Clustering inconsistency for Pitman–Yor mixture models with a prior on the precision but fixed discount parameter

Caroline Lawless CAROLINE.LAWLESS@STATS.OX.AC.UK University of Oxford, Department of Statistics, 24-29 St Giles', Oxford OX1 3LB, UK Louise Alamichel LOUISE.ALAMICHEL@INRIA.FR Univ. Grenoble Alpes, CNRS, Inria, Grenoble INP, LJK, 38000 Grenoble, France Julyan Arbel JULYAN.ARBEL@INRIA.FR Univ. Grenoble Alpes, CNRS, Inria, Grenoble INP, LJK, 38000 Grenoble, France

Guillaume Kon Kam King GUILLAUME.KONKAMKING@INRAE.FR Université Paris-Saclay, INRAE, MaIAGE, 78350 Jouy-en-Josas, France

Abstract

Bayesian nonparametric (BNP) mixture models such as Dirichlet process (DP) and Pitman– Yor process (PY) mixture models are popular for modeling complex data. Their posterior distributions exhibit nice theoretical properties, converging at the optimal minimax rate to the true data-generating distribution, and extensive research has been devoted to developing this theory. However, consistency of the posterior distribution does not imply consistency of the number of clusters, and asymptotic guarantees for the posterior number of clusters of these BNP mixture models have been lacking until recently. Recent research has shown that these models can be inconsistent for the number of clusters. In the case of DP mixture models, this problem can be avoided when a prior is put on the model's concentration hyperparameter α , as is common practice. In this work, we prove that PY mixture models remain inconsistent for the number of clusters when a prior is put on α , in the special case where the true number of components in the data generating mechanism is equal to 1 and the discount parameter $\sigma \in (0, 1)$ is a fixed constant.

1. Introduction

Mixture models, popular for their flexibility and simplicity, are commonly used in the statistical analysis of heterogeneous data where observations are assumed to come from an unknown number of different populations. Since in a mixture, each observation is assumed to come from one population, such models naturally induce a clustering: two data points belong to the same cluster if they come from the same population. We focus on the problem of inferring the number of clusters in the data.

One solution is to fit mixture models with an increasing number of components and select the best model using the Akaike information criterion (AIC), the Bayes information criterion (BIC), etc. This method, however, may be computationally expensive since many models must be fitted. A Bayesian approach could alternatively be taken by putting a parametric prior (such as a Poisson) on the number of components, but inference can be challenging when the dimensionality or the amount of data becomes large (although new strategies have been proposed recently Miller and Harrison, 2018).

In this work, we consider infinite mixture models where the mixing measure is modelled with a nonparametric prior. In such models, the number of components possible has no upper bound. Inference may be performed in a unified way without the need for strong assumptions on the number of components and with no need to fit multiple models.

While the most standard nonparametric prior remains the Dirichlet process (DP) introduced by Ferguson (1973), many extensions now exist. In this work, we focus on the Pitman–Yor process (PY, Pitman and Yor, 1997), a natural extension of the DP with an extra parameter increasing model flexibility. Compared with DP mixtures, PY mixtures are better suited when the sizes of clusters are more evenly distributed. Due to the interpretability of their hyperparameters, ease of implementation, and nice mathematical properties, DP and PY priors are widely used in practice, and in the last two decades a huge amount of research has focused on their properties (see for example Ghosal and Van der Vaart, 2017; Müller et al., 2018). The use of the DP as a mixing measure was first introduced by Lo (1984). Thanks to the wide variety of efficient computational methods which have been introduced for their inference (Escobar and West, 1998; MacEachern and Müller, 1998; Neal, 2000; Blei and Jordan, 2006), nonparametric mixture models have become common in a wide range of modeling applications.

In the context of density estimation, under certain conditions the posterior distribution of DP mixture models concentrates at the true data-generating density at the minimaxoptimal rate (Ghosal and Van der Vaart, 2017; Ghosal et al., 1999). This holds for other types of Bayesian nonparametric priors, such as PY priors (Lijoi et al., 2005). Nguyen (2013) further proved posterior consistency of the mixing distribution in the Wasserstein metric DP and PY mixture models.

It is important to realize that consistency of the posterior distribution for the datagenerating density and even for the mixing measure does not imply consistency of the inferred number of clusters. Empirically, many researchers have observed that DP mixture posteriors tend to overestimate the number of clusters (West and Escobar, 1993; Lartillot and Philippe, 2004; Onogi et al., 2011). More recently, Miller and Harrison (2013, 2014) proved non-consistency for the number of components in DP and PY mixtures. Alamichel et al. (2022) extended this result to the case of Gibbs-type processes and finite-dimensional representations of BNP priors. A possible explanation for this inconsistency result can be found in a result proved by Rousseau and Mengersen (2011), that in overfitted finite or infinite mixture models, the weight attributed to extra cluster goes to zero as the number of observations grows. Provided that the weights for the extra components are infinitesimally small, any mixture can be approximated arbitrarily well by a mixture with a larger number of components.

Despite the above inconsistency results, it can be possible to achieve posterior consistency for the number of clusters in the mixture models we consider. Guha et al. (2021) introduce a fast and simple post-processing procedure for DP mixtures which provides clustering consistency. Alamichel et al. (2022) extend this result to PY mixtures. Zeng et al. (2023) introduce a quasi-Bernoulli stick-breaking process and prove posterior consistency for the number of clusters in the associated mixture model. Consistency in this class of BNP priors requires the prior to be calibrated based on the sample size, hence the model is no longer projective. Ascolani et al. (2022) show that posterior consistency for the number of clusters can be achieved for a projective model by putting a prior on the DP concentration parameter α . DP mixtures modeled in this way can be considered as mixtures of DP mixtures (Antoniak, 1974) and are commonly used in practice. We show that Ascolani et al. (2022)'s result cannot be directly extended to PY mixtures: we prove clustering inconsistency for Pitman–Yor process mixture models with a prior on the concentration parameter, when the true number of clusters in the data generating mechanism, t, is equal to one, and when the discount parameter $\sigma \in (0,1)$ is a fixed constant.

2. Preliminaries

We assume that data $X_{1:n} \in \mathbb{X}^n$ is generated by a mechanism of the following form:

$$X_i \stackrel{\text{iid}}{\sim} P = \sum_{j=1}^t p_j k(\cdot | \theta_j^*), \tag{1}$$

where the p_j are probability weights in (0, 1) summing to one, and where the $k(\cdot|\theta_j^*)$ are probability kernels, each depending on some parameter θ_j^* . The above may alternatively be expressed as a convolution of the component-specific kernel $k(\cdot|\theta)$ with the discrete mixing measure $G = \sum_{j=1}^{t} p_j \delta_{\theta_j^*}$: $P(x) = \int k(x|\theta)G(d\theta)$. We consider the well-specified case where the kernel density $k(\cdot|\theta)$ is known, but where the integer t, the weights p_j , and the latent variables θ_j^* in Equation (1) are all unknown. To allow for an unbounded number of components t in the mixture, we consider nonparametric mixture models with nonparametric priors on the mixing measure G.

Ascolani et al. (2022) consider Dirichlet process mixture models with a prior on the concentration parameter α :

$$X_i | \theta_i \stackrel{\text{ind}}{\sim} k(\cdot | \theta_i), \quad \theta_i | \tilde{P} \stackrel{\text{iid}}{\sim} \tilde{P} \quad \tilde{P} | \alpha \sim \text{DP}(\alpha, Q_0), \quad \alpha \sim \pi_1,$$
(2)

where π_1 is a prior distribution on α , and Q_0 is the DP base measure.

We consider an extension of Ascolani et al. (2022)'s model, which are Pitman–Yor mixture models with a prior on the concentration parameter $\alpha > 0$ and with a fixed discount parameter $\sigma \in (0, 1)$:

$$X_i|\theta_i \stackrel{\text{ind}}{\sim} k(\cdot|\theta_i), \quad \theta_i|\tilde{P} \stackrel{\text{iid}}{\sim} \tilde{P} \quad \tilde{P}|\alpha, \sigma \sim \text{PY}(\alpha, \sigma, Q_0), \quad \alpha \sim \pi_1.$$
(3)

Following the notation of Ascolani et al. (2022), for every pair of numbers $(n, s) \in \mathbb{N}^2$ with $s \leq n$, we let $\tau_s(n)$ denote the set of partitions of $\{1, \ldots, n\}$ into s non empty subsets. Conditional on parameters α and σ , a Pitman–Yor mixture model induces the following prior distribution on the space of partitions on n, for any $n \in \mathbb{N}$, and any $A = \{A_1, \ldots, A_s\} \in \tau_s(n), s \leq n$,

$$p(A|\alpha,\sigma) = \frac{\sigma^{s-1}(1+\frac{\alpha}{\sigma})_{(s-1)}}{(1+\alpha)_{(n-1)}} \prod_{j=1}^{s} (1-\sigma)_{(a_j-1)},$$
(4)

where $\alpha_{(n)} = \alpha \cdots (\alpha + n - 1)$ is the ascending factorial and $a_j = |A_j|$ stands for the cardinality of the set A_j . Conditionally on the partition A, the probability distributions of the data $X_{1:n} = (X_1, \ldots, X_n)$ and of the cluster-specific parameters $\hat{\theta}_{1:s} = (\hat{\theta}_1, \ldots, \hat{\theta}_s)$ are

$$p(X_{1:n}|\hat{\theta}_{1:s}, A) = \prod_{j=1}^{s} \prod_{i \in A_j} k(X_i|\hat{\theta}_j), \quad p(\hat{\theta}_{1:s}|A, \theta) = p(\hat{\theta}_{1:s}|A) = \prod_{j=1}^{s} q_0(\hat{\theta}_j).$$

We use the standard notation K_n to denote the number of clusters in a sample of size n. The concentration parameter α essentially controls the prior mean of K_n , while the discount parameter σ has more impact on the variance (Bystrova et al., 2021). More specifically, the prior number of clusters is known to grow asymptotically with n as a power-law, e.g. in expectation we have $\mathbb{E}K_n \sim \frac{\Gamma(\alpha+1)}{\sigma\Gamma(\alpha+\sigma)} n^{\sigma}$ when $n \to \infty$ (see Section 3.3 of Pitman, 2002). Under our model (3), K_n has the following prior distribution

$$p(K_n = s | \sigma) = \int \sum_{A \in \tau_s(n)} p(A | \alpha, \sigma) \pi_1(\mathrm{d}\alpha)$$

where $p(A|\alpha, \sigma)$ is as above.

To study the asymptotic behavior of the number of clusters, we consider $p(K_n = s|X_{1:n}, \sigma)$. We start with the joint distribution $(X_{1:n}, K_n|\sigma)$ which, for every $x_{1:n} = (x_1, \ldots, x_n) \in \mathbb{X}^n$, is given by:

$$p(X_{1:n} = x_{1:n}, K_n = s | \sigma) = \sum_{A \in \tau_s(n)} p(A | \sigma) \prod_{j=1}^s m(x_{A_j})$$

where $p(A|\sigma) = \int p(A|\alpha, \sigma)\pi_1(d\alpha)$ and $m(x_{A_j}) = \int \prod_{i \in A_j} k(x_i|\theta)q_0(\theta)d\theta$ is the marginal likelihood for the subset of observations identified by A_j , given that they are clustered together.

3. Theoretical result

Throughout, we make the same assumptions as Ascolani et al. (2022) (see also Appendix A). The first set of assumptions A1, A2, and A3, regard the prior π_1 for the precision parameter α : it is assumed to be absolutely continuous with respect to the Lebesgue measure, to have a polynomial behaviour around the origin, and to have subfactorial moments. Ascolani et al. (2022) prove in their Lemma 1 that common families of prior satisfy these assumptions (e.g. distributions with bounded support, the gamma distribution, etc.). The second set of assumptions regards the type of mixture kernels $k(\cdot|\cdot)$ considered: attention is restricted to location families, where the kernel is of the form $k(x|\theta) = g(x - \theta)$ for some density function g on \mathbb{R} . More specifically, assumptions B1 and B2 of Ascolani et al. (2022) require that g be strictly positive and differentiable with bounded derivative on some interval and zero elsewhere. Finally, assumption B3 requires that the BNP process base measure Q_0 be absolutely continuous with respect to the Lebesgue measure, with bounded density q_0 .

Theorem 1 Suppose that the prior π_1 over the concentration parameter α , the kernel k, and density q_0 satisfy assumptions of Ascolani et al. (2022) recalled above. For every P as in (1), for t = 1, we have

$$p(K_n = 1 | X_{1:n}) \not\rightarrow 1 \text{ as } n \rightarrow \infty.$$

The proof of Theorem 1 rests on analysing the ratio $\frac{p(K_n=s|X_{1:n})}{p(K_n=1|X_{1:n})}$, as consistency cannot hold if it does not converge to 0 as $n \to \infty$. Following the strategy of Ascolani et al. (2022), this ratio can be split into the product of two quantities, one capturing the impact of the

prior distribution on the concentration parameter α , and the other independent of the prior on α . In the Dirichlet process case with a prior on α , the first quantity goes to 0 and the second remains bounded. We show that in the Pitman–Yor case, the σ parameter enters the first quantity and prevents it from vanishing as $n \to \infty$, destroying consistency and highlighting a fundamental difference between the DP and PY processes.

4. Simulation study

We illustrate our results through a simulation study. Data is generated using a Gaussian location mixture with t = 3 components:

$$P(x) = \sum_{i=1}^{3} p_i \mathcal{N}(x|\mu_i, \Sigma),$$

where $p = (p_1, p_2, p_3) = (0.5, 0.3, 0.2)$ and $\mathcal{N}(x|\mu_i, \Sigma)$ is a multivariate Gaussian with mean μ_i and covariance matrix Σ with $\mu_1 = (0.8, 0.8), \mu_2 = (0.8, -0.8), \mu_3 = (-0.8, 0.8)$ and $\Sigma = 0.05 I_2$. We adapt the Importance Conditional Sampler for PY mixtures of Canale et al. (2022), with the following prior specification:

$$P \sim \mathrm{PY}(\alpha, \sigma, Q_0), \quad \mu_i \sim \mathcal{N}(b_0, B_0), \quad i = 1, \dots, t,$$

 $\Sigma^{-1} \sim \mathcal{W}(c_0, C_0), \quad C_0 \sim \mathcal{W}(g_0, G_0).$

The Wishart prior on Σ^{-1} and the prior on μ_i are the same as in Malsiner-Walli et al. (2016).

Figure 1 (a) illustrates the inconsistency of Pitman–Yor mixture models for the number of clusters proved in Miller and Harrison (2014) when the parameters α and σ of PY are fixed. The result proved in this paper stated that PY mixture models are also inconsistent for the number of clusters if σ is fixed and there is a prior on α when t = 1, Figure 1 (b) illustrates that this is also the case for the more realistic case of t = 3: the number of clusters does not converge around the true number of components t = 3 (the case t = 1 is in Appendix C). Figure 1 (c) and (d) illustrate cases not covered by current theoretical results, in which a hyperprior is placed on σ and α is either fixed or random. When α is fixed and there is a hyperprior on σ , the model seems to recover the true number of components consistently. In the second scenario, the simulations appear to show inconsistency for the model. Both cases constitute interesting future research topics.

5. Discussion

We have proved inconsistency for the number of clusters when fitting single-component mixtures with Pitman–Yor mixture models with a prior on the concentration parameter α and fixed discount parameter σ . Our result holds when the true number of clusters in the data-generating mechanism is one. While hinting at what to expect, further study would be needed to fully understand clustering consistency for a data-generating mechanism with an arbitrary number of components.

While our result is limited to the setting where the discount parameter σ is kept fixed, it is common in practice to put a prior on both PY parameters α and σ in PY mixture models.

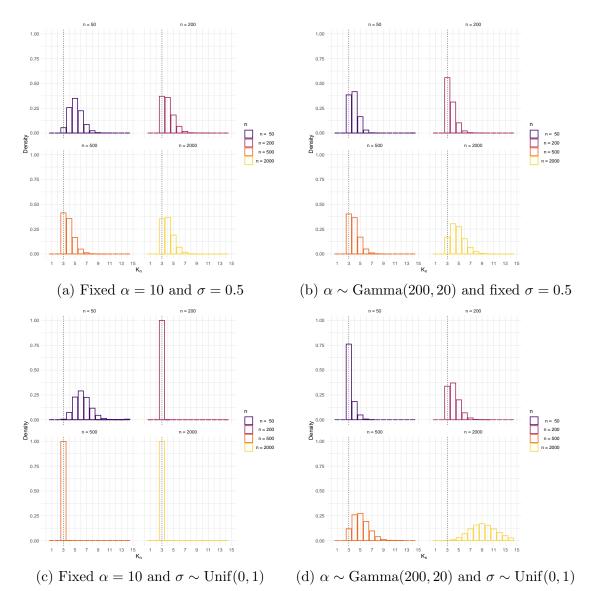


Figure 1: Posterior distribution of the number of clusters K_n under a Pitman–Yor process mixture for various choices of n and with (a) fixed parameters α and σ ; (b) $\alpha \sim \text{Gamma}(200, 20)$ and fixed σ ; (c) fixed α and $\sigma \sim \text{Unif}(0, 1)$; and (d) $\alpha \sim$

The simulation study suggests inconsistency in this case, but consistency when keeping α fixed and putting a prior on σ . Both situations are the subject of current investigations.

Gamma(200, 20) and $\sigma \sim \text{Unif}(0, 1)$.

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Appendix A. Assumptions

Our theoretical result relies on the following three assumptions on the prior π_1 of α .

Assumption 1:

The prior π_1 is absolutely continuous with respect to the Lebesgue measure. Its density is denoted by π_1 .

Assumption 2: There exist ϵ, δ, β such that, for all $\alpha \in (0, \epsilon)$ it holds that $\frac{\alpha^{\beta}}{\delta} \leq \pi_1(\alpha) \leq \delta \alpha^{\beta}$.

Assumption 3: There exist $D, \nu, \rho > 0$ such that $\int \alpha^s \pi(\alpha) d\alpha < D\rho^{-s} \Gamma(\nu + s + 1)$ for every $s \ge 1$.

We assume kernels of the form

$$k(x|\theta) = g(x - \theta), \quad x \in \mathbb{R}.$$

Our results rely on the following assumptions on the function g and the base measure Q_0 of the PYP.

ASSUMPTION 4: Function g is strictly positive on some interval [a, b] and 0 elsewhere.

Assumption 5:

Function g is differentiable with bounded derivative in (a, b).

Assumption 6:

The base measure Q_0 is absolutely continuous with respect to the Lebesgue measure, and its density q_0 is bounded.

Appendix B. Proof of results

The proof of our result relies on the following simple lemma, used by and proved by Ascolani et al. (2022). It justifies working with ratios, which allows us to avoid calculations of marginal likelihoods of the observed data.

Lemma 2 The convergence $p(K_n = t | X_{1:n}) \to 1$ as $n \to \infty$ holds if and only if one has

$$\sum_{s \neq t} \frac{p(K_n = s | X_{1:n})}{p(K_n = t | X_{1:n})} \to 0 \quad as \ n \to \infty.$$

Proof of Theorem 1. By Lemma 2, it will be sufficient to prove that $\frac{p(K_n=s|X_{1:n})}{p(K_n=1|X_{1:n})} \neq 0$ as $n \to \infty$, for some s > 1. We will prove this using s = 2.

In order to prove our result, we make use of results of the asymptotic behavior of certain quantities under the Dirichlet process mixture model of Ascolani et al. (2022). Throughout this proof will thus use the subscript DP to indicate that a quantity is related to the Dirichlet

process model, and we will use the subscript PY to indicate that a quantity is related to the Pitman–Yor model, whenever there is ambiguity.

Under our Pitman–Yor mixture model, by applying Equation (4), we have

$$\frac{p_{\mathrm{PY}}(K_n = 2|X_{1:n})}{p_{\mathrm{PY}}(K_n = 1|X_{1:n})} = \frac{\int \sigma \left(1 + \frac{\alpha}{\sigma}\right) \frac{\pi_1(\alpha)}{(1+\alpha)_{(n-1)}} \mathrm{d}\alpha}{\int \frac{\pi_1(\alpha)}{(1+\alpha)_{(n-1)}} \mathrm{d}\alpha} \frac{\sum_{A \in \tau_2(n)} \prod_{j=1}^2 (1-\sigma)_{(a_j-1)} m(X_{A_j})}{(1-\sigma)_{(n-1)} m(X_{1:n})}$$
$$= C_{\mathrm{PY}}(n, 1, 2) R_{\mathrm{PY}}(n, 1, 2)$$

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where

$$C_{\rm PY}(n,1,2) = \frac{\int \sigma \left(1 + \frac{\alpha}{\sigma}\right) \frac{\pi_1(\alpha)}{(1+\alpha)_{(n-1)}} d\alpha}{\int \frac{\pi_1(\alpha)}{(1+\alpha)_{(n-1)}} d\alpha}$$

and

$$R_{\rm PY}(n,1,2) = \frac{\sum_{A \in \tau_2(n)} \prod_{j=1}^2 (1-\sigma)_{(a_j-1)} m(X_{A_j})}{(1-\sigma)_{(n-1)} m(X_{1:n})}.$$

Similarly, under the Dirichlet process mixture model of Ascolani et al. (2022), one gets

$$\frac{p(K_n = s | X_{1:n})_{\text{DP}}}{p(K_n = t | X_{1:n})_{\text{DP}}} = C_{\text{DP}}(n, t, s) R_{\text{DP}}(n, s, t),$$

where $C_{\text{DP}}(n, t, s)$ is an integral in α over all of the terms involving α , and $R_{\text{DP}}(n, t, s)$ contains all of the remaining factors:

$$C_{\rm DP}(n,t,s) := \frac{\int [\alpha^s \pi_1(\alpha)/\alpha_{(n)}] \mathrm{d}\alpha}{\int [\alpha^t \pi_1(\alpha)/\alpha_{(n)}] \mathrm{d}\alpha}$$

and

$$R_{\rm DP}(n,t,s) := \frac{\sum_{A \in \tau_s(n)} \prod_{j=1}^s (a_j - 1)! \prod_{j=1}^s m(X_{A_j})}{\sum_{B \in \tau_t(n)} \prod_{j=1}^t (b_j - 1)! \prod_{j=1}^t m(X_{B_j})}$$

Ascolani et al. (2022) prove that

$$C_{\rm DP}(n, t, s) \to 0 \text{ as } n \to \infty \quad \forall 0 < t < s.$$
 (5)

Now, since our expression $R_{\rm PY}(n, 1, 2)$ above does not depend on α , it is identical to the corresponding expression in the setup of Miller and Harrison (2014), who prove that it does not converge to zero as $n \to \infty$. What is left to show is that our expression $C_{\rm PY}(n, 1, 2)$ above does not converge to zero as $n \to \infty$.

We then have,

$$C_{\mathrm{PY}}(n,1,2) = \frac{\int \sigma \left(1 + \frac{\alpha}{\sigma}\right) \frac{\pi_1(\alpha)}{(1+\alpha)_{(n-1)}} \mathrm{d}\alpha}{\int \frac{\pi_1(\alpha)}{(1+\alpha)_{(n-1)}} \mathrm{d}\alpha}$$
$$= \sigma + \frac{\int \alpha \frac{\pi_1(\alpha)}{(1+\alpha)_{(n-1)}} \mathrm{d}\alpha}{\int \frac{\pi_1(\alpha)}{(1+\alpha)_{(n-1)}} \mathrm{d}\alpha} = \sigma + \frac{\int \alpha^2 \frac{\pi_1(\alpha)}{(\alpha)_{(n)}} \mathrm{d}\alpha}{\int \alpha \frac{\pi_1(\alpha)}{(\alpha)_{(n)}} \mathrm{d}\alpha}$$
$$= \sigma + C_{\mathrm{DP}}(n,1,2) \to \sigma \text{ as } n \to \infty,$$

where the final line above comes from the special case of Equation (5) where t = 1 and s = 2.

Appendix C. Details on the simulation study

To be closer to the results stated in Section 3, we now consider data generated from a mixture model with only one component. It means that the data are generated from the same Gaussian model,

$$P(x) = \mathcal{N}(x|\mu, \Sigma).$$

The different datasets are of size $n \in \{50, 200, 500, 2000\}$ as in Section 4. The following parameters are considered for the mean and the covariance matrix,

$$\mu = (0.8, 0.8)$$
 and $\Sigma = 0.05 I_2$.

The model and the algorithms used are similar as in Section 4. We choose the hyperparameters of the priors on σ and α such that the mean of these distributions correspond to the fixed values chosen for α and σ . The prior on α also satisfies the conditions introduced in Ascolani et al. (2022).

It can be noted that we need a larger number of iterations to achieve MCMC convergence when we put a prior on σ .

As we choose here a unique component the results are less graphic than in Section 4. Still, we can observe that in Figure 2 (b), the model seems to overestimate K_n as the size increase. Hence, Figure 2 (b) illustrates the theoretical result in Section 3.

Also, the distribution in Figure 2 (c) seems to slowly concentrate on the left, but concentration of the posterior on a single component is probably slower than on three components and it would be necessary to use simulated data with a larger sample size to obtain more striking figures.

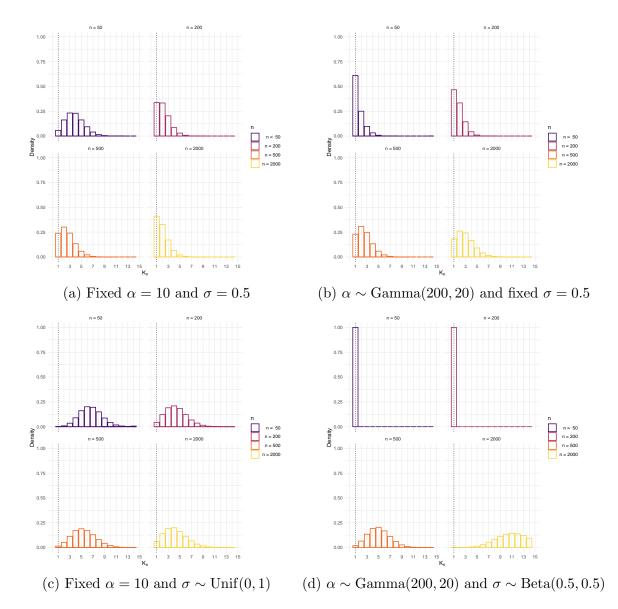


Figure 2: Posterior distribution of the number of clusters K_n under a Pitman–Yor process mixture for various choices of n and with (a) fixed parameters α and σ ; (b) $\alpha \sim \text{Gamma}(200, 20)$ and fixed σ ; (c) fixed α and $\sigma \sim \text{Unif}(0, 1)$; and (d) $\alpha \sim \text{Gamma}(200, 20)$ and $\sigma \sim \text{Unif}(0, 1)$.