#) propose  
467 to model the species sensitivity distribution as a finite mixture, with raises customary issues  
468 of model choice. Using a BNP approach via `BNPdensity` allows generalising this approach  
469 while circumventing the theoretical and technical difficulties of estimating the right number  
470 of components in a mixture.

471 It is also important to use a method which may be applied to small datasets. This is another  
472 motivation for using a BNP approach, where model complexity adapts to the number of data  
473 points, and will tend to suggest simple or even univariate mixtures when few data points  
474 are present. On the contrary, many classical nonparametric approaches to modelling species  
475 sensitivity distribution ([Wang et al. 2015](#); [Verdonck et al. 2001](#)) only work well on large  
476 datasets.

477 To model species sensitivity distribution, we carefully select the parameters in the package  
478 `BNPdensity`. Given that concentrations vary on a wide range, it is common practice to  
479 work on log-transformed concentrations. We choose a fully nonparametric model using  
480 the normalised stable process ([Kingman 1975](#)) as mixing random measure (hence setting  
481  $\text{Alpha} = 1$  and  $\text{Beta} = 0$ ). We favor this process over the more classical Dirichlet process  
482 because it allows specifying less informative prior on the number of components, which  
483 makes it more robust to model misspecification ([Barrios et al. 2013](#)). With this process,  
484 the amount of information from the prior is controlled by the stability parameter  $\gamma$ , which  
485 we set to 0.4 ( $\text{Gama} = 0.4$ ). This choice reflects a compromise between model flexibility  
486 ( $\gamma \rightarrow 1$ ) and computational effort ( $\gamma$  small, see also section 3). As we wish the location  
487 parameter of the clusters  $\mu$  to be estimated freely, we use the default weakly informative  
488 prior of a normal base measure  $f_0^1(\mu|\varphi) = \mathcal{N}(\mu|\varphi_1, \varphi_2)$  with hyperpriors on  $\varphi$  given by  
489  $f(\varphi) = \mathcal{N}(\varphi_1|\psi_1, \psi_2)\text{ga}(\varphi_2|\psi_3, \psi_4)$  (see also [Barrios et al. \(2013\)](#) for more details).

490 For the prior on the scale of the clusters, we want to use two pieces of information: first,  
491 since the data has been scaled, scale parameters are likely to be smaller than 1, the extreme  
492 case being a mixture with a single component. Second, we want to avoid the possibility of  
493 extremely small clusters centred on a data point, because they are not very interesting from  
494 an interpretation point of view, and because they cause numerical problems (the likelihood  
495 diverges when a cluster scale goes to 0). Therefore, we choose a uniform distribution between  
496 0.1 and 1.5 for the prior on the cluster scales.

497 In keeping with the traditional assumption of normality of the species sensitivity distribution,  
498 we choose to use a normal kernel for the mixture (`distr.k = 1`).

499 We now compare three approaches to modelling Species Sensitivity Distribution (SSD):  
500 the most standard and recommended approach of [Wagner & Lokke \(1991\)](#); [Aldenberg &](#)  
501 [Jaworska \(2000\)](#), which is a simple normal model, the most recent proposal by ([Wang et al.](#)  
502 [2015](#)) which is a normal kernel density estimate and the BNP normal mixture made available  
503 with `BNPdensity` that we presented above. As already stated, a quantity of interest is the  
504 5th percentile of the distribution. We choose as an estimator the median of the posterior  
505 distribution of the 5th percentile, while the 95% credible bands are formed by the 2.5%  
506 and 97.5% quantiles of the posterior distribution of the 5th percentile. The 5th percentile  
507 of the Kernel Density Estimate (KDE) is obtained by numerical inversion of the cumulative  
508 distribution function, and the confidence intervals using the nonparametric bootstrap. The 5th  
509 percentile of the normal SSD and its confidence intervals are obtained following the classical  
510 method of [Aldenberg & Jaworska \(2000\)](#).

511 We use data from an ecotoxicity research database as pre-processed in [Hickey et al. \(2012\)](#).  
512 We extract data for the insecticide Carbaryl. The dataset contains 57 species, of which  
513 approximately 40% have censored data. We obtain a non censored version of this dataset by  
514 excluding right or left censored data, and replacing interval censored data by the midpoint of  
515 the interval. [Helsel \(2006\)](#); [Dowse et al. \(2013\)](#); [Kon Kam King et al. \(2014\)](#) have shown  
516 that transforming censored data risks inducing bias, hence the ability of `BNPdensity` to  
517 accommodate censoring is particularly valuable for SSD. There does not appear to be any  
518 easily available approach to use KDE methods on all types of censored data. Figure 7 shows  
519 a comparison of three approaches to SSD. The left hand side of Figure 7 shows that the BNP  
520 model is more flexible than both the KDE and normal model, while the right hand side shows  
521 that it is no less robust, according to a leave-one-out cross validation criterion. The middle  
522 panel shows that although the BNP model is more flexible and takes into account uncertainty  
523 on the number of clusters, the estimation of the 5th percentile is not much more uncertain  
524 than with the other methods. Significantly larger uncertainty would have jeopardised the real  
525 world applicability of the BNP-SSD.

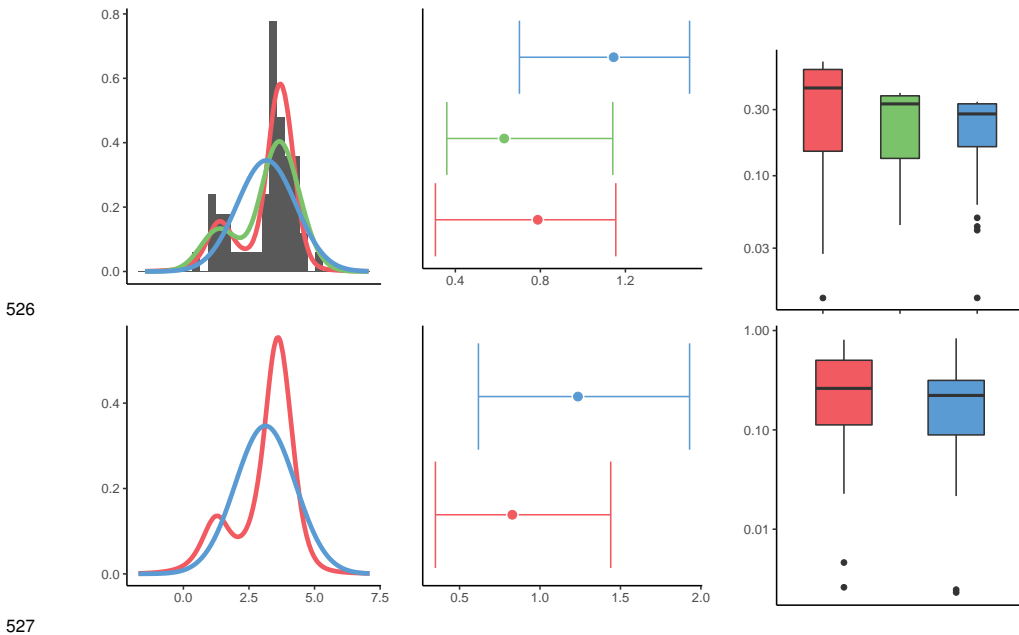
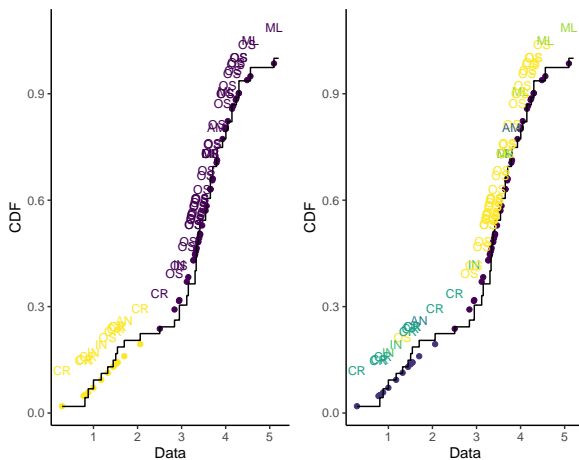


Figure 7. Top panel: non censored data. Bottom panel: censored data. The normal model is represented in blue, the KDE in green and the BNP in red. Left: density plot and histogram for the Carbaryl data using several SSD methods. The histogram is not available for censored data. Center: 5th percentile estimate (not available for KDE with censored data). Right: boxplot of the CPO (for BNP) and Leave-One-Out (LOO) (for normal and KDE, not available for KDE with censored data), one value for each data point.

528

529 An added value of the BNP-SSD is that on top of being more flexible than the classic normal  
 530 SSD and more robust than the nonparametric approach of Wang et al. (2015), as a mixture  
 531 model it naturally induces a clustering of the data which may contain some biologically  
 532 interesting information. We implemented functions to estimate the optimal clustering from  
 533 the MCMC sample and visualise it, potentially including a label on each point to reflect  
 534 available meta data for interpretation. In the context of SSD, it is interesting to know what  
 535 drives species sensitivity: it might be taxonomy, in the sense that taxonomically close species  
 536 will tend to respond in the same way and belong to the same cluster, but other drivers have  
 537 been suggested such as habitat, feeding behaviour or respiration, which may not coincide with  
 538 taxonomy. Figure 8 shows the clustering induced in the case of the insecticide Carbaryl. In  
 539 this case, there is a large cluster mostly composed of fish and molluscs, and a cluster mostly  
 540 composed of insects and crustaceans, showing that the clustering structure is consistent with  
 541 a finer taxonomic structure. This suggests that for Carbaryl, taxonomy may very well be the  
 542 main driver for sensitivity.





543

Figure 8. Graphical representation of the clustering induced by the mixture model for the Carbaryl data. The solid line represents the Turnbull estimate of the CDF, the points loosely represent the data. Interval censored data are represented at the middle of the interval, left and right censored data are not represented. A label describing the taxonomic group of each species is written above each point, AM: Amphibians, AN: Annelids (worms), CR: Crustaceans, IN: Insects, ML: Molluscs, OS: Osteichthyes (fish). On the left panel, the points and the labels are coloured according to the estimated cluster index. On the right panel, the labels are coloured according to the taxonomic group and the points are not coloured.

544

545

### Computational details

546 The results in this paper were obtained using R 4.1.1 with the BNPdensity package version  
 547 2020.3.4. R itself and all packages used are available from the Comprehensive R Archive  
 548 Network (CRAN) at <https://CRAN.R-project.org/>.

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