Bayesian Nonparametric Inference for “Species-sampling” Problems

Cecilia Balocchi∗, Stefano Favaro†, Zacharie Naulet‡

Abstract

“Species-sampling” problems (SSPs) refer to a broad class of statistical problems that, given an observable sample from an unknown population of individuals belonging to some species, call for estimating features of the unknown species composition of additional unobservable samples from the same population. Among SSPs, the problems of estimating coverage probabilities, the number of unseen species and coverages of prevalences have emerged over the past three decades for being the objects of numerous studies, both in methods and applications, mostly within the field of biological sciences but also in machine learning, electrical engineering, theoretical computer science and information theory. In this paper, we present an overview of Bayesian nonparametric (BNP) inference for such three SSPs under the popular Pitman–Yor process (PYP) prior: i) we introduce each SSP in the classical (frequentist) nonparametric framework, and review its posterior analyses in the BNP framework; ii) we improve on computation and interpretability of existing posterior distributions, typically expressed through complicated combinatorial numbers, by establishing novel posterior representations in terms of simple compound Binomial and Hypergeometric distributions. The critical question of estimating the discount and scale parameters of the PYP prior is also considered and investigated, establishing a general property of Bayesian consistency with respect to the hierarchical Bayes and empirical Bayes approaches, that is: the discount parameter can be always estimated consistently, whereas the scale parameter cannot be estimated consistently, thus advising caution in posterior inference. We conclude our work by discussing other SSPs, and presenting some emerging generalizations of SSPs, mostly in biological sciences, which deal with “feature-sampling” problems, multiple populations of individuals sharing species and classes of Markov chains.

Keywords: Bayesian nonparametrics, Bayesian consistency, Coverage of prevalences, Coverage probabilities, Empirical Bayes, Hierarchical Bayes, Pitman–Yor process prior, “Species-sampling” problems, Unseen species.

∗Cecilia Balocchi is Postdoctoral Research Fellow, Department of Economics and Statistics, University of Torino, Torino, Italy (e-mail: cecilia.balocchi@unito.it).
†Stefano Favaro is Professor, Department of Economics and Statistics, University of Torino and Collegio Carlo Alberto, Torino, Italy (e-mail: stefano.favaro@unito.it) and is also affiliated to IMATI-CNR “Enrico Magenes” (Milan, Italy).
‡Zacharie Naulet is Assistant Professor, Department of Mathematics, Université Paris-Sud, Orsay, France (e-mail: zacharie.naulet@universite-paris-saclay.fr).
1 Introduction

“Species-sampling” problems (SSPs) refer to a broad class of statistical problems that deal with the estimation of discrete functionals, of which the number of unseen species is the most popular example [Fisher et al., 1943; Goodman, 1949; Good, 1953; Good and Toulmin, 1956; Efron and Thisted, 1976]. Consider a population of individuals, such that each individual is labeled by a symbol or species’ label belonging to a (possibly infinite) space of symbols. The unseen-species problem assumes that \( n \geq 1 \) observable samples from the population are modeled as a random sample \( (X_1, \ldots, X_n) \) from an unknown distribution \( p \), and calls for estimating

\[
u_{n,m} = |\{X_{n+1}, \ldots, X_{n+m}\} \setminus \{X_1, \ldots, X_n\}|,
\]

namely the number of hitherto unseen symbols that would be observed if \( m \geq 1 \) additional samples \( (X_{n+1}, \ldots, X_{n+m}) \) were collected from the same distribution. The unseen-species problem may be considered as the natural \( m \)-step ahead generalization of the problem of estimating the missing mass, that is the probability of discovering at the \( (n + 1) \)-th draw a symbol not observed in the sample [Good, 1953]. In general, SSPs consist of refinements or generalizations of the unseen-species problem, calling for the estimation of discrete functionals of the \( X_i \)'s that encode features of the species’ composition of the additional unobservable samples. It is a critical feature common to all SSPs that species’ labels identifying the \( X_i \)'s are immaterial in the definition of the functional object of interest, thus making SSPs “invariant” with respect to species labelling. SSPs first appeared in ecology for the estimation of the species richness or diversity of ecological populations, and their importance has grown dramatically in recent years driven by a plethora of applications in biological and physical sciences, machine learning, electrical engineering, theoretical computer science and information theory.

Biological sciences are arguably the field where SSPs have been most investigated over the past three decades, both in methods and applications. A comprehensive and up-to-date review is presented by Deng et al. [2019], from which it emerges the critical role of SSPs for the understanding of genome biology. Although sequencing technologies have greatly advanced the understanding of genome biology, it is well known that observed samples are not perfectly representative of the molecular heterogeneity or species composition of the underlying DNA library, often providing a poor representation due to low-abundance molecules that are hard to sample. Unless DNA libraries can be sequenced up to complete saturation, which is typically not convenient due to budget constraints, it is common to make use of the observed sample to infer the molecular heterogeneity of additional unobservable samples from the library, as well as of the library itself. Deng et al. [2019] identified three main questions that a researcher may ask:

Q1) what is the expected population frequency of a species with frequency \( r \geq 1 \) in the sample?

Q2) how many previously unobserved species in the sample will be observed in additional samples?
Q3) how many species with frequency \( r \geq 1 \) in the sample will be observed in additional samples?

These are examples of SSPs, with Q2) being precisely the unseen-species problem, and they apply to the analysis of sequencing complexity [Daley and Smith, 2013], the design of sequencing experiments [Sims et al., 2014] and the estimation of genetic diversity [Gao et al., 2007], immune receptor diversity [Robins et al., 2009] and genetic variation [Ionita-Laza et al., 2009].

### 1.1 Our contributions

Nonparametric estimation of the number of unseen-species dates back to the 1950s [Goodman, 1949; Good and Toulmin, 1956; Efron and Thisted, 1976], and only recent works have set forth a rigorous and comprehensive treatment of such a problem [Orlitsky et al., 2016; Wu and Yang, 2019; Polyanskiy and Wu, 2020]. Besides providing nonparametric estimators of \( u_{n,m} \) with provable guarantees, these works have introduced a collection of analytical tools that pave the way to nonparametric inference for other SSPs [Wu and Yang, 2021].

In general, nonparametric estimators of SSPs do not rely on any assumption on the underlying distribution \( p \), with provable guarantees that hold uniformly over all distributions. Although this assumption-free framework leads to develop grounded theories in their greatest generality, worst case distributions may severely hamper the empirical performance of the estimators and the study of their provable guarantees, thus leading to unreliable results in concrete applications. To overcome this drawback it is therefore useful to take into account any a priori knowledge on the phenomenon object of study, which in most cases of practical interest results in assumptions on the tail behaviour of the underlying distribution \( p \).

That is, the assumption-free framework of SSPs may be usefully enriched through suitable prior assumptions of regularity on the tail behaviour of \( p \). A common, and flexible, assumption is that of regular variation, which allows for \( p \) to range from geometric tails to heavy power-law tails [Gnedin et al., 2007]. This is well-motivated by the ubiquitous power-law type distributions, which occur in many situations of scientific interest, and nowadays have significant consequences for the understanding of numerous natural and social phenomena [Clauset et al., 2009].

A Bayesian nonparametric (BNP) approach to SSPs has been set forth in Lijoi et al. [2007], and it relies on the specification of a prior on the underlying distribution \( p \), thus being a natural approach to enrich the assumption-free framework of SSPs through prior assumptions on the tail behaviour of \( p \). In this respect, species sampling models [Pitman, 1996] provide a broad class of nonparametric priors for \( p \) [Pitman, 2006, Chapter 3 and Chapter 4]. Among species sampling models, Lijoi et al. [2007] focus their attention on the Pitman–Yor process (PYP) prior [Perman et al., 1992; Pitman and Yor, 1997], whose mathematical tractability and interpretability make it the natural candidate in applications [Favaro et al., 2009, 2012]. The PYP prior is indexed by a discount parameter \( \alpha \in [0, 1) \) and a scale parameter \( \theta > -\alpha \), such that for \( \alpha = 0 \) it reduces to the celebrated Dirichlet process (DP) of Ferguson [1973]. Of special interest is the discount parameter \( \alpha \), as it admits a clear
interpretation in terms of controlling the tail behaviour of the PYP prior, which ranges from geometric tails to heavy power-law tails. In particular, the larger $\alpha$ the heavier the tail of the PYP prior, and as a limiting case for $\alpha \to 0$ one recovers the geometric tail behaviour featured by the DP [Pitman, 2006, Chapter 3]. Such a peculiar parameterization makes the PYP a flexible prior choice, which allows for tuning of the tail behaviour of the prior with respect to the empirical distribution of the data. Among species sampling models, we may say that the PYP prior is a unique match among mathematical tractability, flexibility and interpretability [De Blasi et al., 2015; Bacallado et al., 2017].

In this paper, we present an overview of BNP inference for SSPs under the popular PYP prior. Motivated by the work of Deng et al. [2019], we focus on SSPs corresponding to the aforementioned questions Q1, Q2 and Q3, respectively, which have been proved to be of practical interest also beyond biological sciences. Regarding Q1, we consider the estimation of coverage probabilities, which include the missing mass and the coverage probability of order $r \geq 1$, namely the probability mass of species observed with frequency $r$ in the sample. Regarding Q2, we consider the estimation of the number of unseen species and unseen species’ prevalences of order $r \geq 1$, namely the number of hitherto unseen species that would be observed with frequency $r$ in $m$ additional samples. Finally, regarding Q3, we consider the estimation of coverages of prevalence of order $r \geq 1$, namely the number of species with frequency $r$ in the sample that would be observed in $m$ additional samples. Each SSP is introduced in the classical (frequentist) framework, which is typically the framework where it first appeared in the literature, and then its BNP analysis is presented under the PYP prior. While reviewing posterior analyses of SSPs from the BNP literature, we establish novel representations of posterior distributions. In particular, we show that posterior distributions that are typically expressed in terms of complicated combinatorial numbers, which hamper both the computation and the interpretability of posterior inferences, admit representations in terms of simple compound Binomial distributions and Hypergeometric distributions. This is a remarkable step forward within the BNP approach to SSPs, especially with respect to its practical use in concrete applications, as it contributes to simplify and make more interpretable posterior inferences.

Critical in the BNP approach to SSPs is the estimation of prior’s parameters, namely $(\alpha, \theta)$ under the PYP prior. Two approaches for estimating $(\alpha, \theta)$ are: i) the hierarchical Bayes or fully Bayes approach, which relies on estimates obtained from the posterior distribution of $(\alpha, \theta)$ with respect to a suitable prior specification; ii) the empirical Bayes approach, which relies on estimates obtained by maximizing, with respect to $(\alpha, \theta)$, the marginal likelihood of the observable sample. The empirical Bayes approach is the most used in practice [Lijoi et al., 2007; Favaro et al., 2009; De Blasi et al., 2015], though no provable guarantees have been established for empirical Bayes estimates of the parameter $(\alpha, \theta)$. In particular, the lack of a theoretical understanding of the hierarchical Bayes approach and the empirical Bayes approach has precluded clear guidelines for choosing among them. Here, we consider both the approaches, and we investigate their properties of Bayesian consistency. Under moderate misspecification, we find that the empirical Bayes estimator of $(\alpha, \theta)$ converges to a limit that is interpretable in terms of the true data generating mechanism. When the model
is correct, we find that: i) both the the empirical Bayes estimator and the hierarchical Bayes estimator of $\alpha$ are consistent; ii) $\theta$ can not be tested or estimated consistently, because of a curious anti-concentration result. Under the hierarchical Bayes approach, we characterize the large sample asymptotic behavior of the posterior distribution of the parameter $(\alpha, \theta)$; we find that the limiting posterior distribution of $\theta$ depends on the prior, thus particular caution should be used. As for $\alpha$, we prove a weak form of the Bernstein-von Mises theorem, finding its contraction rates.

1.2 Organization of the paper

The paper is structured as follows. In Section 2 we introduce the classical (frequentist) nonparametric framework and the BNP framework for SSPs, and we review the sampling structure of the PYP prior with emphasis on the interpretation of the prior’s parameter $(\alpha, \theta)$. BNP inference for SSPs under the PYP prior is presented in Section 3 for coverage probabilities, in Section 4 for the number of unseen species, and in Section 5 for coverages of prevalences. In Section 6 we consider the problem of estimating $(\alpha, \theta)$, establishing a general property of Bayesian consistency with respect to the hierarchical Bayes and empirical Bayes approaches. Section 7 contains a discussion of other SSPs, and presents some emerging generalizations of SSPs, mostly in the field of biological sciences, which deal with “feature-sampling” problems, multiple populations of individuals sharing species and classes of Markov chains. Additional material, (technical) results, and proofs of our main results are deferred to the Supplementary Materials.

2 The BNP species sampling framework

The classical (frequentist) nonparametric framework for SSPs, here referred to as the “classical species sampling framework”, assumes that $n \geq 1$ observable samples from a population of individuals belonging to a (possibly infinite) space of species’ labels are modeled as a random sample $X_n = (X_1, \ldots, X_n)$ from an unknown distribution $p$. Following Lijoi et al. [2007], we consider a BNP framework for SSPs that relies on a PYP prior for $p$, namely we assume that

$$X_i \mid P \sim P_{\text{iid}}, \quad i = 1, \ldots, n,$$

$$P \sim \text{PYP}(\alpha, \theta),$$

with $\text{PYP}(\alpha, \theta)$ being the law of the PYP process with parameter $(\alpha, \theta)$. We refer to (1) as the “BNP species sampling framework”. Among possible definitions of the PYP, a simple and intuitive one follows from the stick-breaking construction [Pitman, 1995]. For $\alpha \in [0, 1)$ and $\theta > -\alpha$ let: i) $(V_i)_{i \geq 1}$ be independent random variables with $V_i$ being distributed as a Beta distribution with parameter $(1 - \alpha, \theta + i\alpha)$, for $i \geq 1$; ii) let $(S_j)_{j \geq 1}$ be random variables, independent of the $V_i$’s, and independent and identically distributed as a non-atomic distribution $\nu$ on a measurable space $S$. If we set $P_1 = V_1$ and $P_j = V_j \prod_{1 \leq i \leq j-1} (1 - V_i)$
for \( j \geq 1 \), such that \( P_j \in (0, 1) \) for any \( j \geq 1 \) and \( \sum_{j \geq 1} P_j = 1 \) almost surely, then the random probability measure \( P = \sum_{j \geq 1} P_j \delta_{S_j} \) is a PYP on \( \mathbb{S} \) with base distribution \( \nu \), discount \( \alpha \) and scale \( \theta \). The PYP generalizes the DP by means of \( \alpha \in [0, 1) \), which controls the tail behaviour of \( P \). In particular, for any \( \alpha \in (0, 1) \) let \( P \sim \text{PYP}(\alpha, \theta) \) and let \( (P_{(j)})_{j \geq 1} \) be the decreasingly ordered random probabilities \( P_j \)'s of \( P \). Then, as \( j \to +\infty \) the \( P_j \)'s follow a power-law distribution of exponent \( c = \alpha^{-1} [\text{Pitman and Yor, 1997}] \); that is, \( \alpha \in (0, 1) \) controls the power-law tail behaviour of the PYP through the small \( P_j \)'s: the larger \( \alpha \) the heavier the tail of \( P \). As a limiting case for \( \alpha \to 0 \), the DP features geometric tails \([\text{Pitman, 2006, Chapter 3 and Chapter 4}]\).

### 2.1 Sampling formulae for the PYP prior

According to de Finetti's representation theorem, a random sample \( X_n \) from \( P \sim \text{PYP}(\alpha, \theta) \) is part of an exchangeable sequence \((X_i)_{i \geq 1}\) with directing (de Finetti) measure being the law of the PYP \([\text{Pitman, 2006, Chapter 2 and Chapter 3}]\). Because of the almost sure discreteness of \( P \), the random sample \( X_n \) features \( K_n = k \leq n \) distinct types, labelled by \( \{S^*_1, \ldots, S^*_k\} \), with corresponding frequencies \( N_n = (N_{1,n}, \ldots, N_{K_n,n}) = (n_1, \ldots, n_k) \) such that \( n_i \geq 1 \), for \( i = 1, \ldots, k \), and \( \sum_{1 \leq i \leq k} n_i = n \). In other terms, \( X_n \) induces a random partition \( \Pi_n \) of the set \( \{1, \ldots, n\} \) whose blocks are the (equivalence) classes induced by the equivalence relations \( i \sim j \iff X_i = X_j \) almost surely. In particular, \( \Pi_n \) is an exchangeable random partition, meaning that its distribution is such that the probability of any partition of \( \{1, \ldots, n\} \) into \( k \) blocks with frequency \( (n_1, \ldots, n_k) \) is a symmetric function \( p_{n,k} \) of \( (n_1, \ldots, n_k) \), i.e.

\[
p_{n,k}(n_1, \ldots, n_k) = \frac{\binom{a}{(k)} \prod_{i=1}^{k} \alpha(1 - \alpha)}{(\theta)^{n}} (\alpha(1 - \alpha))_{(n_i - 1)},
\]

where \( \binom{a}{u} \) is the \( u \)-th rising factorial of \( a \), i.e. \( \binom{a}{u} = \prod_{0 \leq i \leq u-1}(a + i) \), for \( a \geq 0 \) and \( u \in \mathbb{N}_0 \). The function \( p_{n,k} \) is referred to as the exchangeable partition probability function \([\text{Kingman, 1978; Pitman, 1995}]\). The sequence \( (\Pi_n)_{n \geq 1} \) defines an exchangeable random partition \( \Pi \) of \( \mathbb{N} \), with exchangeability meaning that the distribution of \( \Pi \) is invariant under finite permutations of its elements, provided that such a sequence is consistent, i.e., \( \Pi_m \) is the restriction of \( \Pi_n \) to the first \( m \) elements, almost surely for all \( m < n \). Consistency implies that

\[
p_{n,k}(n_1, \ldots, n_k) = p_{n+1,k+1}(n_1, \ldots, n_k, 1) + \sum_{i=1}^{k} p_{n+1,k}(n_1, \ldots, n_i + 1, \ldots, n_k)
\]

for all \( n \geq 1 \) \([\text{Hansen and Pitman, 2000; Nacu, 2006}]\). See \textit{Pitman} \([2006, \text{Chapter 2}]\), and references therein, for a detailed account on exchangeable random partitions and generalizations thereof.

Consistency for exchangeable random partitions, and in particular of \( (3) \), implies that the distribution of \( \Pi \) is determined by the distribution of \( (X_i)_{i \geq 1} \) through the predictive probabilities. Let \( X_n \) be a random sample from \( P \sim \text{PYP}(\alpha, \theta) \) featuring \( K_n = k \) distinct types,
labelled by \( \{S^*_i, \ldots, S^*_K\} \), with frequencies \( N_n = (n_1, \ldots, n_k) \). The predictive probability of \( (X_i)_{i \geq 1} \) is

\[
\Pr[X_1 \in \cdot] = \nu(\cdot)
\]

and

\[
\Pr[X_{n+1} \in \cdot | X_n] = \frac{\theta + k\alpha}{\theta + n} \nu(\cdot) + \frac{1}{\theta + n} \sum_{i=1}^{k} (n_i - \alpha) \delta_{S^*_i}(\cdot), \tag{4}
\]

and it determines the distribution of \( \Pi_{n+1} \) from that of \( \Pi_n \), for any \( n \geq 1 \). The probability (4) is a linear combination between: i) the probability \((\theta + k\alpha)/(\theta + n)\) that \( X_{n+1} \) belongs to a new type, i.e. the probability of creating a new block in the random partition of \( \{1, \ldots, n\} \); ii) the probability \((n_i - \alpha)/(\theta + n)\) that \( X_{n+1} \) is of type \( S^*_i \), i.e. the probability of increasing by 1 the size of the block \( S^*_i \) in the random partition of \( \{1, \ldots, n\} \), for \( i = 1, \ldots, k \). For \( \theta > 0 \), an intuitive description of (4) was proposed in Zabell [2005, Chapter 11]. Consider an urn containing a black ball and colored (non-black) balls, where colored balls may be interpreted as the individuals with their associated type (color). Balls are drawn and then replaced, in such a way that the probability of a ball being drawn at any stage is proportional to its weight. Initially the urn contains a black ball with weight \( \theta > 0 \), and at the \( n \)-th draw: i) if we pick a colored ball then it is returned to the urn with a ball of the same color with weight 1; ii) if we pick a black ball, then it is returned to the urn with a black ball of weight \( \alpha \in [0, 1) \) and a ball of a new color with weight \( 1 - \alpha \). If \( X_n \) is the color of the ball returned in the urn after the \( n \)-th draw, and such a color is generated as \( \nu \), then the conditional distribution of \( X_{n+1} \) given \( X_n \) is (4).

Zabell [1992, 1997] provided a meaningful characterization of the PYP through its predictive probability (4), which is referred to as “sufficientness postulate” [Johnson, 1932; Bacallado et al., 2017]. Precisely, for \( \alpha \in (0, 1) \) the PYP is characterized as the sole species sampling model whose predictive probability is such that: i) the probability that \( X_{n+1} \) is of a new type depends on \( X_n \) only through \( n \) and \( K_n \); ii) the probability that \( X_{n+1} \) belongs to \( S^*_i \) depends on \( X_n \) only through \( n \) and \( N_{n,i} \). In particular the DP is the sole species sampling model whose predictive probability is such that the probability that \( X_{n+1} \) belongs is of a new type depends on \( X_n \) only through \( n \) [Regazzini, 1978; Lo, 1991]. Both the “sufficientness postulate” and the Pólya-like urn scheme highlight the critical role of \( \alpha \). The parameter \( \alpha \) drives a combined effect in terms of a reinforcement mechanism and the increase in the rate at which new types are generated according to (4). A new type, say \( S^* \), entering in the sample produces two effects: i) it is assigned a mass proportional to \((1 - \alpha)\) in the \( S^* \) empirical component of (4); ii) it is assigned a mass proportional to \( \alpha \) in the probability of generating a new type. That is, the mass assigned to \( S^* \) is less than proportional to its cluster size, i.e. 1, and the remaining mass is added to the probability of generating new types. The first effect gives rise to the following reinforcement mechanism: if \( S^* \) is re-observed then the mass of \( S^* \) is increased by \( 1/(\theta + n + 1) \), meaning that the sampling procedure tends to reinforce observed types with higher frequencies. The second effect implies that the probability of generating yet another new type, which overall still decreases as a function of \( n \), is increased by \( \alpha/(\theta + n + 1) \). The larger \( \alpha \) the stronger the reinforcement mechanism and the
higher is the probability of generating new types. For $\alpha = 0$ everything is proportional to type’s frequencies, and then the number of observed types does not alter the probability of generating new types.

We conclude by recalling the sampling formula induced by a random sample $X_n$ from $P \sim \text{PYP}(\alpha, \theta)$, which follows from (2) through a combinatorial argument [Pitman, 2006, Chapter 2]. Let $M_{r,n}$ be the number of distinct types with frequency $r$ in $X_n$, for $1 \leq r \leq n$, i.e. $M_{r,n} = \sum_{1 \leq i \leq K_n} I(N_{i,n} = r)$, such that $\sum_{1 \leq r \leq n} M_{r,n} = K_n$ and $\sum_{1 \leq r \leq n} r M_{r,n} = n$. The distribution of $M_n = (M_{1,n}, \ldots, M_{n,n})$ is defined on $\mathcal{M}_{n,k} = \{ k \in \{1, \ldots, n \} \}$ and $(m_1, \ldots, m_n) : m_i \geq 0, \sum_{1 \leq i \leq n} m_i = k; \sum_{1 \leq i \leq n} i m_i = n$, and it is referred to as Ewens-Pitman sampling formula (EPSF). In particular, for $(m_1, \ldots, m_n) \in \mathcal{M}_{n,k}$ it holds

$$
\Pr[M_n = (m_1, \ldots, m_n)] = n! \frac{(\theta)^{\sum_{i=1}^n m_i}}{(\theta)_{(n)}} \prod_{i=1}^n \left( \frac{\alpha(1 - \alpha)(i-1)}{i!} \right)^{m_i} \frac{1}{m_i!}.
$$

See Supplementary Material S2 for an alternative representation of the EPSF in terms of a simple compound Poisson sampling model [Charalambides, 2005, Chapter 7]. The distribution of $K_n$ follows directly from (5) [Pitman, 2006, Chapter 3]. In particular, for $a > 0, b \geq 0$ and $u, v \in \mathbb{N}_0$ with $v \leq u$, let $\mathcal{C}(u, v; a, b)$ be the $(u, v)$-th non-centered generalized factorial coefficient, i.e., $\mathcal{C}(u, v; a, b) = (v!)^{-1} \sum_{0 \leq i \leq v} (-1)^i \binom{v}{i} (i^v - ia - b)^{(u)}$; see Supplementary Material S1 for an account on generalized factorial coefficients. Then, for $x \in \{1, \ldots, n\}$ it holds

$$
\Pr[K_n = x] = \frac{\left( \frac{\theta}{\alpha} \right)^{(x)}}{(\theta)_{(n)}} \mathcal{C}(n, x; \alpha, 0).
$$

For $\alpha = 0$, i.e. under the DP, the distribution of $K_n$ follows directly from (6) by letting $\alpha \to 0$. This distribution is expressed in terms of the $(u, v)$-th signless Stirling number $|s(u, v)|$, which arises by means of $|s(u, v)| = \lim_{a \to 0} a^{-v} \mathcal{C}(u, v; a, 0)$; see Supplementary Material S1.

At the sampling level, the power-law tail behaviour of the PYP emerges from the large $n$ asymptotic behaviour of $K_n$ and $M_{r,n}$. For $\alpha \in (0, 1)$ let $f_\alpha$ be the density function of a positive $\alpha$-stable random variable, and for $\theta > -\alpha$ let $S_{\alpha, \theta}$ be a random variable with density function

$$
f_{S_{\alpha, \theta}}(s) \propto s^{\theta - 1 - \alpha} f_\alpha(s^{-1/\alpha}),
$$

that is a generalized Mittag-Leffler density function. Pitman [2006, Theorem 3.8] shows that, as $n \to +\infty$,

$$
\frac{K_n}{n^\alpha} \to S_{\alpha, \theta} \quad \text{almost surely},
$$

and

$$
\frac{M_{r,n}}{n^\alpha} \to \frac{\alpha(1 - \alpha)(r-1)}{r!} S_{\alpha, \theta} \quad \text{almost surely}.
$$
The random variable $S_{\alpha,\theta}$ is positive and finite (almost surely), and it is referred to as Pitman’s $\alpha$-diversity. See Dolera and Favaro [2020a,b] for a Berry-Esseen type refinements of (8). For $\alpha = 0$, we recall that as $n \to +\infty$, $K(n)/\log n \to \theta$ almost surely [Korwar and Hollander, 1973] and $M_{r,n} \to P_{\theta/r}$ almost surely [Ewens, 1972], where $P_{\theta/r}$ is a Poisson random variable with parameter $\theta/r$. Equation (8) shows that $K_n$, for large $n$, grows as $n^\alpha$. This is the growth of the number of distinct types in $n \geq 1$ random samples from a power-law distribution of exponent $c = \alpha^{-1}$. By combining (8) and (9), it holds that $p_{\alpha,r} = \alpha(1 - \alpha)(r-1)/r!$ is the large $n$ asymptotic proportion of the number of distinct types with frequency $r$. Then $p_{\alpha,r} \approx c_ar^{-\alpha-1}$ for large $r$, for a constant $c_\alpha$. This is the distribution of the number of distinct types with frequency $r$ in $n \geq 1$ random samples from a power-law distribution of exponent $c = \alpha^{-1}$.

3 Coverage probabilities

The estimation of coverage probabilities, or rare probabilities, is a classical problem in statistics, dating back to the work of Alan M. Turing and Irving J. Good at Bletchley Park in 1940s [Goodman, 1949; Good, 1953]. Consider $n$ observable samples to be modeled as a random sample $X_n$ in the classical species sampling framework, and denote by $(N_{j,n})_{j \geq 1}$ the frequencies of species in the sample $X_n$. Then, the coverage probability of order $r \geq 0$ is defined as

$$p_{r,n} = \sum_{j \geq 1} p_j I(N_{j,n} = r).$$

That is, the discrete functional $p_{r,n}$ is the probability mass of species observed with frequency $r \geq 0$ in the sample. Of special interest is $p_0,n$, namely the coverage probability of order 0, which is typically referred to as the missing mass. The problem of estimating $p_{r,n}$ first appeared in ecology [Fisher et al., 1943; Good, 1953; Chao and Lee, 1992; Bunge and Fitzpatrick, 1993], and over the past three decades its importance has grown dramatically in biological sciences [Kroes et al., 1999; Mao, 2004; Gao et al., 2007]. In particular, coverage probabilities arise in DNA sequencing data in the form of sample coverage, or saturation, and frequency estimation. Sample coverage, i.e. the proportion of molecules in the population that are observed in the sample, is strongly related to the estimation of the population abundance of unobserved molecules (the missing mass), as it is equal to $1 - p_0,n$. An accurate estimation of the sample coverage allows to determine if the sample is saturated, i.e. all species have been sampled. Moreover, sequencing experiments with high sample coverage are crucial to avoid sampling bias and to produce robust findings. Given that high sample coverage is often an issue in degraded DNA samples, in metagenomics (such as the study of the microbiome), and in single-cell DNA sequencing, where sample coverage varies in each cell, the correct sample coverage estimation remains critical. See Deng et al. [2019, Section 4] and references therein.

Remark 1. Besides biological and physical sciences, in the recent years the problem of estimating coverage probabilities has found numerous applications in machine learning [Zhang,
A nonparametric estimator of coverage probabilities

The Good-Turing estimator is arguably the most popular estimator of \( p_{r,n} \) [Good, 1953; Good and Toulmin, 1956; Robbins, 1956, 1968]. If \( M_{r,n} = m_r \) is the number of distinct species with frequency \( r \geq 1 \) in the observable sample \( X_n \), then the Good-Turing estimator of \( p_{r,n} \) is

\[
\tilde{p}_{r,n} = (r + 1) \frac{m_{r+1}}{n}.
\]

The Good-Turing estimator (10) is a nonparametric estimator of \( p_{r,n} \), in the sense that it does not rely on any distributional assumption on the unknown \( p \). In the classical species sampling framework, the estimator \( \tilde{p}_{r,n} \) is obtained by comparing expectations of \( p_{r,n} \) and \( M_{r,n} \) [Good, 1953; Robbins, 1968]. The estimator also admits a natural interpretation as a nonparametric empirical Bayes estimator in sense of Robbins [1956, 1964], that is \( \tilde{p}_{r,n} \) may be viewed as a posterior expectation with respect to a nonparametric prior estimated from the sample, i.e. the empirical distribution [Efron and Thisted, 1976; Efron, 2003]. The Good-Turing estimator has been the subject of numerous studies, in both theory and method. These studies include, e.g., classical central limit theorems, local limit theorems and large deviation principles [Esty, 1982, 1983; Zhang and Zhang, 2009; Gao, 2013; Grabchak and Zhang, 2017], admissibility and concentration properties [Robbins, 1968; McAllester and Schapire, 2000; Ohannessian and Dahleh, 2012; Ben-Hamou et al., 2017; Skorski, 2020], consistency and convergence rates [McAllester and Ortiz, 2003; Mossel and Ohannessian, 2019; Ayed et al., 2018], optimality and minimax lower bounds [Orlitsky et al., 2003; Acharya et al., 2018; Ayed et al., 2018].

BNP inference for coverage probabilities

We consider the problem of estimating coverage probabilities under the BNP sampling framework (1). It is assumed that the random sample \( X_n \) features \( K_n = k \) distinct species with frequencies \( N_n = (n_1, \ldots, n_k) \), and \( M_{r,n} = m_r \) is the number of distinct species with frequency \( r \geq 1 \). In the BNP sampling framework, Arbel et al. [2017] computed a closed-form posterior distribution of \( p_{r,n} \), given the sample \( X_n \); see also Bacallado et al. [2017] and references therein. If Beta\((a, b)\) denotes a Beta random variable with parameter \((a, b)\), for \( a, b > 0 \), then

\[
p_{0,n} | X_n \overset{d}{=} \text{Beta}(\theta + \alpha k, n - \alpha k),
\]

and for \( r \geq 1 \)

\[
p_{r,n} | X_n \overset{d}{=} \text{Beta}((r - \alpha)m_r, \theta + n - (r - \alpha)m_r).
\]
According to (11) and (12), for fixed $\alpha \in (0, 1)$ and $\theta > -\alpha$, the number $K_n$ of distinct species in the sample is a sufficient statistic to make inference on $p_{0,n}$, whereas the number $M_{r,n}$ of distinct species with frequency $r$ in the sample is a sufficient statistic to make inference on $p_{r,n}$. If $\alpha = 0$, then the sample size $n$ and $M_{r,n}$ are sufficient statistics to infer $p_{0,n}$ and $p_{r,n}$, respectively. The posterior distributions (11) and (12) are at the basis of BNP inferences for coverage probabilities. Besides leading to BNP estimates of $p_{n,r}$, (11) and (12) are critical to quantify uncertainty of estimates by means of credible intervals obtained through, e.g., Bernstein-type concentration inequalities for Beta distributions [Skorski, 2021] and Monte Carlo sampling Arbel et al. [2017]. This is possible in practice because of the simple form of the posterior distributions, which allow to exploit well known properties of the Beta distribution to deal with BNP inference for coverage probabilities under the PYP prior.

We consider a BNP estimator of $p_{r,n}$ with respect to a squared loss function. Therefore, we make use of the expected values of (11) and (12) as estimators for $p_{0,n}$ and $p_{r,n}$, respectively. That is,

$$\hat{p}_{0,n} = E[p_{0,n} | X_n] = \frac{\theta + k\alpha}{\theta + n},$$

(13)

and for $r \geq 1$

$$\hat{p}_{r,n} = E[p_{r,n} | X_n] = (r - \alpha) \frac{m_r}{\theta + n}.$$

(14)

BNP estimators (13) and (14) first appeared in Lijoi et al. [2007] and Favaro et al. [2012], where it is presented an intuitive derivation of (13) and (14) by means of an application of the predictive probability (4) of the PYP prior. By combining the definition of $p_{0,n}$ and predictive probabilities, the BNP estimator of $p_{0,n}$ under a squared loss function is precisely the probability that the $(n + 1)$-th draw belongs to new species, i.e. a species not observed in the sample. This is the probability $(\theta + k\alpha)/\theta + n$ attached to $\nu$ in (4). Similarly, by combining the definitions of $p_{r,n}$ and predictive probabilities, the BNP estimator of $p_{r,n}$ under a squared loss function is precisely the probability that the $(n + 1) - \text{th}$ draw belongs to a species observed with frequency $r$ in the sample. This is the probability $(r - \alpha)/\theta + n$ attached to the empirical part of (4), i.e. the probability of observing a specific species with frequency $r$ in the sample, multiplied by the number $m_r$ of species with frequency $r$ in the sample.

A peculiar feature of the Good-Turing estimator $\tilde{p}_{r,n}$, which is in contrast with the BNP estimator $\hat{p}_{r,n}$, is that the estimator depends on $m_{r+1}$, and not on $m_r$ as one would intuitively expect for an estimator of $p_{r,n}$. This feature, combined with the irregular behaviour of the $m_r$’s, may lead to absurd estimates, the most common being $\tilde{p}_{r,n} = 0$ when $m_r > 0$ and $m_{r+1} = 0$. To overcome this drawback, Good [1953] suggested to smooth the estimator (10) by replacing the irregular $m_r$’s with more regular $m'_r$’s, with $m'_r$ being, e.g., a suitable parabolic function of $r$, a proportion of the number $k$ of distinct species in the sample, the expectation with respect to a suitable parametric model. The BNP estimator $\hat{p}_{r,n}$ may be interpreted as a smoothed Good-Turing estimator, where the smoothing is induced by the PYP prior. In particular, let $a_n \simeq b_n$ mean that $\lim_{n \to +\infty} a_n/b_n = 1$, namely $a_n$ and $b_n$ are asymptotically equivalent as $n$ tends to infinity. Favaro et al. [2016, Theorem 1] show that,
as $n \to +\infty$, for $r \geq 0$

$$\hat{p}_{r,n} \simeq \frac{(r + 1) m'_{r+1}}{n},$$

where

$$m'_{r+1} = \frac{\alpha(1 - \alpha)(r)}{(r + 1)!} k.$$  \hspace{1cm} (16)

According to (15), the BNP estimator $\hat{p}_{r,n}$ is asymptotically equivalent, for large $n$, to a smoothed Good-Turing estimator, where the smoothed $m'_{r+1}$ in (16) is the proportion $\alpha(1 - \alpha)(r)/(r + 1)!$ of the number $k$ of species in the sample. While smoothing techniques for the Good-Turing estimator were introduced as an ad-hoc tool for post-processing the $m_r$’s in order to improve the performance of $\tilde{p}_{r,n}$, Favaro et al. [2016] show that smoothing emerges naturally from a BNP approach to estimate $p_{r,n}$. See Arbel et al. [2017] for high-order refinements of (15).

4 The number of unseen species

The estimation of the number of unseen species, or unseen-species problem, is the natural $m$-step ahead extension of the problem of estimating the missing mass. Consider $n$ observable samples to be modeled as a random sample $X_n$ in the classical species sampling framework, and assume that $m \geq 1$ additional unobservable samples are also modeled as random sample $(X_{n+1}, \ldots, X_{n+m})$ from the same classical species sampling framework. That is, we are considering a random sample $X_{n+m} = (X_1, \ldots, X_n, X_{n+1}, \ldots, X_{n+m})$ of which only the first $n$ elements are assumed to be observable. If $(N_{j,n})_{j \geq 1}$ and $(N_{j,m})_{j \geq 1}$ denote the frequencies of species in $X_n$ and $(X_{n+1}, \ldots, X_{n+m})$, respectively, then the number of unseen species is defined as

$$u_{n,m} = \sum_{j \geq 1} I(N_{j,n} = 0) I(N_{j,m} > 0).$$

That is, the discrete functional $u_{n,m}$ is the number of hitherto unseen species that would be observed if $m$ additional samples were collected from the same population. Similarly to the estimation of the missing mass, the unseen-species problem first appeared in ecology [Fisher et al., 1943; Good and Toulmin, 1956; Chao, 1984; Chao and Lee, 1992; Bunge and Fitzpatrick, 1993], and over the past three decades its importance has grown dramatically in biological sciences. In molecular biological data, the unseen-species problem arises in the estimation of the complexity of sequencing libraries [Daley and Smith, 2013; Ionita-Laza et al., 2009]. While in low-complexity libraries a large proportion of the sample is composed by only a small number of unique molecules, high-complexity libraries usually display a large number of molecules, providing more information for a fixed level of sequencing. For this reason, high-complexity libraries are often preferred by researchers. To evaluate library complexity, the complexity curve, or Species Accumulation Curve (SAC), is defined as the number of additional species that are observed as the sampling effort increases. This is the number of unseen species, interpreted as a function of $m$. The problem of library complexity estimation
plays a crucial role to predict the benefit of additional sequencing, and optimize resource in the planning stages of experiments. See Deng et al. [2019, Section] and references therein.

Remark 2. As a generalization of the estimation of the missing mass, the unseen-species problem appeared in machine learning and theoretical computer science [Haas et al., 1995; Florencio and Herley, 2007; Hao and Orlitsky, 2020] and in empirical linguistics and natural language processing [Thisted and Efron, 1987; Gale and Sampson, 1995; Ohannessian and Dahleh, 2012]

4.1 A nonparametric estimator of the number of unseen species

Let \( \lambda = m/n \), i.e. the proportion (fraction) of unobserved individuals with respect to observed individuals. For \( \lambda < 1 \), the Good-Toulmin estimator is arguably the most popular estimator of \( u_{n,m} \) [Good and Toulmin, 1956]. If \( M_{r,n} = m_r \) is the number of distinct species with frequency \( r \geq 1 \) in the observable sample \( X_n \), then the Good-Toulmin estimator of \( u_{n,m} \) is

\[
\tilde{u}_{n,m} = \sum_{i \geq 1} (-1)^{i+1} \lambda^i m_i. \tag{17}
\]

For \( \lambda = n^{-1} \), i.e. \( m = 1 \), the estimator (17) reduces to the Good-Turing estimator of \( p_{0,n} \). The Good-Toulmin estimator (17) is a nonparametric estimator of \( u_{n,m} \), in the sense that it does not rely on any distributional assumption on the unknown \( p \). In the classical species sampling framework, the estimator \( \tilde{u}_{n,m} \) is obtained by comparing expectations of \( u_{n,m} \) and \( M_{r,n} \) [Good, 1953; Good and Toulmin, 1956]. The estimator also admits a natural interpretation as a nonparametric empirical Bayes estimator in sense of Robbins [1956] [Efron and Thisted, 1976; Mao and Lindsay, 2002]. Unfortunately, for \( \lambda \geq 1 \) the estimator (17) is useless since the geometrically increasing magnitude of \( \lambda^i \) produces wild oscillations as the number of terms increases. To overcome this drawback, Efron and Thisted [1976] proposed a modification of \( \tilde{u}_{n,m} \) that relies on a Euler-type random truncation of the series (17).

Motivated by the increasing interest in the range \( \lambda > 1 \), especially in biological applications, Efron-Thisted estimator has been the subject of recent breakthrough studies [Orlitsky et al., 2016; Wu and Yang, 2019; Polyanskiy and Wu, 2020]. In particular, Orlitsky et al. [2016] show that Efron-Thisted estimator provably estimates \( u_{n,m} \) all of the way up to \( \lambda \approx \log n \), that such a range is the best possible, and that the estimator’s mean-square error is minimax near-optimal for any \( \lambda \). These provable guarantees do not rely on any assumption on the underlying unknown distribution \( p \), and they hold uniformly over all distributions, thus providing a theory in its greatest generality.

An interesting generalization, or refinement, of the number of unseen species \( u_{n,m} \) is the unseen species’ prevalences. Formally, the unseen species’ prevalence of order \( r \geq 1 \) is defined as

\[
u_{r,n,m} = \sum_{j \geq 1} I(N_{j,n} = 0)I(N_{j,m} = r).
\]

That is, \( u_{r,n,m} \) is the number of hitherto unseen species that would be observed with frequency \( r \) if \( m \) additional samples were collected from the same population. For small values of \( r \),
the unseen species’ prevalence of order \( r \) is also referred to as the number of unseen rare species. This is a critical quantity for the understanding of the species composition of the unobservable individuals. In ecology and biology, for instance, conservation of biodiversity requires a careful control of the number of species with frequency less than a certain threshold, namely rare species [Magurran, 2003; Thompson, 2004]. In genomics, rare species represent a critical issue, the reason being that species that appear only once or twice are often associated with deleterious diseases [Laird and Lange, 2010]. For \( \lambda < 1 \), a nonparametric estimator of \( u_{r,n,m} \) may be obtained by comparing expectations of \( u_{r,n,m} \) and \( M_{r,n} \), which leads to

\[
\tilde{u}_{r,n,m} = \sum_{i \geq 1} (-\lambda)^{i+r-1} \binom{r+i-1}{i-1} m_{i+r-1}.
\]  

(18)

For \( \lambda \geq 1 \), Hao and Li [2020] proposed a modification of \( \tilde{u}_{r,n,m} \) in the spirit of Efron-Thisted estimator, i.e. a Euler-type random truncation of the series (18). Along the same lines of Orlitsky et al. [2016], Hao and Li [2020] show that their estimator provably estimates \( u_{r,n,m} \) all of the way up to \( \lambda \approx r^{-1} \log n \), that such a range is the best possible, and that the estimator’s mean-square error is minimax near-optimal. These provable guarantees do not rely on any assumption on the underlying unknown distribution \( p \), and they hold uniformly over all distributions.

### 4.2 BNP inference for the number of unseen species

We consider the unseen-species problem under the BNP sampling framework (1). It is assumed that the random sample \( X_n \) features \( K_n = k \) distinct species with frequencies \( N_n = (n_1, \ldots, n_k) \), and \( M_{r,n} = m_r \) is the number of distinct species with frequency \( r \geq 1 \). In the BNP sampling framework, Lijoi et al. [2007] first computed a closed-form posterior distribution of \( u_{n,m} \) given the sample \( X_n \) [Favaro et al., 2009]. If \( \alpha \in (0,1) \) then for \( x \in \{0,1,\ldots,m\} \)

\[
\Pr[u_{n,m} = x \mid X_n] = \frac{(k + \frac{\theta}{\alpha})^{(x)}}{(\theta + n)_{(m)}} \mathcal{C}(m, x; -n + k\alpha). \tag{19}
\]

Under a squared loss function, a BNP estimator of \( u_{n,m} \) [Favaro et al., 2009] is the expected value of (19), i.e.,

\[
\hat{u}_{n,m} = \mathbb{E}[u_{n,m} \mid X_n] = \left( k + \frac{\theta}{\alpha} \right) \left( \frac{(\theta + n + \alpha)_m}{(\theta + n)_m} - 1 \right). \tag{20}
\]

For \( \alpha = 0 \), i.e. under the DP, the posterior distribution and the BNP estimator of \( u_{n,m} \) are obtained from (19) and (20), respectively, by letting \( \alpha \to 0 \) [Lijoi et al., 2007]. In particular, for \( b \geq 0 \) let \( |s(u, v; b)| \) be the non-centered signless Stirling number of the first type, which arises from \( \mathcal{C}(u, v; a, b) \) by means of \( |s(u, v; b)| = \lim_{a \to 0} a^{-v} \mathcal{C}(u, v; a, b) \). If \( \alpha = 0 \), then for \( x \in \{0,1,\ldots,m\} \)

\[
\Pr[u_{n,m} = x \mid X_n] = \frac{\theta^k}{(\theta + n)_m} |s(m, x; n)| \tag{21}
\]
\[ \hat{u}_{n,m} = E[u_{n,m} | X_n] = \sum_{i=1}^{m} \frac{\theta}{\theta + n + i - 1}. \] (22)

For \( m = 1 \) the estimator (20) reduces to the estimator (13) of \( p_{0,n} \). As a generalization of the estimators (20) and (22), Favaro et al. [2013] introduced a BNP estimator of the unseen species’ prevalence \( u_{r,n,m} \). See also De Blasi et al. [2015] for details. However, to date no closed-form expressions are available for the posterior distribution of \( u_{r,n,m} \), given the sample \( X_n \).

According to (19), for fixed \( \alpha \in (0, 1) \) and \( \theta > -\alpha \), the number \( K_n \) of distinct species in the sample is a sufficient statistic to make inference on \( u_{n,m} \). If \( \alpha = 0 \), then the sample size \( n \) is a sufficient statistic to infer \( u_{n,m} \). The posterior distributions (19) and (21) are critical to quantify uncertainty of estimates (20) and (22) by means of credible intervals via Monte Carlo sampling. In practice, Monte Carlo sampling of (19) and (21) is doable for small values of \( n \) and \( m \), and it becomes impossible for large values of \( n \) or \( m \). This is because for large \( n \) and \( m \), and even only for large \( m \), the computational burden for evaluating generalized factorial coefficients and Stirling numbers becomes overwhelming.

To overcome this drawback, Favaro et al. [2009] proposed large \( m \) approximations of the posterior distributions (19) and (21). In particular, let \( u_{n,m}(k) \) denote a random variable whose distribution is (19) for \( \alpha \in (0, 1) \) and (21) for \( \alpha = 0 \). For \( \alpha \in (0, 1) \), Favaro et al. [2009, Proposition 2] show that, as \( m \to +\infty \),

\[ \frac{u_{n,m}(k)}{m^\alpha} \to \text{Beta} \left( \frac{\theta}{\alpha} + k, \frac{n}{\alpha} - k \right) S_{\theta,\alpha+n} \text{ almost surely}, \] (23)

where \( S_{\theta,\alpha} \) is the Pitman’s \( \alpha \)-diversity, with \( S_{\theta,\alpha+n} \) being independent of the random variable \( \text{Beta} \left( \frac{\theta}{\alpha} + k, \frac{n}{\alpha} - k \right) \); see also Dolera and Favaro [2020a]. Moreover, for \( \alpha = 0 \), as \( m \to +\infty \)

\[ \frac{u_{n,m}(k)}{\log(m)} \to (\theta + n) \text{ almost surely}. \] (24)

The large \( m \) asymptotics (23) of \( u_{n,m}(k) \) may be viewed as a posterior counterpart of the large \( n \) asymptotic behaviour of \( K_n \) in (8); the limiting random variable (23) is referred to as posterior Pitman’s \( \alpha \)-diversity. We refer to Favaro et al. [2013] for a generalization of (23) and (24) for the unseen species’ prevalences \( u_{r,n,m} \), with weak convergence in place of almost sure convergence.

Favaro et al. [2009] introduced a Monte Carlo scheme for sampling the distribution of the posterior \( \alpha \)-diversity, which is then applied to obtain a large \( m \) approximation of credible intervals for the BNP estimate (20). The critical step of the Monte Carlo scheme consists in sampling the distribution of the Pitman’s \( \alpha \)-diversity \( S_{\theta,\alpha+n} \), whose density function is (7) with \( \theta + n \) in place of \( \theta \). This problem boils down to sample a polynomially tilted positive \( \alpha \)-stable distribution. That is, if \( f_\alpha \) denotes the density function of a positive \( \alpha \)-stable random variable, then the distribution of \( S_{\theta,\alpha+n}^{-1/\alpha} \) has the polynomially tilted positive \( \alpha \)-stable density

\[ \frac{u_{n,m}(k)}{m^\alpha} \to \text{Beta} \left( \frac{\theta}{\alpha} + k, \frac{n}{\alpha} - k \right) S_{\theta,\alpha+n} \text{ almost surely}, \] (23)

where \( S_{\theta,\alpha} \) is the Pitman’s \( \alpha \)-diversity, with \( S_{\theta,\alpha+n} \) being independent of the random variable \( \text{Beta} \left( \frac{\theta}{\alpha} + k, \frac{n}{\alpha} - k \right) \); see also Dolera and Favaro [2020a]. Moreover, for \( \alpha = 0 \), as \( m \to +\infty \)

\[ \frac{u_{n,m}(k)}{\log(m)} \to (\theta + n) \text{ almost surely}. \] (24)
function

\[ f_{S_n,\theta+n}(s) \propto s^{-(\theta+n)} f_{\alpha}(s). \]

The Monte Carlo approach of Favaro et al. [2009] is suitable for scenarios where \( n \) is not large, and \( m \) is much more large than \( n \). This is because: i) for large \( n \) the computational burden for the Monte Carlo sampling of a polynomially tilted positive \( \alpha \)-stable distribution becomes overwhelming [Devroye, 2009; Hofert, 2011]; ii) the large \( m \) asymptotics (23) is of a qualitative nature, in the sense that it does not quantify the error in approximating the posterior distribution (19) with the distribution of the limiting random variable (23). In the next proposition, we present a novel constructive representation of the posterior distributions (19) and (21). Besides providing an intuitive interpretation of (19) in terms of compound Binomial distributions, our representation leads to straightforward Monte Carlo sampling of (19) and (21) for arbitrarily large \( n \) and \( m \). An analogous representation is given for the posterior distribution of the unseen species’ prevalence \( u_{r,n,m} \), thus filling a gap in the literature. We denote by Binomial\((n, p)\) a Binomial random variable with parameter \((n, p)\), \( n \in \mathbb{N} \) and \( p \in (0, 1) \).

**Proposition 1.** Let \( X_n \) be a random sample from \( P \sim PY_{\alpha,\theta} \), for \( \alpha \in [0, 1) \) and \( \theta > -\alpha \), and let \( X_n \) feature \( K_n = k \) distinct species with frequencies \( N_n = (n_1, \ldots, n_k) \). If \( K^*_m \) is the number of distinct species in \( m \geq 1 \) random samples from \( P \sim PY_{\alpha,\theta+n} \), then

i) for \( \alpha \in (0, 1) \)

\[ u_{n,m} | X_n \overset{d}{=} \text{Binomial} \left( K^*_m, \text{Beta} \left( \frac{\theta}{\alpha} + k, \frac{n}{\alpha} - k \right) \right), \quad (25) \]

with the random variable \( \text{Beta}(\theta/\alpha + k, n/\alpha - k) \) being independent of the random variable \( K^*_m \);

ii) for \( \alpha = 0 \)

\[ u_{n,m} | X_n \overset{d}{=} \text{Binomial} \left( K^*_m, \frac{\theta}{\theta + n} \right), \quad (26) \]

If \( M^*_r,m \) is the number of distinct species with frequency \( r \geq 1 \) in \( m \geq 1 \) random samples from \( P \sim PY_{\alpha,\theta+n} \), then

iii) for \( \alpha \in (0, 1) \)

\[ u_{r,n,m} | X_n \overset{d}{=} \text{Binomial} \left( M^*_r,m, \text{Beta} \left( \frac{\theta}{\alpha} + k, \frac{n}{\alpha} - k \right) \right), \quad (27) \]

with the random variable \( \text{Beta}(\theta/\alpha + k, n/\alpha - k) \) being independent of the random variable \( M^*_r,m \);

iv) for \( \alpha = 0 \)

\[ u_{r,n,m} | X_n \overset{d}{=} \text{Binomial} \left( M^*_r,m, \frac{\theta}{\theta + n} \right). \quad (28) \]
We refer to Supplementary Material S3 for the proof of Proposition 1. The constructive representations of Proposition 1 are a consequence of the conjugacy and quasi conjugacy properties of the DP and the PYP, respectively [Ferguson, 1973; Pitman, 1996]. From (25) the posterior distribution (19) coincides with the distribution of the number of successes in a random number $K^*_m$ of independent Bernoulli trials with a Beta random probability $\text{Beta}(\theta/\alpha + k, n/\alpha - k)$. Note that the expectation of $\text{Beta}(\theta/\alpha + k, n/\alpha - k)$ is precisely the BNP estimator of the missing mass (13). In particular, we may write the BNP estimator (20) as

$$\hat{u}_{n,m} = \frac{\theta + k\alpha}{\theta + n} E[K^*_m],$$

where a simple closed-form expression for $E[K^*_m]$ is available in Pitman [2006, Chapter 3].

From (26), the posterior distribution (21) coincides with the distribution of the number of successes in a random number $K^*_m$ Bernoulli of independent trials with probability $\theta/(\theta + n)$, i.e. the BNP estimator of the missing mass (13). In particular, we may write the BNP estimator (22) as

$$\hat{u}_{n,m} = \frac{\theta}{\theta + n} E[K^*_m].$$

Along the same lines, from (27) and (28) we write the BNP estimator $u_{r,n,m}$ [Favaro et al., 2013] as

$$\hat{u}_{r,n,m} = \frac{\theta + k\alpha}{\theta + n} E[M^*_r],$$

where a simple closed-form expression for $E[M^*_r]$ is available in Favaro et al. [2013, Proposition 1]. Note that, according to the compound Binomial representation (27), for fixed $\alpha \in (0, 1)$ and $\theta > -\alpha$ the number $K_n$ of distinct species in the sample is a sufficient statistic to make inference on $u_{r,n,m}$. If $\alpha = 0$, i.e. under the DP, then the sample size $n$ is a sufficient statistic to infer $u_{r,n,m}$.

The representations (25) and (26) are useful for Monte Carlo sampling of the posterior distributions (19) and (21). They allow for Monte Carlo sampling of (19) and (21) for arbitrarily large values of $n$ and $m$, thus avoiding the use of the large $m$ approximation proposed in Favaro et al. [2009]. For fixed $\alpha \in (0, 1)$ and $\theta > -\alpha$, Monte Carlo sampling of (19) consists of three steps: i) sample the random variable $\text{Beta}(\theta/\alpha + k, n/\alpha - k)$; ii) independently of step i), sample the random variable $K^*_m$ under $P \sim \text{PYP}(\alpha, \theta + n)$; iii) given step i) and step ii), sample the random variable $\text{Binomial}(K^*_m, \text{Beta}(\theta/\alpha + k, n/\alpha - k))$. If $\alpha = 0$, i.e. under the DP, then Monte Carlo sampling of (21) consists of two steps: i) sample the random variable $K^*_m$ under $P \sim \text{PYP}(0, \theta + n)$; ii) given step i), sample the random variable $\text{Binomial}(K^*_m, \theta/(\theta + n))$. Sampling Beta and Binomial random variables is straightforward, for arbitrarily large $n$ and $m$, and routines are available in standard software. Sampling $K^*_m$ is also straightforward, for arbitrarily large $n$ and $m$, and it exploits the predictive probabilities of the PYP (4). In particular, let $\text{Bernoulli}(p)$ be Bernoulli random variable with parameter $p$, for $p \in (0, 1)$. Sampling $K^*_m$ then reduces to sample $m - 1$ Bernoulli random variables as follows:

1) Set $k = 1$;
2) For $i = 1$ to $m - 1$

Set $b$ to be a sample from $\text{Bernoulli}((\theta + n + \alpha k)/(\theta + n + i))$;

Set $k = k + b$;

3) Return $k$.

Along the same lines, the compound Binomial representations (27) and (28) are a critical tool for Monte Carlo sampling of the posterior distribution of $u_{r,n,m}$, given $X_n$. This requires to sample the random variable $M_{r,m}^*$ rather than $K_m^*$. Sampling of $M_{r,m}^*$ still exploits the predictive probabilities of the PYP although, regrettably, it does not reduce to sample Bernoulli random variables.

5  Coverages of prevalences

The estimation of coverages of prevalences, or saturations, is the natural $m$-step ahead extension of the problem of estimating coverage probabilities. As for the unseen-species problem, here we consider $n$ observable samples to be modeled as a random sample $X_n$ in the classical species sampling framework, and we assume that $m \geq 1$ additional unobservable samples are also modeled as random sample $(X_{n+1}, \ldots, X_{n+m})$ from the same classical species sampling framework. If $(N_{j,n})_{j \geq 1}$ and $(N_{j,m})_{j \geq 1}$ denote the frequencies of species in $X_n$ and $(X_{n+1}, \ldots, X_{n+m})$, respectively, then the coverage of prevalence of order $r \geq 0$ is defined as

$$f_{r,n,m} = \sum_{j \geq 1} I(N_{j,n} = r) I(N_{j,m} > 0).$$

That is, the discrete functional $f_{r,n,m}$ is the number of species observed $r$ times that would be observed if $m$ additional samples were collected from the same population. Note that $f_{0,n,m}$, i.e. the coverage of prevalence of order 0, is the number of unseen species $u_{n,m}$.

The problem of estimating coverages of prevalences first appeared in linguistics to answer the question “Did Shakespeare write a newly-discovered poem?” [Thisted and Efron, 1987]. The estimated coverages of prevalences was applied to test the consistency of the word usage in a previously unknown poem attributed to Shakespeare with the word usage in the entire Shakespearean canon. Similar questions, though under different vests, appear in biological sciences. In genomics data, they appear in relation to coverage depth, i.e. the average number of reads that are aligned to known reference bases [Deng et al., 2019]. Depending on the specific application, different levels of coverage might be required. This leads to the problem of determining whether additional sequencing is needed, which can be motivated by a required minimum coverage threshold, or investigating rare events. The estimation of coverages of prevalences can be valuable in this setting, as it allows researchers to estimate how many molecules observed with a given frequency would be observed again if the sampling efforts were increased.
5.1 A nonparametric estimator of coverages of prevalences

Let \( \lambda = m/n \), i.e. the proportion (fraction) of unobserved individuals with respect to observed individuals. If \( M_{r,n} = m_r \) is the number of distinct species with frequency \( r \geq 1 \) in the observable sample \( X_n \), then Thisted and Efron [1987] introduced an estimator of \( \tilde{f}_{r,n,m} \) of the form

\[
\tilde{f}_{r,n,m} = \sum_{j \geq 1} (-1)^{i+j+1} \lambda^i \binom{r+i}{i} m_{r+i}.
\] (29)

For \( \lambda = n^{-1} \), i.e. \( m = 1 \), the estimator (29) reduces to the Good-Turing estimator of \( p_{r,n} \). The estimator (29) is a nonparametric estimator of \( f_{r,n,m} \), in the sense that it does not rely on any distributional assumption on the unknown \( p \). Under the Multinomial model for \( X_n \), the estimator \( \tilde{f}_{r,n,m} \) is obtained by comparing expectations of \( f_{r,n,m} \) and \( M_{r,n} \). The estimator also admits a natural interpretation as a nonparametric empirical Bayes estimator in sense of Robbins [1956]. Because of its moment-based derivation, for \( r = 0 \) the estimator (29) reduces to the Good-Toulmin estimator \( \tilde{u}_{n,m} \). Differently from \( \tilde{u}_{n,m} \), to date the study of provable guarantees of \( \tilde{f}_{r,n,m} \) has not been considered in the literature of “species-sampling” problem. Thisted and Efron [1987] showed that \( \tilde{f}_{r,n,m} \) empirically estimates \( f_{r,n,m} \) for \( \lambda < 1 \), but without provable guarantees. For \( \lambda > 1 \) we expect that \( \tilde{f}_{r,n,m} \) will suffer the same variance issue of \( \tilde{u}_{n,m} \), that is the geometrically increasing magnitude of \( \binom{r+i}{i} \lambda^i \) may produce wild oscillations as the number of terms increases. Because of the additional Binomial term \( \binom{r+i}{i} \lambda^i \), it is natural to expect that such a variance issue worsens as \( r \) increases. Therefore, it seems natural the need of a suitable Euler-type random truncation of the series (29). As for the study of its provable guarantees, we expect that the theory developed to study minimax optimality \( \tilde{u}_{n,m} \) for \( \lambda \geq 1 \) [Wu and Yang, 2016, 2019; Polyanskiy and Wu, 2020] is not of a direct applicability to \( \tilde{f}_{r,n,m} \).

5.2 BNP inference for coverages of prevalences

We consider the problem of estimating coverages of prevalences under the BNP sampling framework (1). It is assumed that the random sample \( X_n \) features \( K_n = k \) distinct species with frequencies \( N_n = (n_1, \ldots, n_k) \), and \( M_{r,n} = m_r \) is the number of distinct species with frequency \( r \geq 1 \). For \( r \geq 1 \), in the next proposition we compute a closed-form posterior distribution of \( f_{r,n,m} \), given the sample \( X_n \). Before stating this result, it is useful to recall the (general) hypergeometric distribution [Johnson et al., 2005, Chapter 6.2.5] and the generalized factorial distribution [Charalambides, 2005, Chapter 2]. For \( u \in \mathbb{N} \) and \( b, c > 0 \), a random variable \( U_{b,c,u} \) on \( \{0, 1, \ldots, u\} \) has a generalized factorial distribution if, for \( x \in \{1, \ldots, u\} \),

\[
\Pr[U_{b,c,u} = x] = \frac{1}{(bc)_u} \mathcal{C}(u, x; b, 0)(c)_x;
\] (30)

see Supplementary Material S1. Moreover, for \( u, v \in \mathbb{N} \) and \( a > 0 \) such that \( a > u \), a random variable \( H_{a,u,v} \) on \( \{0, 1, \ldots, u\} \) has a (general) hypergeometric distribution if, for
for the proof of Equation 32.

The next proposition presents a constructive representation of the posterior distribution of \( f_{r,n,m} \), given \( X_n \), in terms of a compound (general) hypergeometric distribution. We denote by \( \text{Hypergeometric}(a, u, v) \) a (general) hypergeometric random variable with parameter \((a, u, v)\).

**Proposition 2.** Let \( X_n \) be a random sample from \( P \sim PYP(\alpha, \theta) \), for \( \alpha \in [0, 1) \) and \( \theta > -\alpha \), and let \( X_n \) feature \( K_n = k \) distinct species with frequencies \( N_n = (n_1, \ldots, n_k) \). If \( M_{r,n} = m_r \) is the number of distinct species with frequency \( r \geq 1 \) in the random sample \( X_n \), then

\[
 f_{r,n,m} \mid X_n \overset{d}{=} m_r - \text{Hypergeometric}\left(\frac{\theta + n}{r - \alpha} - 1, m_r, U_{r-a,\alpha, r-a, m}\right)
\]

We refer to Supplementary Material S4 for the proof of Proposition 2. According to (32), for fixed \( \alpha \in [0, 1) \) and \( \theta > -\alpha \), the number \( M_{r,n} \) of distinct species with frequency \( r \geq 1 \) in the sample is a sufficient statistic to make inference on \( f_{r,n,m} \). The posterior distribution is at the basis of BNP inferences for coverages of prevalences, e.g. estimation and uncertainty quantification for \( f_{r,n,m} \). Under a squared loss function, a BNP estimator of \( f_{r,n,m} \) is the expected value of (32), i.e.,

\[
 \hat{f}_{r,n,m} = E[f_{r,n,m} \mid X_n] = m_r \left(1 - \frac{(\theta + n - r + \alpha)(m)}{(\theta + n)(m)}\right).
\]

We refer to Supplementary Material S5 for the proof of Equation 33. For \( m = 1 \) the estimator (33) reduces to the estimator (14) of \( p_{r,n} \). The estimator (33) may be interpreted as the proportion

\[
 w_{r,n,m}(\alpha, \theta) = 1 - \frac{(\theta + n - r + \alpha)(m)}{(\theta + n)(m)} \in (0, 1),
\]

of the number \( m_r \) of distinct species with frequency \( r \). Uncertainty quantification of the estimate (33) is obtained by means of credible intervals via Monte Carlo sampling of the posterior distribution (32). Monte Carlo sampling of (32) is doable for small values of \( n \) and \( m \), and it becomes impossible for large values of \( n \) or \( m \). This is because for large \( n \) and \( m \), and even only for large \( m \), the computational burden for evaluating the generalized factorial coefficients in the distribution of \( U_{r-a,\alpha, (\theta+n)/(r-\alpha), m} \). To overcome this drawback, we propose an approximation of the posterior distribution (32) for large \( n \) and \( m \). Let \( a_{n,m} \sim b_{n,m} \) mean that \( \lim_{n \to +\infty} \lim_{m \to +\infty} a_{n,m} / b_{n,m} = 1 \), namely \( a_{n,m} \) and \( b_{n,m} \) are asymptotically equivalent as \( n \) and \( m \) tend to infinity. Then, as \( n, m \to +\infty \) with \( m > 0 \), for \( x \in \{0, 1, \ldots, m_r\} \) it holds true

\[
 \Pr(f_{r,n,m} = x \mid X_n) \simeq \frac{m_r}{x} \left[1 - \left(\frac{n}{n + m}\right)^{r-\alpha}\right]^x \left[\left(\frac{n}{n + m}\right)^{r-\alpha}\right]^{m_r-x},
\]

\[x \in \{0, 1, \ldots, u\},\]

\[
 \Pr[H_{a,u,v} = x] = \frac{\binom{a}{x} \binom{v}{u-x}}{\binom{a+v}{u}}.
\]
and hence
\[
\hat{f}_{r,n,m} \simeq m_r \left[ 1 - \left( \frac{n}{n + m} \right)^{r-\alpha} \right].
\]

We refer to Supplementary Material S6 for the proof of Equation 34. According to (34), for large \( n \) and \( m \) with \( m > 0 \), the posterior distribution (32) admits a first order local approximation in terms of a Binomial distribution with parameters \((m_r, 1 - (n/(n+m))^{r-\alpha})\), with \( m_r \) being the number of trials and \( 1 - (n/(n+m))^{r-\alpha} \) being the probability of success at the single trial.

### 6 Estimation of prior’s parameter \((\alpha, \theta)\) and Bayesian consistency

We investigate the estimation of the parameters \((\alpha, \theta)\) of the PYP over the space \( \Phi = \{(\alpha, \theta) \in (0, 1) \times \mathbb{R} : \theta > -\alpha\} \) using maximum likelihood estimation, i.e. the empirical Bayes approach, and hierarchical Bayes modeling. We consider the model where we observe a partition \( \Pi_n \) of \([1, \ldots, n]\) induced by a random sample \( X_n \) from a distribution \( p \) over a set of symbols. We do not, however, necessarily assume that \( p \) has a PYP prior distribution with \( \alpha_0 \) and \( \theta_0 \); that is we carry the analysis under potential misspecification of the model. To guarantee that the sequence of maximum likelihood estimators \((\hat{\alpha}_n, \hat{\theta}_n)\) converges to a limit \((\alpha^*, \theta^*)\) as \( n \to \infty \), we require the misspecification to be moderate, as stated in the next assumption.

**Assumption 1.** The distribution \( p \) is discrete with \( p = \sum_{j \geq 1} p_j \delta_{s_j} \). Furthermore, defining \( \bar{F}_p(x) = \sum_{j \geq 1} I(p_j > x) \), there exist \( L > 0 \) and \( \alpha_* \in (0, 1) \) such that as \( x \to 0 \)
\[
\bar{F}_p(x) = Lx^{-\alpha_*} + o\left[\frac{1}{-x^{\alpha_*}\log(x)}\right].
\]

Assumption 1 considers a deterministic distribution \( p \), but all the results can be extended to the case of a random \( P \) if the event on which the assumption is satisfied occur with a large probability. In particular, Assumption 1 is motivated by the fact that if \( P \sim \text{PYP}(\alpha, \theta) \), then results in Pitman [2003] show that \( \lim_{x \to 0} x^\alpha \bar{F}_P(x) = S_{\alpha, \theta}/\Gamma(1-\alpha) \) almost-surely, with \( \Gamma \) being the Gamma function [Pitman, 2006, Chapter 3 and Chapter 4]. As shown in the next theorem, the assumption also guarantees that \((\alpha_*, \theta_*)\) are interpretable even though the model is misspecified. Indeed, the limiting value of \( \hat{\alpha}_n \) is precisely \( \alpha_* \) as defined in the Assumption 1, the so-called tail-index of \( \bar{F}_p \). Regarding the limiting value of \( \hat{\theta}_n \), it is related to the value of \( L \) in a non-trivial but unique way. To be more precise, \( \theta_* \) is defined through the relation
\[
L = \frac{\exp\{\psi(\theta_*/\alpha_* + 1) - \alpha_*\psi(\theta_* + 1)\}}{\Gamma(1-\alpha_*)},
\]
where \( \psi \) denote the digamma function; that is \( \psi \) is the derivative of \( \log \Gamma \). A standard analysis of the digamma function shows that for any \( L > 0 \) there exists a unique value of \( \theta_* \in (-\alpha_*, \infty) \).
Theorem 1. Let \( L_n : \Phi \rightarrow \mathbb{R}_+^* \) be the likelihood function of the PYP random partition model, corresponding to the observation of the partition \( \Pi_n \) of \( \{1, \ldots, n\} \) induced by a iid sample \( (X_1, \ldots, X_n) \) from a distribution \( p \) over a set of symbols. Then, the following item are true.

1. The mapping \( \alpha \mapsto \log L_n(\alpha, 0) \) is concave on \((0, 1)\) and it admits a unique maximizer \( \hat{\alpha}_n^0 \) whenever \( K_n \neq n \) and \( K_n \neq 1 \). Furthermore, if Assumption 1 is satisfied,

\[
\log(n)|\hat{\alpha}_n^0 - \alpha_*| = o_p(1).
\]

2. Let Assumption 1 be satisfied. Then the set \( \arg \max_{(\alpha, \theta) \in \Phi} L_n(\alpha, \theta) \) is not empty with probability \( 1 + o(1) \) as \( n \to \infty \). Furthermore, \( (\hat{\alpha}_n, \hat{\theta}_n) \in \arg \max_{(\alpha, \theta) \in \Phi} L_n(\alpha, \theta) \) must satisfy \( \hat{\alpha}_n = \hat{\alpha}_n^0 + O_p \left( \frac{\log(n)}{n^{\alpha}} \right) \) [thus \( \hat{\alpha}_n = \alpha_* + o_p(1) \)], and \( \hat{\theta}_n = \theta_* + o_p(1) \).

Interestingly, Theorem 1 establishes that if the misspecification is moderate, then \((\alpha_*, \theta_*)\) can be directly interpreted in terms of key functionals of the true data generative mechanism. This also sheds some lights in the meaning of the parameter \((\alpha, \theta)\) when the model is correct. The next anti-concentration result shows that we shall, however, be really careful about the estimation of \( \theta \).

Proposition 3. Let \( \ell_n = \log L_n \) denote the log-likelihood function and let Assumption 1 be satisfied. For all \( 0 < c < d \) there exists a constant \( A > 0 \) such that as \( n \to \infty \)

\[
\sup_{\theta + \alpha_* \in [c, d]} \left\{ \ell_n(\hat{\alpha}_n, \theta) - \sup \ell_n \right\} \geq -A + o_p(1).
\]

Proposition 3 states that the likelihood function, as function of \( \theta \), is nearly flat on all compact sets. As a consequence, under well-specification of the model, the parameter \( \theta \) can not be estimated nor even tested consistently as \( n \to \infty \). This is because testing is always easier than estimation, and we know by Neyman-Pearson’s lemma that the most powerful test (assuming \( \alpha_* \) known for simplicity) for \( H_0 : \theta = \theta_1 \) against \( H_1 : \theta = \theta_2 \) is given by the likelihood-ratio test: this test can’t be consistent because of the flatness of the likelihood. This is not surprising since under well-specification we have that \( L = S_{\alpha, \theta} / \Gamma(1 - \alpha) \) almost-surely; whence in the true model \( \theta_* \) is a random variable related to Pitman’s \( \alpha \)-diversity. Consequently, it can only contain a weak information about the true value of \( \theta \). If we work, however, conditional on the PYP, we get one realization of \( S_{\alpha, \theta} \) and \( L \) becomes fixed (and interpretable!). Then we can use maximum likelihood to derive a good estimator of \( L \) via the result of Theorem 1. Regarding hierarchical Bayes estimation however, the flatness of the likelihood implies that the prior distribution can substantially influence the Bayesian estimates. Therefore, in the absence of strong prior belief on \( \theta \) it is unclear if a full Bayes approach is meaningful for this parameter.

We conclude by investigating in more details the large \( n \) asymptotic behaviour of a hierarchical Bayes approach. In particular, we consider the case where we put a prior distribution over the parameter \( \alpha \in (0, 1) \) and the shifted parameter \( \gamma = \theta + \alpha \), such that \( \alpha \) and \( \gamma \) are independent. This slight change of parameterization is convenient since we have that \( (\alpha, \gamma) \in (0, 1) \times (0, \infty) \) instead of \( (\alpha, \theta) \in \Phi \), which clearly forbid to have \( \alpha \) independent of \( \theta \). The next theorem characterizes the asymptotic behaviour of the posterior distribution of \((\alpha, \gamma)\).
and define a probability distribution is needed, see for instance the assumptions 1 Favaro and Naulet [1].

Then under Assumption 1, the posterior distribution of $(\alpha, \gamma)$ given $\Pi_n$, written here $G(\cdot \mid \Pi_n)$, satisfies as $n \to \infty$

$$
\sup_{A,B} |G(\hat{\gamma}_n^{1/2}(\alpha - \hat{\alpha}_n) \in A, \gamma \in B \mid \Pi_n) - \phi(A)H_*(B)| = o_p(1),
$$

where the supremum is taken over all measurable sets, $\hat{V}_n = -\partial_\alpha^2 \ell_n(\hat{\alpha}_n^0, 0)$, and $\phi(A)$ is the probability that a standard normal random variable lies in $A$.

We see from the previous theorem that if $(\alpha, \gamma)$ are independent a priori, then they are asymptotically independent a posteriori (but dependent for all fixed $n$). As expected from the result of Proposition 3 the limiting marginal distribution for $\gamma$ is neither converging toward a point mass, nor even Gaussian, which is a consequence of the flatness of the likelihood. For this reason, we shall be careful with posterior analysis involving the parameter $\gamma$ (equivalently $\theta$), since the limiting distribution heavily depends on the prior $G_\gamma$ (a fact that will remain true even if $\alpha$ and $\gamma$ are dependent a priori). The limiting marginal distribution for $\hat{V}_n^{1/2}(\alpha - \hat{\alpha}_n)$ is however Gaussian, which can be seen as a weak form of Bernstein-von Mises’ (BvM) theorem. It is not a true BvM because the centering is taken at $\hat{\alpha}_n$ instead of $\alpha_*$ and the scaling is the “empirical” Fisher information instead of Fisher’s information. Obtaining a true BvM would be interesting but not necessarily easy. It requires to understand the limiting law of $\hat{V}_n^{1/2}\hat{\alpha}_n$ for which there is no generic probabilistic result (because $\Pi_n$ is a random partition and not an iid sample, which makes the analysis tedious). Finally, let us mention that $\hat{V}_n \sim n^{\alpha_*}$ on an event of probability $1 + o(1)$, so the Theorem 2 does imply that the posterior distribution for $\alpha$ contracts near $\hat{\alpha}_n$ at rate $n^{-\alpha_* / 2}$. The rate of convergence of $\hat{\alpha}_n$ to $\alpha_*$, however, can be arbitrarily slow. To obtain a rate of convergence for $\hat{\alpha}_n - \alpha_*$, a finer second order assumption than Assumption 1 is needed, see for instance the assumptions in Favaro and Naulet [2021].

7 Discussion

SSPs form a broad class of statistical problems that are of interest in many scientific fields. In this paper, we considered three SSPs, namely coverage probabilities, the number of unseen species and coverages of prevalences, and we presented an overview of BNP inference for

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1This is not a strong restriction since it allows to use all proper priors, as well as many improper priors.
such three problems under the PYP prior. The choice of the PYP prior is motivated by its
uniqueness with respect to mathematical tractability, flexibility and interpretability, which
makes it the natural candidate for applications; the choice of the SSPs is motivated by the
fact that they have emerged over the past three decades for being the objects of numerous
studies, both in methods and applications, mostly within the field of biological sciences but
also in machine learning, electrical engineering, theoretical computer science and information
theory. We believe that the chosen combination of prior distribution and SSPs provides a
sensible trade-off between the broadness of BNP inference for SSPs and its effectiveness
in concrete (modern) applications. For the three SSPs object of our work, we reviewed
the main posterior analyses from the BNP literature, and also improved remarkably the
existing results, with respect to both the computation and the interpretability of posterior
inferences, by showing that posterior distributions admit representations in terms of simple
compound Binomial and Hypergeometric distributions; in particular, we discussed how our
novel posterior representations provide useful tools in the application of the BNP approach.
Furthermore, we considered the problem of estimating the discount and scale parameters
of the PYP prior, which is known to be critical in the BNP approach to SSPs, and we
established a general property of Bayesian consistency with respect to the hierarchical Bayes
approach and empirical Bayes approaches, that is: the discount parameter can be always
estimated consistently, whereas the scale parameter cannot be estimated consistently, thus
advising caution in posterior inference.

Beyond the SSPs presented in this paper, it is worth mentioning a popular SSP arising in
disclosure risk for data confidentiality [Willenborg and Waal, 2001]. Consider a microdata
sample of \( n \geq 1 \) units (individuals) from a population of \( N > n \) units, such that each unit
contains identifying and sensitive information. Identifying information consists of categorical
variables which might be matchable to known units of the population. A threat of disclosure
results from the possibility of identifying an individual through such a matching, and hence
disclose its sensitive information. To quantify disclosure risk, microdata units are partitioned
according to a categorical variable formed by cross-classifying the identifying variables; that
is, units are partitioned into non-empty cells containing individuals with the same combi-
nations of values of identifying variables. Intuitively, a risk of disclosure arises from cells
with frequency 1 since, assuming no errors in matching processes or data sources, for these
cells the match is guaranteed to be correct [Bethlehem et al., 1990; Skinner et al., 1994;
Skinner and Elliot, 2002]. Formally, if microdata units are modeled as a random sample \( X_N \)
in the classical species sampling framework, and \( (N_{j,n})_{j \geq 1} \) and \( (N_{j,m})_{j \geq 1} \)
are the frequen-
cies of cells (species) in \( X_n \) and \( (X_{n+1}, \ldots, X_{n+N}) \), respectively, then a popular measure of
disclosure risk is
\[
d_{n,m} = \sum_{j \geq 1} I(N_{j,n} = 1)I(N_{j,m} = 0),
\]

namely the number of cells with frequency 1 in the observable sample that are also of
frequency 1 in the population. We refer to Camerlenghi et al. [2021] and Favaro et al. [2021b]
for a detailed study on the estimation of \( d_{n,m} \) in the classical and the BNP species sampling
frameworks.
7.1 Some generalizations of SSPs

“Feature-sampling” problems (FSPs) generalize SSPs by allowing an individual in the population to belong to more than one species, which are referred to as features. To introduce FSPs, consider a population of individuals such that each individual is endowed with a finite set of features’ labels belonging to a (possibly infinite) space of features. The classical (frequentist) nonparametric framework for FSPs assumes that \( n \geq 1 \) observable samples from the population are modeled as a random sample \( (Y_1, \ldots, Y_n) \), where \( Y_i = (Y_{i,j})_{j \geq 1} \) is a sequence of independent Bernoulli random variables with unknown feature probabilities \( (p_j)_{j \geq 1} \), such that \( Y_r \) is independent of \( Y_s \) for any \( r \neq s \). In principle, each of SSPs discussed in this paper admits a corresponding feature sampling counterpart. Within the broad class of FSPs, in recent years there has been a growing interest, especially biological sciences, in the estimation of

\[
\sum_{j \geq 1} I \left( \sum_{i=1}^{n} Y_{i,j} = 0 \right) I \left( \sum_{i=1}^{m} Y_{n+i,j} > 0 \right),
\]

namely the number of hitherto unseen features that would be observed if \( m \) additional samples \( (Y_{n+1}, \ldots, Y_{n+m}) \) were collected from the same \( (p_j)_{j \geq 1} \). We refer to Ionita-Laza et al. [2009], Gravel [2014], Zou et al. [2016], Orlitsky et al. [2016] Chakraborty et al. [2019] for parametric and nonparametric approaches to estimate (35). The FSP (35) provides the natural feature sampling counterpart of the problem of the unseen-species problem; we refer to Ayed et al. [2021] for classical (frequentist) nonparametric inference of a feature sampling counterpart of the problem of estimating the missing mass. Recently Masoero et al. [2022] and Masoero et al. [2021] proposed a BNP approach to estimate (35), which rely on placing suitable prior distributions on the underlying probabilities \( (p_j)_{j \geq 1} \). Despite these recent works, BNP inference for FSPs remains still a mostly unexplored field for both methods and applications.

SSPs may be generalized to multiple populations of individuals sharing species. Consider \( r > 1 \) populations of individuals, such that each individual is labeled by a symbol or species’ label belonging to a (possibly infinite) space of symbols. That is, species’ labels are shared among the populations. Following the classical species sampling framework, it is assumed that \( r \) observables samples of individuals from the populations, the \( i \)-th sample being of size \( n_i \), are modeled as a random sample \( \{(X_{i,1}, \ldots, X_{i,n_i})\}_{i=1, \ldots, r} \) from a collection of \( r \) unknown distributions \( (p_1, \ldots, p_r) \). Then, interest is in estimating discrete functionals that encode features of additional unobservable samples from the same populations; of special interest are functionals encoding information of the number of shared species among populations. In recent years, SSPs with multiple populations have become critical in microbiome studies, i.e. microbial ecology and biology, where next generation sequencing has been applied to obtain inventories of bacteria in many different environments (populations); see Jeganathan and Holmes [2021] and references therein. Nonparametric inference for SSPs with multiple populations pose challenging mathematical hurdles to overcome [Raghuhanathan et al., 2017; Hao and Li, 2020]. In particular, the BNP approach requires to place a nonparametric prior on the underlying collection of distributions \( (p_1, \ldots, p_r) \), in such
a way to model the unknown species compositions of the populations and the dependency among these compositions. Hierarchical priors [Teh et al., 2006; Camerlenghi et al., 2019] and compound priors [Griffin and Leisen, 2017] are arguably the most promising priors for \((p_1, \ldots, p_r)\), being mathematically tractable and flexible in terms of prior’s parameters. However, to date, BNP inference for SSPs in multiple populations is mostly unexplored, being difficult to obtain posterior inferences that are analytically tractable and, most importantly, computationally efficient in concrete applications.

In the classical species sampling framework, the observable samples are assumed to be modeled by independent random variables identically distributed as unknown underlying distribution \(p\). The assumption of independence is unrealistic in many applications, though it yields results that are interesting in themselves, and upon which more sophisticated frameworks may be built. For instance, in a natural language the probability of appearance of a word strongly depends on the previous words, both for grammatical and semantic reasons. Likewise, the nucleotides in a DNA sequence do not form a random sample. Recently, there has been interest in the estimation of the missing mass and coverage probabilities when observable samples are modeled as Markov chains [Asadi et al., 2014; Falahatgar et al., 2016; Hao et al., 2018; Wolfer and Kontorovich, 2019; Skorski, 2020; Cha et al., 2021]. In BNPs, Bacallado et al. [2013] considered SSPs for observable samples modeled as reversible Markov chains. This is motivated by the analysis of benchtop and computer experiments that produce dynamical data associated with the structural fluctuations of a protein in water, with species being protein conformational states [Pande et al., 2010]. In particular, Bacallado et al. [2013] introduced a flexible nonparametric prior for the unknown transition kernel of a reversible Markov chain, such that: i) the state space of chain is uncountable; ii) the prediction for the next state visited by the chain is not solely a function of the number of transitions observed in and out of the last state, but transition probabilities out of different states share statistical strength. While the model of Bacallado et al. [2013] can be used to predict any characteristic of future unobservable trajectories of reversible Markov chains, i.e. protein dynamics, the major goals of the paper were: i) the prediction of how soon the chain will return to a specific state of interest; ii) the prediction of the number of states that the Markov chain has not yet visited in the first (observable) transitions and that will appear in subsequent (unobservable) transitions.

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Supplemental Materials for
Bayesian nonparametric inference for
"species-sampling" problems
Cecilia Balocchi, Stefano Favaro, Zacharie Naulet

S1 Combinatorial numbers

We recall some basic identities on factorial numbers, Stirling numbers, generalized factorial coefficients and generalizations thereof, which will be critical to prove the results of the present paper. We refer to Charalambides (2005) for a comprehensive account on these combinatorial numbers. For \( t \in \mathbb{R}^+ \) and \( u \in \mathbb{N}_0 \), let \( (t)_u = \prod_{0 \leq i \leq u-1} (t + i) \) be the rising factorial of \( t \) of order \( u \). For \( t > 0 \), the \( (u,v) \)-th signless Stirling number of the first type, denoted by \( \mid s(u,v) \mid \), is the defined as the \( v \)-th coefficient in the expansion of \( (t)_u \) into powers, i.e.,

\[
(t)_u = \sum_{v=0}^{u} \mid s(u,v) \mid t^v.
\]

For \( t \in \mathbb{R}^+ \) and \( u \in \mathbb{N}_0 \), let \( (t)_u = \prod_{0 \leq i \leq u-1} (t - i) \) be the falling factorial of \( t \) of order \( u \), such that it holds \( (t)_u = (-1)^u (-t)_u \). The \( (u,v) \)-th Stirling number of the second type, denoted by \( S(u,v) \), is the defined as the \( v \)-th coefficient in the expansion of \( t^u \) into falling factorials, i.e.,

\[
t^u = \sum_{v=0}^{u} S(u,v) (t)_v.
\]

It is assumed: \( \mid s(0,0) \mid = S(0,0) = 1 \), \( \mid s(u,0) \mid = S(u,0) = 0 \) for \( u > 0 \) and \( \mid s(u,v) \mid = S(u,v) = 0 \) for \( v > u \). An generalization of Stirling numbers is given by the coefficients of the expansion of non-centered rising factorials into powers and of powers into non-centered falling factorials, i.e.,

\[
(t + b)_u = \sum_{v=0}^{u} \mid s(u,v; b) \mid t^v
\]

and

\[
t^u = \sum_{v=0}^{u} S(u,v; b)(t - b)_v.
\]

It is assumed: \( \mid s(0,0; b) \mid = S(0,0; b) = 1 \), \( \mid s(u,0; b) \mid = (b)_u \) for \( u > 0 \), \( S(u,0; b) = b^u \) for \( u > 0 \) and \( \mid s(u,v; b) \mid = S(u,v;b) = 0 \) for \( v > u \). The coefficients \( \mid s(u,v; b) \mid \) and \( S(u,v;b) \) are typically referred to as signless non-centered Stirling number of the first type and non-centered Stirling number of the second type, respectively. An explicit expression for the
non-centered Stirling number of the second type can be deduced by applying its definition, that is it holds
\[ S(u, v; b) = \frac{1}{v!} \sum_{j=0}^{v} (-1)^{v-j} \binom{v}{j} (j + b)^u. \]

The following convolutional identities show some useful relationships between Stirling numbers of the first and of the second type and their corresponding non-centered Stirling numbers, i.e.,

i) \[ |s(u, v; b)| = \sum_{j=v}^{u} \binom{j}{v} b^{j-v} |s(u, j)| = \sum_{j=v}^{u} \binom{u}{j} (b)_{u-j} |s(j, v)|; \]

ii) \[ S(u, v; b) = \sum_{j=v}^{u} \binom{u}{j} b^{u-j} S(j, v) = \sum_{j=v}^{u} \binom{j}{v} (b)_{j-v} S(u, j). \] (S1.1)

A variation of the convolutional identity (S1.1), which will be useful in our context, is the following
\[ S(u, v; b) = \sum_{j=v}^{u} (-1)^{u-j} \binom{j}{v} S(u, j) (b + v)_{j-v}. \] (S1.2)

For \( t \in \mathbb{R}^+, a \in \mathbb{R} \) and \( u \in \mathbb{N}_0 \), let us consider the rising factorial of \( at \) of order \( u \), i.e., \( (at)_{(u)} = \prod_{0 \leq i \leq u-1} (at + i) \). The \( (u, v) \)-th (centered) generalized factorial coefficient, denoted by \( C(u, v; a) \), is defined as the \( v \)-th coefficient in the expansion of \( (at)_{(u)} \) into rising factorials, i.e.,
\[ (at)_{(u)} = \sum_{v=0}^{u} C(u, v; a) (t)_{(v)}. \] (S1.3)

It is assumed: \( C(0, 0; a) = 1, C(u, 0; a) = 0 \) for \( u > 0 \), \( C(u, v; a) = 0 \) for \( v > u \). Similarly to the non-centered Stirling number, a generalization of the (centered) generalized factorial coefficient is defined as the \( v \)-th coefficient in the expansion of \( (at - b)_{(u)} \) into rising factorials, i.e.,
\[ (at - b)_{(u)} = \sum_{v=0}^{u} C(u, v; a, b) (t)_{(v)}. \] (S1.4)

It is assumed: \( C(0, 0; a, b) = 1, C(u, 0; a, b) = (-b)_{(u)} \) for \( u > 0 \), \( C(u, v; a, b) = 0 \) for \( v > u \). The coefficient \( C(u, v; a, b) \) is referred to as the non-centered generalized factorial coefficient. An explicit expression for the non-centered generalized factorial coefficients can be deduced, i.e.,
\[ C(u, v; a, b) = \frac{1}{v!} \sum_{j=0}^{v} (-1)^j \binom{v}{j} (-ja - b)_{(u)}. \] (S1.5)
The following convolutional identities show the interplay between the (centered) generalized factorial coefficient and the non-centered generalized factorial coefficient, and the interplay between the non-centered generalized factorial coefficient and the non-centered Stirling number, i.e.,

i)\[ C(u, v; a, b) = \sum_{j=v}^{u} \binom{u}{j} C(j, v; a)(-b)_{u-j}; \quad (S1.6) \]

ii)\[ C(u, v; a_1a_2, a_1a_2 + b) = \sum_{j=v}^{u} C(u, j; a_1, b_1)C(j, v; a_2, b_2); \]

iii)\[ \lim_{a \to 0} \frac{C(u, v; a, b)}{a^k} = |s(u, v; -b)|; \quad (S1.7) \]

iv)\[ \lim_{a \to +\infty} \frac{C(u, v; a, ab)}{b^n} = (-1)^{u-v}S(u, v; b). \]

**S2 A compound Poisson perspective of EPSF**

We conclude present representation of the EPSF in terms of compound Poisson sampling models [Charalambides, 2005, Chapter 7], thus providing an intuitive construction of the EPSF that sheds light on the sampling structure of the PYP prior. We consider a population of individuals with a random number \( K \) of distinct types, and we assume that \( K \) is distributed as a Poisson distribution with parameter \( \lambda = z[1 - (1 - q)^\alpha] \) such that \( q \in (0, 1), \alpha \in (0, 1) \) and \( z > 0 \). For \( i \geq 1 \) let \( N_i \) denote the random number of individuals of type \( i \) in the population, and assume the \( N_i \)’s to be independent of \( K \), independent of each other and such that for \( x \in \mathbb{N} \)

\[ \Pr[N_i = x] = -\frac{1}{[1 - (1 - q)^\alpha]} \binom{\alpha}{x} (-q)^x \quad (S2.1) \]

for all \( i \geq 1 \). Let \( S = \sum_{1 \leq i \leq K} N_i \) and \( M_r = \sum_{1 \leq i \leq K} I(N_i = r) \) for \( r = 1, \ldots, S \), that is \( M_r \) is the random number of \( N_i \)’s equal to \( r \) such that \( \sum_{r \geq 1} M_r = K \) and \( \sum_{r \geq 1} rM_r = S \). If \( M(n, z) = (M_1(n, z), \ldots, M_s(n, z)) \) is a random variable whose distribution coincides with the conditional distribution of \( (M_1, \ldots, M_S) \) given \( S = n \), then it holds [Charalambides, 2007, Section 3]

\[ \Pr[M(n, z) = (m_1, \ldots, m_n)] = \frac{n!}{\sum_{j=0}^{n} \mathcal{C}(n, j; \alpha, 0)z^j} \prod_{i=1}^{n} \frac{z^{\alpha(1-\alpha)(i-1)}}{m_i!}. \quad (S2.2) \]
The distribution (S2.2) is referred to as the negative Binomial compound Poisson sampling formula. See Charalambides [2005, Chapter 7] for an account on compound Poisson sampling models and their distributional properties, and to Dolera and Favaro [2020c] for a comprehensive treatment of the large $n$ asymptotic behaviour of $M(n, z)$ under the negative Binomial compound Poisson sampling model. See also Dolera and Favaro [2020a,b] and references therein.

By letting $\alpha \to 0$ the distribution (S2.1) reduces to the log-series distribution, whereas (S2.2) reduces to the well-known log-series compound Poisson sampling formula. The equivalence between the Ewens sampling formula, i.e. (5) with $\alpha = 0$, and the log-series compound Poisson sampling formula is known from Watterson [1974]. For $\alpha \in (0, 1)$, it exists an interplay between the EPSF (5) and the negative Binomial compound Poisson sampling formula (S2.2). Let $G_{a,b}$ denote a Gamma random variable with scale parameter $b > 0$ and shape parameter $a > 0$, and let $S_{\alpha,\theta}$ be the Pitman’s $\alpha$-diversity random variable in (8). For $\alpha \in (0, 1)$ and $\theta > -\alpha$, let $G_{\theta+n, 1}$ and $S_{\alpha,\theta}$ be independent random variables and define the scale mixture random variable

$$
\bar{X}_{\alpha,\theta,n} = G_{\theta+n, 1}^\alpha S_{\alpha,\theta}.
$$

If $M_n$ is distributed as the EPSF (5), with $\alpha \in (0, 1)$, and $M(n, z)$ is distributed as the negative Binomial compound Poisson formula (S2.2), then Dolera and Favaro [2020c, Theorem 2.2] show that

$$
M_n \overset{d}{=} M(n, \bar{X}_{\alpha,\theta,n}).
$$

(S2.3)

According to (S2.3) the EPSF admits a representation in terms of a randomized negative Binomial compound Poisson sampling formula. The randomization acts on the parameter $z$ with respect to the distribution of the scaled Pitman’s $\alpha$-diversity random variable $\bar{X}_{\alpha,\theta,n}$. This is an instance of a compound mixed Poisson sampling model [Charalambides, 2005, Chapter 7], where the distribution of $K$ is a mixture of Poisson distributions with respect to the distribution of $\bar{X}_{\alpha,\theta,n}$. We refer to Dolera and Favaro [2020c] for a detailed account of (S2.3), and its role in quantifying the large $n$ asymptotic behaviours of $K_n$ and $M_{r,n}$ in (8) and (9), respectively.

**S3 Proof of Proposition 1**

We start by proving statement i), and then statement ii) by letting $\alpha \to 0$. For $\alpha \in (0, 1)$ and $\theta > -\alpha$, the falling factorial moment of order $d \geq 0$ of $K^*_m$ [Favaro et al., 2009, Proposition 1] is

$$
E[(K^*_m)_{(d)}] = (-1)^d d! \left( \binom{\theta+n}{m} \right) \mathcal{C}(m, d; -\alpha, -\theta - n).
$$

(S3.1)

Let $Z_{n,p} \overset{d}{=} \text{Binomial}(n, p)$, and let recall the moment of order $d$ of $Z_{n, p}$ [Johnson et al., 2005, Chapter 3.3], i.e.,

$$
E[(Z_{n, p})_{(d)}] = \sum_{t=0}^{r} S(d, t)(n)_{(t)} p^t.
$$

(S3.2)
for \(d \geq 0\). By a direct application of Proposition 1 in Favaro et al. [2009], the following identities hold

\[
\begin{align*}
\mathbb{E}[(u_{n,m})^d | X_n] &= \sum_{i=0}^{d} (-1)^{d-i} \left( k + \frac{\theta}{\alpha} \right) S(d, i; k + \frac{\theta}{\alpha}) \frac{(\theta + n + i\alpha)_{(m)}}{\Gamma(m)} \\
&= \sum_{i=0}^{d} (-1)^{d-i} \frac{(\theta + n + i\alpha)_{(m)}}{\Gamma(m)} \sum_{t=i}^{d} (-1)^t \binom{t}{i} S(d, t) \left( k + \frac{\theta}{\alpha} \right) \\
&= \sum_{t=0}^{d} S(d, t) \frac{(\theta + n + i\alpha)_{(m)}}{\Gamma(m)} \sum_{i=0}^{d} (-1)^{d-i} \binom{t}{i} \left( \frac{\theta + n + i\alpha}{\alpha} \right)_{(m)} \\
&= \sum_{t=0}^{d} S(d, t) \frac{(\theta + n + i\alpha)_{(m)}}{\Gamma(m)} \mathbb{E}[(K_m^{*})_{[t]}] \\
&= \sum_{t=0}^{d} S(d, t) \frac{(\theta + n + i\alpha)_{(m)}}{\Gamma(m)} \frac{\Gamma(\frac{\theta + n + i\alpha}{\alpha} + t) \Gamma(\frac{n}{\alpha} - k)}{\Gamma(\frac{\theta + n + i\alpha}{\alpha} + t)} \mathbb{E}[(K_m^{*})_{[t]}] \\
&= \sum_{t=0}^{d} S(d, t) \mathbb{E}[(K_m^{*})_{[t]}] \frac{\Gamma(\frac{\theta + n + i\alpha}{\alpha} + t) \Gamma(\frac{n}{\alpha} - k)}{\Gamma(\frac{\theta + n + i\alpha}{\alpha} + t)} \\
&= \sum_{t=0}^{d} S(d, t) \mathbb{E}[(K_m^{*})_{[t]}] \left[ \text{Beta} \left( \frac{\theta}{\alpha} + k, \frac{n}{\alpha} - k \right) \right]^t \\
&= \mathbb{E} \left[ \left( Z_{K_m^{*}, \text{Beta}(\frac{\theta}{\alpha} + k, \frac{n}{\alpha} - k)} \right)^d \right].
\end{align*}
\]

This completes the proof of statement i) of Proposition 1. The proof of statement ii) follows along similar lines, and by letting \(\alpha \to 0\). By combining Equation (S3.1) with Equation
it holds

\[
\mathbb{E}[(K^*_m)^d] = \lim_{\alpha \to 0} (-1)^d d! \left( \frac{\theta + n}{\alpha} \right)^{d(\theta + n)} (\theta + n - d) \mathcal{G}(m, d; -\alpha, -\theta - n)
\]

\[
= \frac{(\theta + n)^d}{(\theta + n)(m)} d! s(m, d; \theta + n)
\]

for \( d \geq 0 \). Then, still using Proposition 1 in Favaro et al. [2009], the following identities hold true

\[
\mathbb{E}[(u_{n,n})^d | X_n] = \lim_{\alpha \to 0} \sum_{i=0}^{d} (-1)^{d-i} \left( k + \frac{\theta}{\alpha} \right) S \left( d, i; k + \frac{\theta}{\alpha} \right) \frac{\theta + n + i\alpha}{\alpha} (\theta + n)(m)
\]

[by Equation (S1.2) and Equation (S1.5)]

\[
= \lim_{\alpha \to 0} \sum_{t=0}^{d} S(d, t) \frac{\theta^t}{(\theta + n)(m)} (\theta + n)^t (-1)^t! \mathcal{G}(m, t; -\alpha, -\theta - n)
\]

[by Equation (S1.7)]

\[
= \sum_{t=0}^{d} S(d, t) \frac{\theta^t}{(\theta + n)(m)} (\theta + n)^t t! s(m, t; \theta + n)
\]

[by Equation (S3.3)]

\[
= \sum_{t=0}^{d} S(d, t) \frac{\theta^t}{(\theta + n)(m)} (\theta + n)^t t! s(m, t; \theta + n)
\]

[by Equation (S3.2)]

\[
= \mathbb{E} \left[ \left( Z_{K^*_m, \theta + n} \right)^d \right].
\]

This completes the proof of statement ii). Now, we consider the proof of statement iii). For \( \alpha \in (0, 1) \) and \( \theta > -\alpha \), the falling factorial moment of order \( d \geq 0 \) of \( M^*_r,m \) [Favaro et al., 2013, Proposition 1] is

\[
\mathbb{E}[(M^*_r,m)^d] = (m)_{[dr]} \left( \frac{(\theta + n)^{d-r}}{r!} \right)^d \left( \frac{\theta + n + d\alpha}{\alpha} \right) \frac{\theta + n + d\alpha}{\alpha} (\theta + n)(m).
\]

Then, by combining Theorem 2 in Favaro et al. [2013] with Equation (S1.5) the following identities hold

\[
\mathbb{E}[(u_{r,n})^d | X_n]
\]
\[
\begin{align*}
&= \sum_{t=0}^{d} S(d, t)(m)_{[r]} \left( \frac{(1 - \alpha)(r-1)}{r!} \right)^{t} \left( k + \frac{\theta}{\alpha} \right) \left( \frac{\theta + n + t\alpha}{(\theta + n)_{(m)}} \right) \\
&= \sum_{t=0}^{d} S(d, t) \left( k + \frac{\theta}{\alpha} \right)_{[t]}\left( \frac{(1 - \alpha)(r-1)}{r!} \right)^{t} \left( \frac{\theta + n + t\alpha}{(\theta + n)_{(m)}} \right) \\
\text{[by Equation (S3.4)]} \\
&= \sum_{t=0}^{d} S(d, t) \left( k + \frac{\theta}{\alpha} \right)_{[t]}\left( \frac{(1 - \alpha)(r-1)}{r!} \right)^{t} \left( \frac{\theta + n + t\alpha}{(\theta + n)_{(m)}} \right) \\
\text{[by the identity \( \Gamma(\frac{\alpha + n}{\alpha}) = \int_{0}^{1} x^{\frac{\alpha + n}{\alpha} - 1} (1 - x)^{\frac{n}{\alpha} - 1} dx \)]} \\
&= \sum_{t=0}^{d} S(d, t) \left[ \Gamma\left( \frac{\alpha + n}{\alpha} \right) \Gamma\left( \frac{n}{\alpha} - k \right) \right] \left( \frac{\theta + n + t\alpha}{(\theta + n)_{(m)}} \right) \\
&= \sum_{t=0}^{d} S(d, t) \left[ \Gamma\left( \frac{\alpha + n}{\alpha} \right) \right] \left( \frac{\theta + n + t\alpha}{(\theta + n)_{(m)}} \right) \\
\text{[by Equation (S3.2)]} \\
&= \sum_{t=0}^{d} S(d, t) \left[ \Gamma\left( \frac{\alpha + n}{\alpha} \right) \right] \left( \frac{\theta + n + t\alpha}{(\theta + n)_{(m)}} \right) \\
\end{align*}
\]

This completes the proof of statement iii) of Proposition 1. The proof of statement iv) follows along similar lines, and by letting \( \alpha \to 0 \) from Equation (S3.4) we can write the following identity

\[E[(M_{r,m}^{*})_{[d]}] = \lim_{\alpha \to 0} \left( m \right)_{[d]} \left( \frac{\alpha(1 - \alpha)(r-1)}{r!} \right)^{d} \left( \frac{\theta + n + d\alpha}{(\theta + n)_{(m)}} \right) \]

\[= \left( m \right)_{[d]} \left( \frac{\theta + n}{r} \right)^{d} \left( \frac{\theta + n + d\alpha}{(\theta + n)_{(m)}} \right) \]

for \( d \geq 0 \). Then, still by using Theorem 2 in Favaro et al. [2013], the following identities hold true

\[E[(u_{r,n,m})_{[d]} \mid X_{n}] \]
\[
\lim_{\alpha \to 0} \sum_{t=0}^{d} S(d,t)(m)_{[tr]} \left( \frac{\alpha(1-\alpha)(r-1)}{r!} \right)^t \left( k + \frac{\theta}{\alpha} \right) \frac{(\theta + n + t\alpha)(m-tr)}{(\theta + n)(m)}
\]

\[
= \sum_{t=0}^{d} S(d,t)(m)_{[tr]} \left( \frac{\theta}{r} \right)^t \frac{(\theta + n)(m-tr)}{(\theta + n)}
\]

\[
= \sum_{t=0}^{d} S(d,t) \left( \frac{\theta}{\theta + n} \right)^t (m)_{[tr]} \left( \frac{\theta + n}{r} \right)^t \frac{(\theta + n)(m-tr)}{(\theta + n)}
\]

\[
= [\text{by Equation (S3.5)}]
\]

\[
= \sum_{t=0}^{d} S(d,t) \left( \frac{\theta}{\theta + n} \right)^t E[(M^*_{r,m})_{[l]}]
\]

\[
= [\text{by Equation (S3.2)}]
\]

\[
= E \left( Z_{M^*_{r,m},\theta+n}^d \right).
\]

This completes the proof of statement iv).

**S4 Proof of Proposition 2**

We consider the case \( \alpha \in (0,1) \) and \( \theta > -\alpha \), whereas the case \( \alpha = 0 \) and \( \theta > 0 \) holds by letting \( \alpha \to 0 \). By means of the definition of \( f_{r,n,m} \) and an application of the Binomial theorem, we write

\[
E[(f_{r,n,m})^d | X_n] = E \left[ \left( \sum_{j \geq 1} 1_{\{N_{j,n}=r\}} 1_{\{N_{j,m}>0\}} \right)^d | X_n \right]
\]

\[
= E \left[ \left( \sum_{j \geq 1} 1_{\{N_{j,n}=r\}} (1 - 1_{\{N_{j,m}=0\}}) \right)^d | X_n \right]
\]

\[
= E \left[ \left( \sum_{j \geq 1} 1_{\{N_{j,n}=r\}} - \sum_{j \geq 1} 1_{\{N_{j,n}=r\}} 1_{\{N_{j,m}=0\}} \right)^d | X_n \right]
\]

\[
= E \left[ \left( m_r - \sum_{j \geq 1} 1_{\{N_{j,n}=r\}} 1_{\{N_{j,m}=0\}} \right)^d | X_n \right]
\]

\[
= \sum_{i=0}^{d} \binom{d}{i} \binom{m_r}{d-i} (-1)^i E \left[ \left( \sum_{j \geq 1} 1_{\{N_{j,n}=r\}} 1_{\{N_{j,m}=0\}} \right)^i | X_n \right]. \quad (S4.1)
\]

Now, let

\[
\mathbf{d}_{r,n,m} = \sum_{j \geq 1} 1_{\{N_{j,n}=r\}} 1_{\{N_{j,m}=0\}} \quad (S4.2)
\]
be the the random variable whose conditional moment of order \(i\), given \(X_n\) is in Equation (S4.1). The first part of the proof considers the problem of computing the conditional moment of order \(d\), given \(X_n\), of the random variable (S4.2). For \(u \in \mathbb{N}\) and \(b, c > 0\), recall that a random variable \(U_{b,c,u}\) on \(\{1, \ldots, u\}\) has a generalized factorial distribution if, for \(x \in \{1, \ldots, u\}\) it holds

\[
\Pr[U_{b,c,u} = x] = \frac{1}{(bc)_x} \mathcal{C}(u, x; b, 0)(c)_x.
\] (S4.3)

See Supplementary Material S1. For \(u, v \in \mathbb{N}\) and \(a > 0\) such that \(a > u\), recall that a random variable \(H_{a,u,v}\) on \(\{0,1,\ldots,u\}\) has a (general) hypergeometric distribution if, for \(x \in \{0,1,\ldots,u\}\) it holds

\[
\Pr[H_{a,u,v} = x] = \frac{(a)_x (u-x)_{a-u}}{(a+v)_x}.
\]

Recall the moment of order \(d\) of the random variable \(H_{a,u,v}\) [Johnson et al., 2005, Chapter 6.3], that is

\[
E[H_{a,u,v}^d] = \sum_{i=1}^{d} S(d, i)! \binom{u}{i} \frac{\Gamma(a + 1 + v - i) \Gamma(a + 1)}{\Gamma(a + 1 - i) \Gamma(a + 1 + v)}.
\] (S4.4)

for \(d \geq 0\). Now, let \(C_{n,x}\) be a combinatorial set of combinations defined as follows: \(C_{n,0} = \emptyset\) and \(C_{n,x} = \{(c_1, \ldots, c_x) : c_k \in \{1, \ldots, n\}, c_k \neq c_l, \text{ if } k \neq l\}\) for any \(x \geq 1\). Then, we can write

\[
E[(d_{r,n,m})^d | X_n] = E[(d_{r,n,m})^d | N_n = (n_1, \ldots, n_k), K_n = k]
\]

\[
= E \left[ \left( \sum_{j=1}^{k} \mathbb{I}_{\{N_j,n=r\}} \mathbb{I}_{\{N_j,m=0\}} \right)^d | N_n = (n_1, \ldots, n_k), K_n = k \right]
\]

\[
= \sum_{x=1}^{d} S(d, x)! \sum_{(c_1, \ldots, c_x) \in C_{k,x}} \mathbb{E} \left[ \prod_{t=1}^{x} \mathbb{I}_{\{N_{c_t,m}=0\}} | N_n = (n_1, \ldots, n_k), K_n = k \right]
\]

\[
= \sum_{x=1}^{d} S(d, x)! \sum_{(c_1, \ldots, c_x) \in C_{k,x}} \mathbb{E} \left[ \prod_{t=1}^{x} \mathbb{I}_{\{N_{c_t,m}=0\}} | N_n = (n_1, \ldots, n_k), K_n = k \right]
\]

\[
= \sum_{x=1}^{d} S(d, x)! \sum_{(c_1, \ldots, c_x) \in C_{k,x}} \mathbb{P}[N_{c_1,m} = 0, \ldots, N_{c_x,m} = 0 | N_n = (n_1, \ldots, n_k), K_n = k].
\] (S4.5)
The conditional probability in (S4.5) can be computed from Favaro et al. [2013, Lemma 1]. Let $V_m$ be the number of $X_{n+i}$'s that do not coincide with any of the $S_j^*$'s in the random sample $X_n$. From Favaro et al. [2013, Equation 38 and Equation 40] we can write the following distributions

i) $\Pr[N_{c_1,m} = 0, \ldots, N_{c_x,m} = 0 \mid N_n = (n_1, \ldots, n_k), K_n = k, V_m = v]$

\[
= \frac{(n - \sum_{i=1}^{x} n_{c_i} - (k - x)\alpha)(m-v)}{(n-k\alpha)_{(m-v)}};
\]

ii) $\Pr[V_{N-n} = v \mid N_n = (n_1, \ldots, n_k), K_n = k]$

\[
= \binom{m}{v} (n - k\alpha)_{(m-v)} \sum_{j=0}^{v} \frac{\prod_{i=0}^{k+j-1}(\theta+i\alpha)}{\prod_{i=0}^{k+j-1}(\theta}_{(n)} \mathcal{C}(v, j; \alpha) \frac{\alpha^j}{\alpha^j},
\]

such that

$\Pr[N_{c_1,m} = 0, \ldots, N_{c_x,m} = 0 \mid N_n = n, K_n = k]$ (S4.6)

\[
= \sum_{j=0}^{m} \frac{1}{\alpha^j} \frac{\prod_{i=0}^{k+j-1}(\theta+i\alpha)}{\prod_{i=0}^{k+j-1}(\theta}_{(n)} \sum_{v=j}^{m} \binom{m}{s} \mathcal{C}(v, j; \alpha)(n - \sum_{i=1}^{x} n_{c_i} - (k - x)\alpha)(m-v)
\]

[by Equation (S1.6)]

\[
= \sum_{j=0}^{m} \frac{\prod_{i=0}^{k+j-1}(\theta+i\alpha)}{\prod_{i=0}^{k+j-1}(\theta}_{(n)} \mathcal{C}(m, j; \alpha, -n + \sum_{i=1}^{x} n_{c_i} + (k - x)\alpha)
\]

\[
= \frac{1}{\theta + n}_{(m)} \sum_{j=0}^{m} \binom{\theta + k}{j} \mathcal{C}(m, j; \alpha, -n + \sum_{i=1}^{x} n_{c_i} + (k - x)\alpha)
\]

[by Equation (S1.4)]

\[
= \frac{\theta + n - \sum_{i=1}^{x} n_{c_i} + x\alpha}_{(m)}.
\]

Then, by a direct combination of Equation (S4.5) with Equation S4.6 we can write the following identities

$\mathbb{E}[(\delta_{r,n,m})^d \mid X_n]$
\[
\begin{align*}
\sum_{x=1}^{d} S(d, x)x! \sum_{(c_1, \ldots, c_2) \in \mathcal{C}_{k,x}} \prod_{t=1}^{x} \mathbb{1}_{\{N_{c_t,n} = r\}} \Pr[N_{c_1,m} = 0, \ldots, N_{c_x,m} = 0 \mid \mathbf{N}_n = (n_1, \ldots, n_k), K_n = k] \\
= \sum_{x=1}^{d} S(d, x)x! \sum_{(c_1, \ldots, c_2) \in \mathcal{C}_{k,x}} \prod_{t=1}^{x} \mathbb{1}_{\{N_{c_t,n} = r\}} \frac{(\theta + n - \sum_{i=1}^{x} n_{c_i} + x\alpha)}{(\theta + n)}(m) \\
= \sum_{x=1}^{d} S(d, x)x! \sum_{(c_1, \ldots, c_2) \in \mathcal{C}_{k,x}} \prod_{t=1}^{x} \mathbb{1}_{\{N_{c_t,n} = r\}} \frac{(\theta + n - \sum_{i=1}^{x} n_{c_i} + x\alpha)}{(\theta + n)}(m) \\
\text{[by the definition of } \mathcal{C}_{k,x}] \\
= \frac{1}{(\theta + n)(m)} \sum_{x=1}^{d} S(d, x)x! \left( m_r \frac{(\theta + n - x\alpha)}{(\theta + n)}(m) \right) \\
= \frac{1}{(\theta + n)(m)} \sum_{x=1}^{d} S(d, x)x! \left( m_r \left( r - \alpha \right) \left( \frac{\theta + n}{r - \alpha} - x \right) \right)(m) \\
\text{[by Equation (S1.3)]} \\
= \frac{1}{(\theta + n)(m)} \sum_{x=1}^{d} S(d, x)x! \left( m_r \sum_{i=0}^{m} \mathcal{C}(m, i; \theta - \alpha) \frac{\theta + n}{r - \alpha} - x \right)(i) \\
= \frac{1}{(\theta + n)(m)} \sum_{i=0}^{m} \mathcal{C}(m, i; \theta - \alpha) \sum_{x=1}^{d} S(d, x)x! \left( m_r \frac{\theta + n}{r - \alpha} + i - x \right) \frac{\Gamma \left( \frac{\theta + n}{r - \alpha} + i \right)}{\Gamma \left( \frac{\theta + n}{r - \alpha} \right)} \\
\times \sum_{x=1}^{d} S(d, x)x! \left( m_r \frac{\theta + n}{r - \alpha} + i - x \right) \frac{\Gamma \left( \frac{\theta + n}{r - \alpha} \right)}{\Gamma \left( \frac{\theta + n}{r - \alpha} + i \right)} \\
\text{[by Equation (S4.3) and (S4.4)]} \\
= \mathbb{E}[f_{r,n,m}^d \mid X_n]. \\
\text{Then, by combining the last expression with (S4.1), the moment } \mathbb{E}[f_{r,n,m}^d \mid X_n] \text{ can be written as} \\
\mathbb{E}[f_{r,n,m}^d \mid X_n] = \sum_{i=0}^{d} \binom{d}{i} m_r^{d-i} (-1)^i \mathbb{E}\left[ (d_{r,n,m})^i \mid X_n \right] \\
= \sum_{i=0}^{d} \binom{d}{i} m_r^{d-i} (-1)^i \mathbb{E}\left[ (H_{\frac{\theta + n}{r - \alpha} - 1, m_r, U_{\frac{\theta + n}{r - \alpha}} r - \alpha})^i \right] \\
= \mathbb{E}\left[ \left( m_r - H_{\frac{\theta + n}{r - \alpha} - 1, m_r, U_{\frac{\theta + n}{r - \alpha}} r - \alpha} \right)^d \right]. \\
The proof for } \alpha \in (0, 1) \text{ and } \theta > -\alpha \text{ is completed. The case } \alpha = 0 \text{ and } \theta > 0 \text{ follows by letting } \alpha \to 0.
S5  Proof of Equation (33)

Let \( X_n \) be a random sample from \( P \sim \text{PYP}(\alpha, \theta) \) with \( \alpha \in [0, 1) \) and \( \theta > -\alpha \), and let \( X_n \) feature \( K_n = k \) distinct symbols with frequencies \( N_n = (n_1, \ldots, n_k) \), and \( M_{r,n} = m_r \) is the number of distinct species with frequency \( r \geq 1 \). From the proof of Proposition 2 in Supplementary Material S4, the moment of order \( d \geq 1 \) of the posterior distribution of \( f_{r,n,m} \), given \( X_n \), is

\[
E[(f_{r,n,m})^d | X_n] = \sum_{i=1}^{d} \binom{d}{i} m_r^{d-i} (-1)^i \sum_{x=1}^{i} S(i, x)x! \left( \frac{m_r}{x} \right) \frac{(\theta + n - xr + x\alpha)(m)}{(\theta + n)(m)},
\]

(S5.1)

and hence

\[
E[f_{r,n,m} | X_n] = m_r - \frac{(\theta + n - r + \alpha)(m)}{(\theta + n)(m)}.
\]

This completes the proof for \( \alpha \in [0, 1) \) and \( \theta > -\alpha \).

S6  Proof of Equation (34)

Let \( X_n \) be a random sample from \( P \sim \text{PYP}(\alpha, \theta) \) with \( \alpha \in [0, 1) \) and \( \theta > -\alpha \), and let \( X_n \) feature \( K_n = k \) distinct symbols with frequencies \( N_n = (n_1, \ldots, n_k) \), and \( M_{r,n} = m_r \) is the number of distinct species with frequency \( r \geq 1 \). From the proof of Proposition 2 in Supplementary Material S4, the moment of order \( d \geq 1 \) of the posterior distribution of \( f_{r,n,m} \), given \( X_n \), is

\[
E[(f_{r,n,m})^d | X_n] = \sum_{i=1}^{d} \binom{d}{i} m_r^{d-i} (-1)^i \sum_{x=1}^{i} S(i, x)x! \left( \frac{m_r}{x} \right) \frac{(\theta + n - xr + x\alpha)(m)}{(\theta + n)(m)},
\]

(S6.1)

Recall that by means of Stirling formula \( \Gamma(n + i)/\Gamma(n) \simeq n^i \) as \( n \to +\infty \) is a first order approximation of the Gamma function. By applying Stirling formula to (S6.1), as \( n \to +\infty \) and \( m \to +\infty \).

\[
E[(f_{r,n,m})^d | X_n] \\
= \sum_{i=1}^{d} \binom{d}{i} m_r^{d-i} (-1)^i \sum_{x=1}^{i} S(i, x)x! \left( \frac{m_r}{x} \right) \frac{(\theta + n - xr + x\alpha)(m)}{(\theta + n)(m)} \\
= \sum_{i=1}^{d} \binom{d}{i} m_r^{d-i} (-1)^i \sum_{x=1}^{i} S(i, x)x! \left( \frac{m_r}{x} \right) \frac{\Gamma(\theta + n + m - xr + x\alpha)}{\Gamma(\theta + n + m)} \frac{\Gamma(\theta + n + m - xr + x\alpha)}{\Gamma(\theta + n)} \\
\simeq \sum_{i=1}^{d} \binom{d}{i} m_r^{d-i} (-1)^i \sum_{x=1}^{i} S(i, x)x! \left( \frac{m_r}{x} \right) \left\{ \left( \frac{n}{n + m} \right)^{r-\alpha} \right\}^x.
\]

(S6.2)

Formula (S6.2) is the moment of order \( d \) of the random variable \( m_r - \text{Binomial}(m_r, (n/(n + m))^{r-\alpha}) \) with \( m_r \) being the number of trials and \( (n/(n + m))^{r-\alpha} \) being the probability of
success in the single trial [Johnson et al., 2005, Section 3.3]. This completes the proof for \( \alpha \in [0, 1) \) and \( \theta > -\alpha \).

**S7 Proof of Theorem 1, Proposition 3, and Theorem 2**

In order to prove these results, we need to write the likelihood \( L_n \) under a convenient form. We can obtain from the equation (5) that \( L_n \) factorizes as

\[
L_n(\alpha, \theta) = \frac{\prod_{i=0}^{K_n-1}(\theta/\alpha + i)}{\prod_{i=0}^{n-1}(\theta + i)} L_n(\alpha, 0) = \frac{\Gamma(\theta + 1)\Gamma(\theta/\alpha + K_n)}{\Gamma(\theta/\alpha + 1)\Gamma(\theta + n)} L_n(\alpha, 0) / \alpha.
\]  

(S7.1)

We note that \( \alpha \mapsto L_n(\alpha, 0) \) is the likelihood of the \( \alpha \)-stable Poisson-Kingman partition model Pitman [2006] which has been investigated in Favaro and Naulet [2021]. In the whole proof, we denote \( \ell_n = \log L_n \) the log-likelihood function of the model.

**S7.1 Proof of the item 1 in Theorem 1**

The concavity of \( \alpha \mapsto \ell_n(\alpha, 0) \), uniqueness, and existence of its maximizer when \( K_n \neq 1 \) and \( K_n \neq n \) is a consequence of the fact that

\[
\ell_n(\alpha, 0) = (K_n - 1) \log(\alpha) + \sum_{i=1}^{n-1} \left( \sum_{\ell=i+1}^{n} M_{n,\ell} \right) \log(i - \alpha).
\]

(S7.2)

In particular, we see that \( \lim_{\alpha \to 0} \partial_\alpha \ell_n(\alpha, 0) = \infty \) and \( \lim_{\alpha \to 1} \partial_\alpha \ell_n(\alpha, 0) = -\infty \); and also \( \partial_\alpha^2 \ell_n(\alpha, 0) < 0 \) for all \( \alpha \in (0, 1) \). The same result has been established with more details in Theorem 1 of Favaro and Naulet [2021].

The second claim is a classical consistency analysis of the maximum likelihood estimator; it is also similar to Theorem 2 in Favaro and Naulet [2021] but here we use weaker conditions, which changes a bit the analysis of the misspecification bias. For the sake of completeness, we give the complete proof.

We show that for all \( \epsilon > 0 \) the condition \( \log(n)|\hat{\alpha}_n^0 - \alpha_*| > \epsilon \) contradicts \( \partial_\alpha \ell_n(\hat{\alpha}_n^0, 0) = 0 \) on a event of probability \( 1 + o(1) \). Since \( \ell_n(\cdot, 0) \) is concave, \( \partial_\alpha \ell_n(\cdot, 0) \) is monotone decreasing on \( (0, 1) \). Therefore,

\[
\inf_{|\alpha-\alpha_*| > \delta} |\partial_\alpha \ell_n(\alpha, 0)| = \min \{|\partial_\alpha \ell_n(\alpha_* - \delta)|, |\partial_\alpha \ell_n(\alpha_* + \delta)|\}.
\]

Hence, the theorem follows if we show that with probability \( 1 + o(1) \) we have \( |\partial_\alpha \ell_n(\alpha_* - \delta)| > 0 \) and \( |\partial_\alpha \ell_n(\alpha_* + \delta)| > 0 \) for \( \delta = \epsilon / \log(n) \) [and for all \( \epsilon > 0 \)]. We do so by proving in Proposition 4 that \( S_{p,n}(\alpha) = \mathbb{E}_p[\partial_\alpha \ell_n(\alpha, 0)] \) satisfies \( S_{p,n}(\alpha \pm \delta) \gg 0 \) and by proving in Proposition 5 that var\( p(\partial_\alpha \ell_n(\alpha \pm \delta)) \ll S_{p,n}(\alpha \pm \delta)^2 \).

**Proposition 4.** Let \( p \) satisfy Assumption 1. Then, there exists a constant \( B > 0 \) depending only on \( (L, \alpha_*\) such that for all \( \epsilon > 0 \) and all \( \alpha \in (0, 1) \) as \( n \to \infty \)

\[
\log(n)|\alpha - \alpha_*| > \epsilon \implies |S_{p,n}(\alpha)| \geq \frac{Bn^{\alpha_*}|\alpha - \alpha_*|}{\min(\alpha, 1 - \alpha)}(1 + o(1))
\]
Proof. By Lemma 1, 

\[ S_{p,n}(\alpha) = -\frac{1}{\alpha} - \sum_{k=1}^{n-1} \frac{n-k}{k-\alpha} \binom{n}{k} \int_0^1 \tilde{F}_p(x)x^k (1-x)^{n-k-1}dx + \frac{n}{\alpha} \int_0^1 \tilde{F}_p(x)(1-x)^{n-1}dx. \]

We now define \( \Delta(x) = \tilde{F}_p(x) - Lx^{-\alpha_*} \), so that we can decompose \( S_{p,n} \) as 

\[ S_{p,n}(\alpha) = -\frac{1}{\alpha} + \frac{Ln}{\alpha} \int_0^1 x^{-\alpha_*}(1-x)^{n-1}dx + \frac{n}{\alpha} \int_0^1 \Delta(x)(1-x)^{n-1}dx \]

\[ - Ln \sum_{k=1}^{n-1} \frac{n-k}{k-\alpha} \binom{n}{k} \int_0^1 x^{k-\alpha_*}(1-x)^{n-k-1}dx \]

\[ + \sum_{k=1}^{n-1} \frac{n-k}{k-\alpha} \binom{n}{k} \int_0^1 \Delta(x)x^k (1-x)^{n-k-1}dx. \]

That is, after splitting the last summation in two at \( k_n = \lfloor n^{1-\alpha_*} \log(n)/\epsilon \rfloor \) for an arbitrary small \( \epsilon > 0 \), 

\[ S_{p,n}(\alpha) = -\frac{1}{\alpha} + \frac{Ln}{\alpha} \int_0^1 x^{-\alpha_*}(1-x)^{n-1}dx + \frac{n}{\alpha} \int_0^1 \Delta(x)(1-x)^{n-1}dx - Ln \sum_{k=1}^{n-1} \frac{n-k}{k-\alpha} \binom{n}{k} \int_0^1 x^{k-\alpha_*}(1-x)^{n-k-1}dx \]

\[ + \sum_{k=1}^{n-1} \frac{n-k}{k-\alpha} \binom{n}{k} \int_0^1 \Delta(x)x^k (1-x)^{n-k-1}dx. \]

By Lemma 2 and by Stirling’s formula, 

\[ |f_2(\alpha)| = \frac{1}{\alpha} \cdot o \left[ \frac{n\Gamma(n)}{\Gamma(n+1-\alpha_*) \log(n)} \right] = \frac{1}{\alpha} \cdot o \left[ \frac{n^{\alpha_*}}{\log(n)} \right]. \]

Similarly, 

\[ |f_3(\alpha)| = o \left[ \frac{1}{\log(n)} \cdot \sum_{k=1}^{k_n} \frac{n-k}{k-\alpha} \binom{n}{k} \frac{\Gamma(n-k)\Gamma(k+1-\alpha_*)}{\Gamma(n+1-\alpha_*)} \right] \]

\[ \leq o \left[ \frac{n^{\alpha_*}}{\log(n)} \cdot \sum_{k=1}^{k_n} \frac{1}{k} \frac{\Gamma(k+1-\alpha_*)}{k!} \right]. \]
\[ \leq \frac{1}{1 - \alpha} \cdot o\left[ \frac{n^{\alpha}}{\log(n)} \right]. \]

Also,

\[
|f_4(\alpha)| \leq \frac{1}{k_n - \alpha} \int_0^1 |\Delta(x)| \sum_{k=0}^{n-1} (n - k) \binom{n}{k} x^k (1 - x)^{n-k-1} \, dx
\]

\[
= \frac{n}{k_n - \alpha} \int_0^1 |\Delta(x)| \sum_{k=0}^{n-1} \binom{n-1}{k} x^k (1 - x)^{n-k-1} \, dx
\]

\[
= \frac{n}{k_n - \alpha} \int_0^1 |\Delta(x)| \, dx
\]

\[
= o\left[ \frac{n^{\alpha}}{\log(n)} \right]
\]

because \( \epsilon \) can be chosen as small as we want and because \( \int_0^1 \bar{F}_p(x) \, dx = 1 \) and \( \int_0^1 x^{-\alpha} \, dx < \infty \).

Finally, we note that,

\[
f_1(\alpha) = \frac{Ln!}{\Gamma(n - \alpha + 1)} \sum_{k=1}^{n-1} \frac{\Gamma(k - \alpha)}{k!}
\]

\[
= \frac{Ln(1 - \alpha)\Gamma(n + 1)}{\alpha\Gamma(n - \alpha + 1)} - \frac{Ln(\alpha + \Gamma(n - \alpha))}{\alpha\Gamma(n - \alpha + 1)}
\]

\[
= \frac{Ln(1 - \alpha)\Gamma(n + 1)}{\alpha\Gamma(n - \alpha + 1)} + O(1),
\]

and,

\[
f_1(\alpha) - f_1(\alpha_*) = \frac{Ln!}{\Gamma(n - \alpha_* + 1)} \sum_{k=1}^{n-1} \frac{\Gamma(k - \alpha_*)}{k!} \left\{ \frac{k - \alpha_*}{k - \alpha} - 1 \right\}
\]

\[
= (\alpha - \alpha_*) \cdot \frac{Ln!}{\Gamma(n - \alpha + 1)} \sum_{k=1}^{n-1} \frac{\Gamma(k - \alpha_*)}{k!(k - \alpha)}. \]

Combining all of the previous equations, we find that,

\[
S_{p,n}(\alpha) = -\frac{1}{\alpha} + \left( \frac{\alpha_*}{\alpha} - 1 \right) \frac{Ln(1 - \alpha_*)n!}{\alpha_\alpha\Gamma(n - \alpha_* + 1)}
\]

\[
- (\alpha - \alpha_*) \cdot \frac{Ln!}{\Gamma(n - \alpha_* + 1)} \sum_{k=1}^{n-1} \frac{\Gamma(k - \alpha_*)}{k!(k - \alpha)} + O\left[ \frac{n^{\alpha_*}}{\min(\alpha, 1 - \alpha) \log(n)} \right].
\]

The conclusion of the proposition follows from the last display.
Proposition 5. The following is true for all $\alpha \in (0, 1)$ and all $p$

$$\text{var}_p(\partial_\alpha \ell_n(\alpha, 0)) \leq \max \left\{ \frac{1}{\alpha^2}, \frac{2}{(1-\alpha)^2} \right\} \mathbb{E}_p[K_n].$$

We also recall the result from Gnedin et al. [2007] that if $F_p(x) \sim Lx^{-\alpha^*}$ as $x \to 0$ [which is the case under Assumption 1] then $\mathbb{E}_p[K_n] \sim L(1-\alpha_*)n^{\alpha^*}$ as $n \to \infty$.

Proof. We bound the variance of $\partial_\alpha \ell_n(\alpha)$ using an Efron-Stein argument. For simplicity we write $\varphi \equiv -\alpha \partial_\alpha \ell_n(\alpha)$. For every $n = 1, \ldots, n$, we define the random variables $C_{n,k} = \sum_{\ell=k}^n M_{n,\ell} = \sum_{j \geq 1} 1_{Y_{n,j} \geq k}$, $Y_{n,j}^{(i)} = Y_{n,j} - 1_{X_i = j}$, and $C_{n,k}^{(i)} = \sum_{j \geq 1} 1_{Y_{n,j}^{(i)} \geq k}$. We note that $Y_{n,j}$ does not depend on $X_i$, so does $C_{n,k}^{(i)}$. Also remark that $\varphi = \sum_{k=1}^{n-1} \frac{\alpha}{k-\alpha} C_{n,k+1} - C_{n,k-1}$.

Defining $\varphi_i = \sum_{k=1}^{n-1} \frac{\alpha}{k-\alpha} C_{n,k+1}^{(i)} - C_{n,k}^{(i)}$, we have by Efron-Stein’s bound [Boucheron et al., 2013, Theorem 3.1]

$$\text{var}_p(\varphi) \leq \sum_{i=1}^n \mathbb{E}_p[(\varphi - \varphi_i)^2].$$

But,

$$C_{n,k} - C_{n,k}^{(i)} = \sum_{j \geq 1} (1_{Y_{n,j} \geq k} - 1_{Y_{n,j}^{(i)} \geq k}) = \sum_{j \geq 1} 1_{Y_{n,j} = k} 1_{X_i = j},$$

where the second equality follows because $Y_{n,j} \geq Y_{n,j}^{(i)} \geq Y_{n,j} - 1$ almost-surely, hence $1_{Y_{n,j} \geq k} - 1_{Y_{n,j}^{(i)} \geq k}$ is either zero or one, and it is one iff $Y_{n,j} = k$ and $Y_{n,j}^{(i)} = k - 1$; that is iff $Y_{n,j} = k$ and $X_i = j$. Therefore,

$$(\varphi - \varphi_i)^2 = \left( \sum_{k=1}^{n-1} \frac{\alpha}{k-\alpha} (C_{n,k+1} - C_{n,k+1}^{(i)}) - (C_{n,1} - C_{n,1}^{(i)}) \right)^2$$

$$= \left\{ \sum_{j \geq 1} 1_{X_i = j} \left( \sum_{k=1}^{n-1} \frac{\alpha}{k-\alpha} 1_{Y_{n,j} = k+1} - 1_{Y_{n,j} = 1} \right) \right\}^2.$$

It follows,

$$\sum_{i=1}^n (\varphi - \varphi_i)^2 = \sum_{j \geq 1} \left( \sum_{i=1}^n 1_{X_i = j} \right) \left( \sum_{k=1}^{n-1} \frac{\alpha}{k-\alpha} 1_{Y_{n,j} = k+1} - 1_{Y_{n,j} = 1} \right)^2$$

$$= \sum_{j \geq 1} Y_{n,j} \left( \sum_{k=1}^{n-1} \frac{\alpha}{k-\alpha} 1_{Y_{n,j} = k+1} - 1_{Y_{n,j} = 1} \right)^2$$

$$= \sum_{j \geq 1} 1_{Y_{n,j} = 1} + \sum_{j \geq 1} Y_{n,j} 1_{Y_{n,j} \neq 1} \left( \sum_{k=1}^{n-1} \frac{\alpha}{k-\alpha} 1_{Y_{n,j} = k+1} \right)^2$$

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\[ M_n,1 + \sum_{k=1}^{n-1} \alpha \sum_{j=1}^{n-k-1} Y_{n,j} 1_{Y_{n,j} \neq 1} 1_{Y_{n,j} = k+1} Y_{n,j} = k' + 1 \]

\[ = M_n,1 + \sum_{k=1}^{n-1} \left( \frac{\alpha}{k - \alpha} \right)^2 \sum_{j=1}^{n-k-1} Y_{n,j} 1_{Y_{n,j} = k+1}. \]

Hence we have shown,

\[ \sum_{i=1}^{n} \mathbb{E}_p[(\varphi - \varphi_i)^2] = \mathbb{E}_p[M_{n,1}] + \sum_{k=1}^{n-1} \left( \frac{\alpha}{k - \alpha} \right)^2 (k + 1) \mathbb{E}_p[M_{n,k+1}] \]

\[ \leq \mathbb{E}_p[M_{n,1}] + \frac{2\alpha^2}{(1 - \alpha)^2} \sum_{k=1}^{n-1} \mathbb{E}_p[M_{n,k+1}] \]

\[ \leq \max \left\{ 1, \frac{2\alpha^2}{(1 - \alpha)^2} \right\} \mathbb{E}_p[K_n], \]

where the second line follows because \((k + 1)/(k - \alpha)^2 \leq 2/(1 - \alpha)^2\) for all \(k \geq 1\); and the third line because \(\sum_{\ell=1}^{n} M_n,\ell = K_n. \)

\[ \square \]

### S7.2 Auxiliary results for the proof of the item 1 in Theorem 1

This section gathers a series of Lemma that are used in the proof of the Proposition 4.

**Lemma 1.** For any \(p\), any \(n \geq 1\), and any \(0 \leq k \leq n - 1\),

\[ \mathbb{E}_p\left[ \sum_{\ell=k+1}^{\ell=n-1} M_{n,\ell} \right] = (n-k) \binom{n}{k} \int_0^1 \tilde{F}_p(x) x^k (1 - x)^{n-k-1} dx. \]

**Proof.** Let \(Y_{n,j} = \sum_{i=1}^{j} 1_{X_i = j}\) so that \(M_{n,\ell} = \sum_{j=1}^{\ell} 1_{Y_{n,j} = \ell}\). Thus,

\[ \mathbb{E}_p[M_{n,\ell}] = \sum_{j=1}^{\ell} \mathbb{E}_p[1_{Y_{n,j} = \ell}] \]

\[ = \binom{n}{\ell} \sum_{j=1}^{\ell} p_j^j (1 - p_j)^{n-\ell} \]

\[ = \binom{n}{\ell} \sum_{j=1}^{\ell} \int_0^{p_j} \left\{ x^{\ell-1} (1 - x)^{n-\ell} - (n-\ell)x^{\ell} (1 - x)^{n-\ell-1} \right\} dx. \]

Since \(\tilde{F}_p(x) = \sum_{j=1}^{\ell} 1_{p_j > x}\) we deduce that

\[ \mathbb{E}_p[M_{n,\ell}] = \binom{n}{\ell} \int_0^1 \tilde{F}_p(x) x^{\ell-1} (1 - x)^{n-\ell-1} (\ell - nx) dx. \]
Finally, we observe that
\[
\sum_{\ell=k+1}^{n} \binom{n}{\ell} x^{\ell-k} (1-x)^{n-\ell} (\ell-nx) = (n-k) \binom{n}{k} x^k (1-x)^{n-k-1}.
\]
\[\text{Lemma 2.} \quad \text{Suppose } (k_n) \text{ is a sequence such that for some } 0 < \eta \leq 1 \text{ it holds } k_n = O(n^{1-\eta}) \text{ as } n \to \infty. \text{ Then, under Assumption 1}
\]
\[
\sup_{k=0,\ldots,k_n} \frac{\int_0^1 |F_p(x) - Lx^{-\alpha}| x^k (1-x)^{n-k-1} \, dx}{\Gamma(n-k) \Gamma(k+1-\alpha) / \Gamma(n+1-\alpha)} = o\left[ \frac{1}{\log(n)} \right].
\]
\[\text{Proof.} \quad \text{For all } \epsilon > 0 \text{ there is } x_0 > 0 \text{ such that } |F_p(x) - Lx^{-\alpha}| \leq \epsilon x^{-\alpha} / \log(1/x) \text{ for all } x \in (0,x_0). \text{ Further, } F_p \text{ is monotone decreasing and } x \mapsto x^{-\alpha} \text{ too. Therefore,}
\]
\[
\int_0^1 |F_p(x) - Lx^{-\alpha}| x^k (1-x)^{n-k-1} \, dx \leq \epsilon \int_0^{x_0} \frac{x^{k-\alpha}(1-x)^{n-k-1} \, dx}{\log(1/x)} + (F_p(x_0) + Lx_0^{-\alpha}) \int_{x_0}^1 x^k (1-x)^{n-k-1} \, dx.
\]
But,
\[
\int_{x_0}^1 x^k (1-x)^{n-k-1} \, dx \leq \int_0^1 x^k (1-x)^{n-k-1} \, dx
\]
\[
= \frac{\Gamma(k+1) \Gamma(n-k)}{\Gamma(n+1)}
\]
\[
= \frac{\Gamma(n-k) \Gamma(k+1-\alpha)}{\Gamma(n+1-\alpha)} \cdot \frac{\Gamma(k+1) \Gamma(n+1-\alpha)}{\Gamma(n+1) \Gamma(k+1-\alpha)}.
\]
Hence, for a universal constant \( A > 0 \) [in particular not depending on \( x_0 \) nor \( k_n \)]
\[
\sup_{k=1,\ldots,k_n} \frac{\int_{x_0}^{x_0} x^k (1-x)^{n-k-1} \, dx}{\Gamma(n-k) \Gamma(k+1-\alpha) / \Gamma(n+1-\alpha)} \leq \frac{Ak_n^{\alpha}}{n^{\alpha}}.
\]
On the other hand, for any \( c > 1 \) [since \( k_n/n \to 0 \) we assume without loss of generality that \( k/n \ll x_0 \)]
\[
\int_0^{x_0} \frac{x^{k-\alpha}(1-x)^{n-k-1} \, dx}{\log(1/x)} = \int_0^{ck/n} \frac{x^{k-\alpha}(1-x)^{n-k-1} \, dx}{\log(1/x)} + \int_{ck/n}^{x_0} \frac{x^{k-\alpha}(1-x)^{n-k-1} \, dx}{\log(1/x)}
\]
\[
\leq \frac{\int_0^{x_0} x^{k-\alpha}(1-x)^{n-k-1} \, dx}{\log[n/(ck)]} + \frac{\int_{ck/n}^{x_0} x^{k-\alpha}(1-x)^{n-k-1} \, dx}{\log(1/x_0)}
\]
\[
= \frac{\Gamma(n-k) \Gamma(k+1-\alpha)}{\Gamma(n+1-\alpha) \log[n/(ck)]} + \frac{\int_{ck/n}^{x_0} x^{k-\alpha}(1-x)^{n-k-1} \, dx}{\log(1/x_0)}.
\]
But, introducing $Z$ a random variable that has a Beta distribution with parameters $k+1-\alpha_*$ and $n-k$,

$$
\int_{ck/n}^{1} x^{k-\alpha_*(1-x)^n-k-1} dx = \frac{\Gamma(n-k)\Gamma(k+1-\alpha_*)}{\Gamma(n+1-\alpha_*)} \mathbb{P}(Z > ck/n)
$$

Note that $\mathbb{E}[Z] = (k+1-\alpha_*(n+1-\alpha_*)$, and thus if $c$ is taken large enough [but depending only on $\alpha_*]$

$$
\sup_{k=1,\ldots,k_n} \mathbb{P}(Z > ck/n) = \sup_{k=1,\ldots,k_n} \mathbb{P}(Z - \mathbb{E}[Z] > ck/(2n)) \\
\leq \sup_{k=1,\ldots,k_n} \frac{\text{var}(Z)}{c^2k^2/(4n^2)} \\
= \sup_{k=1,\ldots,k_n} \frac{4n^2(k+1-\alpha_*)n-k)}{c^2k^2(n+1-\alpha_*)^2(n+2-\alpha_*)} \\
\leq \frac{8}{c^2}.
$$

Taking for instance $c = \sqrt{n/k}$, we obtain finally,

$$
\sup_{k=1,\ldots,k_n} \frac{\int_0^1 |\bar{F}_p(x) - Lx^{-\alpha_*}|x^{k-\alpha_*(1-x)^n-k-1} dx}{\Gamma(n-k)\Gamma(k+1-\alpha_*)/\Gamma(n+1-\alpha_*)} \\
\leq \frac{2\epsilon}{\log(n/k_n)} + \frac{8\epsilon}{\log(1/x_0)} \cdot \frac{k_n}{n} \\
+ A(\bar{F}_p(x_0) + Lx_0^{-\alpha_*}) \cdot \frac{k_n^{\alpha_*}}{n^{\alpha_*}}.
$$

Since $k_n/n$ decays polynomially in $n$ and since this is true for all $\epsilon > 0$, the conclusion follows.

\[ \square \]

**S7.3 Proof of the item 2 in Theorem 1**

We prove the item 2 in several steps. We define two subsets of $\Phi$ by $\Phi_1 = \{(\alpha, \theta) \in \Phi : |\alpha - \hat{\alpha}_n| \leq b_1n^{-\delta}\}$ and $\Phi_2 = \{(\alpha, \theta) \in \Phi : -\hat{\alpha}_n + b_2 \leq \theta \leq \hat{\alpha}_n + b_2 \log(n)\}$, where $b_1, b_2, b_2' > 0$ and $\delta > 0$ are constants to be chosen accordingly. Then, we show that no maximizer of $L_n$ can be found in $\Phi_1^c$ [Proposition 6], and neither in $\Phi_2^c$ [Proposition 7]. As a consequence, if there is a maximizer, it must be in $\Phi_1 \cap \Phi_2$. We analyze $L_n$ over the domain $\Phi_1 \cap \Phi_2$ in Proposition 9 which establishes the final result.

In the whole proof, we use the well-known fact [Gnedin et al., 2007] that $K_n \asymp n^{\alpha_*}$ and $M_{n,2} \asymp n^{\alpha_*}$ on an event of probability $1 + o(1)$. Hence, from now we assume without loss of generality that $K_n \asymp n^{\alpha_*}$ and $M_{n,2} \asymp n^{\alpha_*}$.

**Proposition 6.** If the constant $b_1 > 0$ is large enough and the constant $\delta > 0$ is small enough, then there exists a constant $c > 0$ such that with probability $1 + o(1)$ as $n \to \infty$

$$
\sup_{(\alpha, \theta) \in \Phi_1^c} \{\ell_n(\alpha, \theta) - \sup \ell_n\} \leq -cn^{\alpha_*-\delta}.
$$
Proof. We first get a very rough localization and show that \( \hat{\alpha}_n \) must be within \([c_0, c_1]\) with probability \( 1 + o(1) \), for suitable constants \( 0 < c_0 < c_1 < 1 \). By combining the results of the Lemma 3, 4 and 5, we find that

\[
\sup_{\alpha \in [c_0, c_1]} \{ \ell_n(\alpha, \theta) - \ell_n(\hat{\alpha}_n) \} \leq \sup_{\alpha \in [c_0, c_1]} \left\{ -2 \log(\alpha) + \ell_n(\alpha, 0) - \ell_n(\hat{\alpha}_n, 0) \right\} + O_p(n^{\alpha^*}).
\]

For \( c_0 \) small enough (but bounded away from zero) and \( c_1 \) large enough (but bounded away from 1), the equation (S7.2) and the fact that \( K_n \approx n^{\alpha^*} \) and \( M_{n,2} \approx n^{\alpha^*} \) guarantee that the last display is smaller than \( \lesssim -n^{\alpha^*} \) on an event of probability \( 1 + o(1) \).

Then it is enough to consider \( \alpha \in [c_0, c_1] \) and refine the previous result. We start with the region \( \theta > c_2 \) for some \( c_2 > 0 \) large enough. We can use Stirling’s formula to obtain

\[
\log \left\{ \frac{\Gamma(\theta + 1)}{\Gamma(\theta/\alpha + K_n)} \right\} = (\theta + 1) \log(\theta + 1) + \frac{1}{2} \log \frac{\theta + n}{\theta + 1} - \frac{1}{2} \log \frac{\theta + n}{\theta + 1} - \frac{1}{2} \log \frac{\theta + n}{\theta + 1} \]

\(
+ (\theta + K_n) \log(\theta + K_n) - K_n - (\theta + n) \log(\theta + n) + n + O\left(\frac{1}{c_2}\right).
\)

We observe that,

\[
\frac{1}{2} \log \frac{\theta + n}{\theta + 1} - \frac{1}{2} \log \frac{\theta + n}{\theta + 1} = O(\log(n)).
\]

Hence

\[
\ell_n(\alpha, \theta) \leq h_{n,\alpha}(\theta) + \ell_n(\alpha, 0) + n - K_n + O(\log(n)), \quad (S7.3)
\]

where

\[
h_{n,\alpha}(\theta) = (\theta + 1) \log(\theta + 1) - (\theta + 1) \log(\theta + 1) + (\theta + K_n) \log(\theta + K_n) - (\theta + n) \log(\theta + n).
\]

We now analyze the function \( h_{n,\alpha} \). First,

\[
h'_{n,\alpha}(\theta) = \frac{1}{\alpha} \log \frac{\theta + K_n}{\theta + 1} - \frac{1}{\alpha} \log \frac{\theta + n}{\theta + 1} = \frac{1}{\alpha} \log \left[ 1 + \frac{K_n - 1}{\theta + 1} \right] - \log \left[ 1 + \frac{n - 1}{\theta + 1} \right] \quad (S7.4)
\]

We want to ensure the unique existence of a solution to \( h'_{n,\alpha}(\theta) = 0 \) and guarantee that solution maximizes \( h_{n,\alpha} \). We differentiate a second time

\[
h''_{n,\alpha}(\theta) = \frac{1}{\theta + 1} - \frac{1}{\theta + n} + \frac{1}{\alpha^2 \theta + K_n} - \frac{1}{\alpha^2 \theta + 1}.
\]

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\[
\frac{n-1}{(\theta + 1)(\theta + n)} - \frac{1}{\alpha^2(\theta/\alpha + K_n)(\theta/\alpha + 1)} \frac{K_n - 1}{n-1} \frac{1}{(\theta + 1)(\theta + n)} - \frac{K_n - 1}{(\theta + \alpha K_n)(\theta + \alpha)} \frac{1}{(n-1)(\theta + \alpha K_n)(\theta + \alpha)} - \frac{(K_n - 1)(\theta + 1)(\theta + n)}{(\theta + 1)(\theta + n)}(\theta + \alpha K_n)(\theta + \alpha) .
\]

So, the sign of \( h''_{n,\alpha}(\theta) \) is the same as the sign of (recall \( \theta > -\alpha > -1 \))

\[
N_0 = (n-1)(\theta + \alpha K_n)(\theta + \alpha) - (K_n - 1)(\theta + 1)(\theta + n) = A\theta^2 + B\theta + C,
\]

where \( A = n-K_n, B = (K_n+1)(n-1)\alpha -(n+1)(K_n-1), \) and \( C = -n(K_n-1)+(n-1)K_n\alpha^2 \).

We observe that \( A = n(1+o_p(1)), B = -(-1-\alpha)nK_n+O_p(n), \) and \( C = -nK_n(1-\alpha^2)+O_p(n) \).

By studying the polynomial \( x \mapsto Ax^2+Bx+C \) on \( \mathbb{R} \), we find that it has two roots, given by

\[
r_1 = K_n(1-\alpha)(1+o_p(1)), \quad r_2 = -\frac{1-\alpha^2}{1-\alpha} + o_p(1).
\]

Remark that \( r_2 + \alpha = -1 + o_p(1) \), so indeed with probability \( 1+o(1) \) the root \( r_2 \) is strictly smaller than \(-\alpha\). Hence, with probability \( 1+o(1) \) the equation \( h''_{n,\alpha}(\alpha) = 0 \) has only one solution on \((-\alpha, \infty)\). Further, \( A > 0 \) with probability \( 1+o(1) \), then on a event of probability \( 1+o(1) \) we have \( h''_{n,\alpha} < 0 \) on \((-\alpha, r_1)\) and \( h''_{n,\alpha}(\theta) > 0 \) on \((r_1, \infty)\). Also,

\[
h'_{n,\alpha}(r_1) = \frac{1}{\alpha} \log \left\{ 1 + \frac{K_n(1+o_p(1))}{(1-\alpha)K_n/\alpha} \right\} - \log \left\{ 1 + \frac{n(1+o_p(1))}{(1-\alpha)K_n} \right\}
\]

\[= - \log(n/K_n) + O_p(1) .\]

On the other hand with probability \( 1+o(1) \) it is also the case that \( \lim_{\theta \to -\alpha} h'_{n,\alpha}(\theta) = +\infty \) and \( \lim_{\theta \to \infty} h'_{n,\alpha}(\theta) = 0 \). Therefore, we have established that with probability \( 1+o(1) \) we have \( h'_{n,\alpha} \) is monotonically decreasing on \((-\alpha, r_1)\) with \( \lim_{\theta \to -\alpha} h'_{n,\alpha}(\theta) = +\infty \) and \( h'_{n,\alpha}(r_1) < 0 \); and \( h'_{n,\alpha} \) is monotonically increasing on \((r_1, \infty)\) with \( h'_{n,\alpha}(r_1) < 0 \) and \( \lim_{\theta \to \infty} h'_{n,\alpha}(\theta) = 0 \). Thus, in probability, \( h'_{n,\alpha}(\theta) = 0 \) has a unique solution \( \tilde{\theta} \), and this solution must be within \((-\alpha, r_1)\). Clearly \( \tilde{\theta} \) is the global maximizer of \( h_{n,\alpha} \) and it must be the case that \( \tilde{\theta} = o_p(K_n) \).

Then, by equation (S7.4), we deduce that \( \tilde{\theta} \) must satisfy

\[
\frac{\tilde{\theta} + \alpha}{(\tilde{\theta} + 1)^\alpha} = \frac{\alpha K_n}{n^\alpha(1+o_p(1))}. \tag{S7.5}
\]

So letting \( E \) large enough, either we have \( K_n \leq En^\alpha \) and it must be that \( \tilde{\theta} \in (\alpha, D) \) for some constant \( D \), or \( K_n > En^\alpha \) and we must have that \( \tilde{\theta}^{1-\alpha} \propto n^{-\alpha} K_n = (K_n/n)^\alpha K_n^{1-\alpha} \).

This establishes that \( \tilde{\theta} = O_p\left[ \max(1, K_n(K_n/n)^{\alpha/(1-\alpha)}) \right] \). It follows that,

\[
\sup_{\theta > -\alpha} h_{n,\alpha}(\theta) \leq (\tilde{\theta}/\alpha + K_n) \log(\tilde{\theta}/\alpha + K_n) - (\tilde{\theta} + n) \log(\tilde{\theta} + n)
\]

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\[
= K_n \log K_n - n \log n + O_p \left( \bar{\theta} \max \left( 1, \log \frac{K_n^{1/\alpha}}{n} \right) \right)
\]
\[
= K_n \log K_n - n \log n + O_p (n^{\alpha - \delta})
\]
for some \( \delta > 0 \), because \( K_n \asymp n^{\alpha} \). Then, by combining the last display with equation (S7.3) and the result of the Lemma 3 [after applying Stirling’s formula to both the \( \log \Gamma(K_n) \) and \( \log \Gamma(n) \) terms], we find
\[
\sup_{(\alpha, \theta) \in \Phi_1} \{ \ell_n(\alpha, \theta) - \sup \ell_n \} \leq \sup_{|\alpha - \hat{\alpha}^0_n| > b_1 n^{-\delta}} \{ \ell_n(\alpha, 0) - \ell_n(\hat{\alpha}_n, 0) \} + O_p (n^{\alpha - \delta}).
\]
The equation (S7.2) and the fact that \( K_n \asymp n^{\alpha} \) and \( M_{n,2} \asymp n^{\alpha} \) guarantee that the last display is smaller than \( \lesssim -n^{\alpha - \delta} \) on an event of probability \( 1 + o(1) \) if \( b_1 \) is large enough.

It remains to consider the region \(-\alpha < \theta \leq c_2 \) and \( \alpha \in [c_0, c_1] \). But in this case \( \log \Gamma(\theta + 1) \lesssim 1 \), \( \log(\theta/\alpha + 1) \lesssim 1 \), and by Stirling’s formula \( \log \Gamma(\theta/\alpha + K_n) = \log \Gamma(K_n) + (\theta/\alpha) \log(K_n) + o_p(1) \) and \( \log(\theta/n) = \log \Gamma(n) + \theta \log(n) + o(1) \). By Lemma 3
\[
\sup_{(\alpha, \theta) \in \Phi_2} \{ \ell_n(\alpha, \theta) - \sup \ell_n \} \leq \sup_{|\alpha - \hat{\alpha}^0_n| > b_1 n^{-\delta}} \{ \ell_n(\alpha, 0) - \ell_n(\hat{\alpha}_n, 0) \} + O_p \left( \log(n) \right).
\]
Hence the conclusion follows by the same argument as before. \( \square \)

**Proposition 7.** There exists a constant \( c > 0 \) such that for all \( 0 < b_2 \ll \hat{\alpha}^0_n \) small enough and \( b'_2 > 0 \) large enough \( 1 + o(1) \) as \( n \rightarrow \infty \)
\[
\sup_{(\alpha, \theta) \in \Phi_1 \cap \Phi_2} \{ \ell_n(\alpha, \theta) - \sup \ell_n \} \leq -c \min \left\{ b'_2 \log(n), \log \left( \frac{\hat{\alpha}^0_n}{b_2} \right) \right\}
\]
with probability \( 1 + o(1) \).

**Proof.** We first consider the region where \( \theta > b'_2 \log(n) \), we note that the bound of the equation (S7.3) in the proof of Proposition 6 holds here too. Further, we have proven that \( h_{n,\alpha} \) has a unique maximizer \( \bar{\theta} \) which must satisfy the equation (S7.5). Here, we have in addition that \( |\alpha - \hat{\alpha}^0_n| \lesssim n^{-\delta} \), and by the item 1 of the Theorem \( \log(n)|\hat{\alpha}^0_n - \alpha| = o_p(1) \). Since \( K_n \asymp n^{\alpha} \), it must be that \( \bar{\theta} = O_p(1) \). We also proved that \( h_{n,\alpha}'(\theta) < 0 \) for all \( \theta > \bar{\theta} \), guaranteeing for all \( z > 0 \)
\[
\sup_{\theta > \bar{\theta} + z} h_{n,\alpha}(\theta) = h_{n,\alpha}(\bar{\theta} + z) = h_{n,\alpha}(\bar{\theta}) + \frac{1}{2} h_{n,\alpha}''(\bar{\theta} + \bar{z}) z^2
\]
for some \( \bar{z} \in (0, z) \), by a Taylor expansion and because \( \bar{\theta} \) maximizes \( h_{n,\alpha} \). By definition of \( h_{n,\alpha} \), and since \( \bar{\theta} = O_p(1) \) and \( K_n/n^{\alpha} \asymp 1 \)
\[
h_{n,\alpha}(\bar{\theta}) = K_n \log K_n - n \log(n) + O_p(1).
\]
By the computations in the proof of Proposition 6, if $\theta \leq 1$ we have

$$h''_{n,\alpha}(\theta) = \frac{A\theta^2 + B\theta + C}{(\theta + 1)(\theta + n)(\theta + \alpha K_n)(\theta + \alpha)}$$

$$= (1 + o_p(1))\frac{n\theta^2 - (1 - \alpha)nK_n\theta - (1 - \alpha^2)nK_n}{(\theta + 1)(\theta + n)(\theta + \alpha K_n)(\theta + \alpha)}$$

$$\leq (1 + o_p(1))\frac{- (1 - \alpha^2)nK_n}{(\theta + 1)(\theta + n)(\theta + \alpha K_n)(\theta + \alpha)} \lesssim -1,$$

while if $1 < \theta \leq o(K_n)$

$$h''_{n,\alpha}(\theta) \leq (1 + o_p(1))\frac{- (1 - \alpha)nK_n\theta}{(\theta + 1)(\theta + n)(\theta + \alpha K_n)(\theta + \alpha)} \lesssim -\frac{1}{\theta}.$$ 

Taking $z = D \log(n)$ for some constant $D > 0$ large enough, we necessarily have that

$$\bar{\theta} + \bar{z} = O(\log(n)) = o_p(K_n).$$

It follows the existence of a universal constant $E > 0$ (in particular not depending on $D$), such that with probability $1 + o(1)$

$$\sup_{\theta > \bar{\theta} + D \log(n)} h_{n,\alpha}(\theta) \leq K_n \log K_n - n \log(n) - E \cdot D \log(n).$$

By combining the last display with equation (S7.3) and the result of the Lemma 3 [after applying Stirling’s formula to both the $\log \Gamma(K_n)$ and $\log \Gamma(n)$ terms], when $b'_2 > 0$ is large enough there is a constant $c > 0$ such that with probability $1 + o(1)$

$$\sup_{(\alpha,\theta) \in \Phi_1 \cap \theta > b'_2 \log(n)} \{\ell_n(\alpha, \theta) - \sup \ell_n\} \leq -c b'_2 \log(n).$$

It remains to consider the region where $\theta < -\hat{\alpha}_n^0 + b_2$ and $(\alpha, \theta) \in \Phi_1$. But by Stirling’s formula,

$$\log \Gamma(\theta/\alpha + K_n) = (\theta/\alpha + K_n) \log(\theta/\alpha + K_n) - (\theta/\alpha + K_n) + \frac{1}{2} \log \frac{2\pi}{\theta/\alpha + K_n} + O(K_n^{-1})$$

$$= \frac{\theta \log K_n}{\alpha} + K_n \log K_n - K_n + \frac{1}{2} \log \frac{2\pi}{K_n} + O\left[\max(1, \theta^2)\right],$$

and

$$\log \Gamma(\theta + n) = \theta \log(n) + n \log(n) - n + \frac{1}{2} \log \frac{2\pi}{n} + O\left[\max(1, \theta^2)\right].$$

So we have because of Lemma 3 and another application of Stirling’s formula

$$\ell_n(\alpha, \theta) - \sup \ell_n \leq \Psi_n(\alpha, \theta) - \Psi_n(\hat{\alpha}_n^0, \hat{T}_n)$$

$$- \log \frac{\alpha}{\hat{\alpha}_n^0} + \ell_n(\alpha, 0) - \ell_n(\hat{\alpha}_n^0, 0) + O\left[\max(1, \theta^2)\right].$$  \hspace{1cm} (S7.6)
But $\Psi_n(\hat{\alpha}_0, \hat{T}_n) = O_p(1)$ by Lemma 3. $\ell_n(\alpha, 0) - \ell_n(\hat{\alpha}_0, 0) \leq 0$ by construction, and $\lim_{\theta \to -\alpha} \Psi_n(\alpha, \theta) = -\infty$. Furthermore, $\log \Gamma(z) \sim \log(1/z)$ as $z \to 0$. Hence, there exists a constant $c > 0$ such that for small enough $0 < b_2 \ll \hat{\alpha}_0$

$$\sup_{(\alpha, \theta) \in \Phi_1 \theta < -\hat{\alpha}_0 + b_2} \{\ell_n(\alpha, \theta) - \sup \ell_n\} \leq -c \log \left(\frac{\hat{\alpha}_0}{b_2}\right)$$

with probability $1 + o(1)$. \hfill \Box

To facilitate the analysis of $L_n$ over $\Phi_1 \cap \Phi_2$ we introduce an auxiliary estimator $\hat{T}_n$ of $\theta^*$ as in the next Proposition.

**Proposition 8.** Define a function $\Psi_n : \Phi \to \mathbb{R}$ by $\Psi_n(\alpha, \theta) = \log \Gamma(\theta + 1) - \log \Gamma(\theta/\alpha + 1) + \theta \log \frac{K_1^{1/\alpha}}{n}$. Then for each fixed $\alpha \in (0, 1)$ the map $\theta \mapsto \Psi_n(\alpha, \theta)$ is concave and has a unique maximizer on $(-\alpha, \infty)$. Call this maximizer $\hat{T}_{n, \alpha}$ and let $\hat{T}_n = \hat{T}_{n, \hat{\alpha}_0}$. If the Assumption 1 is satisfied, then the sequence $(\hat{T}_n)_{n \geq 1}$ converges in probability to $\theta^* \in (-\alpha^*, \infty)$.

**Proof.** Let $\alpha \in (0, 1)$ arbitrary. Recall that $\psi$ is the derivative of $\log \Gamma$ by definition. Hence, by differentiating $\Psi_n$ with respect to $\theta$, we find that

$$\partial_\theta \Psi_n(\alpha, \theta) = \psi(\theta + 1) - \alpha^{-1} \psi(\theta/\alpha + 1) + \log \frac{K_1^{1/\alpha}}{n}. \tag{S7.7}$$

Standard analysis of the digamma function shows that $\lim_{z \to 0} \psi(z) = -\infty$ and $\psi(z) = \log(z) + O(z^{-1})$ as $z \to \infty$. Thus $\lim_{\theta \to -\alpha} \partial_\theta \Psi_n(\alpha, \theta) = +\infty$ and $\lim_{\theta \to \infty} \partial_\theta \Psi_n(\alpha, \theta) = \infty$ [Olver et al., 2010]. Since $\theta \mapsto \partial_\theta \Psi_n(\alpha, \theta)$ is continuous, there exists a solution in $\theta$ to $\partial_\theta \Psi_n(\alpha, \theta) = 0$. Furthermore, it is well-known that [Olver et al., 2010]

$$\psi(z + 1) = -\gamma + \sum_{k=1}^{\infty} \left(\frac{1}{k} - \frac{1}{k + x}\right),$$

where $\gamma$ is Euler’s gamma constant, $\gamma \approx 0.577$. It follows that

$$\partial_\theta^2 \Psi_n(\alpha, \theta) = \sum_{k=1}^{\infty} \left[\frac{1}{(k + \theta)^2} - \frac{1}{(\alpha k + \theta)^2}\right] < 0. \tag{S7.8}$$

This establishes that $\theta \mapsto \Psi_n(\alpha, \theta)$ has a unique maximizer on $(-\alpha, \infty)$ as well as the (strict) concavity of this map. By computations analogous to the one made in the proof of Proposition 4, we find that under Assumption 1 we have

$$\mathbb{E}_p[K_n] = n \int_0^1 \bar{F}_p(x)(1 - x)^{n-1}dx$$

$$= L \Gamma(1 - \alpha^*) \{1 + o\left(\frac{1}{\log(n)}\right)\},$$

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and by Lemma A.3 in Favaro and Naulet [2021] we have \( \text{var}_p(K_n) \leq \mathbb{E}_p[K_n] \). Since \( \log(n)|\hat{\alpha}_n - \alpha_0| = o_p(1) \) by the Item 1, we find that \( K_n/n^{\hat{\alpha}_n} = \Gamma(1-\alpha_0) + o_p(1) \). Since \( \partial_\theta \Psi_n(\hat{\alpha}_n, \hat{T}_n) = 0 \), by equation (S7.7),

\[
\Gamma(1-\hat{\alpha}_n^0) = \exp\{\psi(\hat{T}_n/\hat{\alpha}_n^0 + 1) - \hat{\alpha}_n^0 \psi(\hat{T}_n + 1)\} + o_p(1).
\]

The final claim follows by a continuity argument. \( \square \)

**Proposition 9.** Any maximizer \((\hat{\alpha}_n, \hat{\theta}_n)\) of \( \ell_n \) must satisfy \( \hat{\alpha}_n = \hat{\alpha}_n^0 + O_p\left(\frac{\log(n)}{n^{\alpha_*}}\right) \) and \( \hat{\theta}_n = \hat{T}_n + O_p\left(\frac{\log(n)^2}{n^{\alpha_*}}\right) \).

**Proof.** By Propositions 6 and 7, it is enough to consider \((\alpha, \theta) \in \Phi_1 \cap \Phi_2 \). It is easily seen that the bound of equation (S7.6) also holds true here. Then, by a Taylor expansion, there is \( \hat{\alpha} \) in a neighborhood of \( \hat{\alpha}_n \) such that

\[
\Psi_n(\alpha, \theta) - \Psi_n(\hat{\alpha}_n, \hat{T}_n) = \partial_\alpha \Psi_n(\hat{\alpha}_n, \theta)(\alpha - \hat{\alpha}_n) + \Psi_n(\hat{\alpha}_n, \theta) - \Psi_n(\hat{\alpha}_n, \hat{T}_n).
\]

But,

\[
\partial_\alpha \Psi_n(\hat{\alpha}_n, \theta) = \frac{\theta}{\hat{\alpha}_n^2} \{- \log K_n + \psi(\theta/\hat{\alpha}_n + 1)\} = O[\theta \max(\log K_n, \log \theta)],
\]

where the second estimate follows because \( \theta/\hat{\alpha}_n \) is bounded away from \(-1\) with probability \(1 + o(1)\) by the previous results, and hence \( \psi(\theta/\hat{\alpha}_n + 1) \) is of order constant for small \(-\hat{\alpha}_n^0 + b_2 \leq \theta \leq 1\) and never more than \(O(\log(\theta))\) for \( \theta \geq 1 \). So on \( \Phi_1 \cap \Phi_2 \), we must have

\[
\Psi_n(\alpha, \theta) - \Psi_n(\hat{\alpha}_n, \hat{T}_n) = \Psi_n(\hat{\alpha}_n, \theta) - \Psi_n(\hat{\alpha}_n, \hat{T}_n) + O_p[\theta \log(n) \cdot (\alpha - \hat{\alpha}_n^0)].
\]

By concavity of \( \theta \mapsto \Psi_n(\hat{\alpha}_n, \theta) \)

\[
\sup_{|\theta - \hat{T}_n| > \varepsilon} \left\{ \Psi_n(\alpha_0, \theta) - \Psi_n(\hat{\alpha}_n, \hat{T}_n) \right\} \leq \sup_{x \in (0, \varepsilon)} \partial_\theta^2 \Psi_n(\hat{T}_n + x, \alpha_0) \cdot \frac{\varepsilon^2}{2}.
\]

But by the equation (S7.8),

\[
\partial_\theta^2 \Psi_n(\alpha, \theta) \leq \frac{1}{(1 + \theta)^2} - \frac{1}{(\alpha + \theta)^2} = \frac{-(1 - \alpha)^2 - 2\theta(1 - \alpha)}{(\alpha + \theta)(1 + \theta)} \leq \frac{-(1 - \alpha)^2 + 2\alpha(1 - \alpha)}{(\alpha + \theta)(1 + \theta)} = -\frac{(1 - \alpha)^2}{(\alpha + \theta)(1 + \theta)}.
\]

Hence, for \( \varepsilon > 0 \) small enough \( \ell_n(\alpha, \theta) - \sup \ell_n \lesssim -\varepsilon^2 + O_p(n^{-3} \log(n)^2) \) whenever \( |\theta - \hat{T}_n| \geq \varepsilon \) with \( \theta \leq b_2 \log(n) \). So we have shown that any maximizer of \( \ell_n \) must lie in the region
\[ |\alpha - \hat{\alpha}_n| \leq b_0 n^{-\delta} \text{ and } |\theta - \hat{T}_n| \leq b_3 n^{-\delta/2} \log(n) \text{ for some } b_3 > 0 \text{ large enough. In this region, and by the same arguments as before, we can refine the bound of equation (S7.6) onto} \]
\[
\ell_n(\alpha, \theta) - \sup \ell_n \leq \frac{1}{2} \partial^2_n \Psi_n(\hat{T}, \hat{\alpha}_n)(\theta - \hat{T}_n)^2 + \frac{1}{2} \partial^2_n \ell_n(\hat{\alpha}, 0)(\alpha - \hat{\alpha}_n)^2 \\
+ O_p[\log(n) \cdot (\alpha - \hat{\alpha}_n) + n^{-\alpha_0}] 
\]
for some \( \alpha \) in a neighborhood of \( \hat{\alpha}_n \) and some \( \hat{T} \) in a neighborhood of \( \hat{T}_n \). The conclusion follows because with probability 1 + \( o(1) \) it is true that \( \partial^2_n \Psi_n(\hat{T}, \hat{\alpha}_n) \lesssim -1 \) by the previous, and \( \frac{1}{2} \partial^2_n \ell_n(\alpha, 0) \lesssim -n^{\alpha_0} \) by equation (S7.2) and classical arguments. \[ \square \]

**S7.4 Auxiliary results for the proof of the item 2 in Theorem 1**

This section gathers a series of Lemma that are used in the proof of the Propositions 6, 7, and 9 of the previous section.

**Lemma 3.** The following lower bound is true.
\[
\sup \ell_n \geq \Psi_n(\hat{\alpha}_n, \hat{T}_n) - \log \hat{\alpha}_n + \ell_n(\hat{\alpha}_n) + \log \Gamma(K_n) - \log \Gamma(n) + O_p(K_n^{-1}).
\]
Furthermore, observe that \( \Psi_n(\hat{\alpha}_n, \hat{T}_n) = O_p(1) \) because of the item ?? of the Theorem.

**Proof.** Obviously, \( \sup \ell_n \geq \ell_n(\hat{\alpha}_n, \hat{T}_n) \). Then, the conclusion follows by equation (S7.1), the definition of \( \Psi_n \), by Stirling’s formula applied to \( \Gamma(\hat{T}_n/\hat{\alpha}_n + K_n) \), to \( \Gamma(\hat{T}_n + n) \), to \( \Gamma(K_n) \), and to \( \Gamma(n) \), and because \( K_n = O_p(n^{\alpha_0}) \), and \( \hat{T}_n > -\hat{\alpha}_n \). \[ \square \]

**Lemma 4.** For all \( \theta > 0 \) and for all \( \alpha \in (0, 1) \)
\[
L_n(\alpha, \theta) \leq \frac{\Gamma(K_n)e^{K_n}}{\alpha \Gamma(n)} L_n(\alpha, 0).
\]

**Proof.** The starting point is the following observation. If \( Z \sim \text{Gamma}(\theta/\alpha, 1) \) and \( W \sim \text{Gamma}(K_n) \) are independent random variables, then
\[
\mathbb{E}[e^Z (1 - \frac{Z^{1/\alpha}}{W^{1/\alpha}})^{n-1} 1_{W > z}] = \frac{1}{\Gamma(\theta/\alpha) \Gamma(K_n)} \int_0^\infty w^{K_n-1} e^{-w} \int_0^w z^{\theta/\alpha-1} \left(1 - \frac{z^{1/\alpha}}{w^{1/\alpha}} \right)^{n-1} dz dw \\
= \frac{\alpha}{\Gamma(\theta/\alpha) \Gamma(K_n)} \int_0^\infty w^{K_n+\theta/\alpha-1} e^{-w} dw \int_0^1 u^{\theta-1} (1 - u)^{n-1} du \\
= \frac{\alpha \Gamma(\theta/\alpha + K_n)}{\Gamma(\theta/\alpha) \Gamma(K_n) \Gamma(\theta + n)} \Gamma(n) \Gamma(\theta) \Gamma(\theta + n).
\]

Therefore, by Chernoff’s bound on the Gamma distribution
\[
\frac{\Gamma(\theta)}{\Gamma(\theta/\alpha) \Gamma(\theta + n)} = \frac{\Gamma(K_n)}{\alpha \Gamma(n)} \mathbb{E}[e^Z (1 - \frac{Z^{1/\alpha}}{W^{1/\alpha}})^{n-1} 1_{W > z}]
\]
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\[ \frac{\Gamma(K_n)}{\alpha \Gamma(n)} \mathbb{E}[e^Z \mathbb{P}(W > Z)] \leq \frac{\Gamma(K_n)}{\alpha \Gamma(n)} \left[ e^Z \min \left\{ 1, e^{K_n - Z \left( \frac{K_n}{Z} \right)^K_n} \right\} \right] \]

\[ = \frac{\Gamma(K_n)}{\alpha \Gamma(n)} \left[ \min \left\{ e^Z, e^{K_n \left( \frac{K_n}{Z} \right)^K_n} \right\} \right] \]

\[ \leq \frac{\Gamma(K_n)}{\alpha \Gamma(n)} e^{K_n \left( \frac{K_n}{Z} \right)^K_n}. \]

Then, since \( \theta > 0 \),

\[ L_n(\alpha, \theta) = \frac{\Gamma(\theta)}{\Gamma(\theta / \alpha)} \frac{\Gamma(\theta / \alpha + K_n)}{\Gamma(\theta + n)} L_n(\alpha, 0) \leq \frac{\Gamma(K_n)}{\alpha \Gamma(n)} L_n(\alpha, 0). \]

\[ \square \]

**Lemma 5.** Let \( K_n \geq 2 \). Then, there is a generic constant \( C > 0 \) such that for all \( \alpha \in (0, 1) \) and all \( -\alpha < \theta \leq 0 \)

\[ L_n(\alpha, \theta) \leq \frac{C n \Gamma(K_n)}{\alpha^2 \Gamma(n)} L_n(\alpha, 0). \]

**Proof.** We note that there exist constants \( A, B > 0 \) such that for all \( 0 < z \leq 1 \) it holds \( A \leq z \Gamma(z) \leq B \). Hence, we can find a generic constant \( C > 0 \) such that

\[ \frac{\Gamma(\theta + 1)}{\Gamma(\theta / \alpha + 1)} \leq C \frac{\theta / \alpha + 1}{\theta + 1} \leq \frac{\theta + \alpha}{\theta + 1} \leq \frac{C}{\alpha}. \]

Then, by Gautschi’s inequality, we can bound,

\[ \frac{\Gamma(\theta / \alpha + K_n)}{\Gamma(\theta + n)} = \frac{\Gamma(K_n)}{\Gamma(n)} \cdot \frac{\Gamma(\theta / \alpha + K_n)}{\Gamma(K_n)} \cdot \frac{\Gamma(n)}{\Gamma(n + \theta)} \]

\[ \leq \frac{\Gamma(K_n)}{\Gamma(n)} \cdot (K_n - 1)^{\theta / \alpha} \cdot n^{-\theta} \]

\[ \leq \frac{n \Gamma(K_n)}{\Gamma(n)}. \]

\[ \square \]

**S7.5 Proof of Proposition 3**

For every \( c, d > 0 \), we can find \( \eta > 0 \) such that \( \{(\alpha, \theta) \in \Phi : \theta + \alpha_\ast \in [c, d]\} \subseteq B \) where \( B = \{(\alpha, \theta) \in \Phi : \theta > -\alpha_\ast + c, |\theta - \hat{\theta}_n| \leq \eta\} \). Hence, it is enough to consider the infimum over \( B \). For the same reasons, we can assume that \( c \) is arbitrarily small and \( \eta \) arbitrarily
large. Let $H(\phi)$ be the Hessian matrix of $\ell_n$ at $\phi = (\alpha, \theta)$. Since $\hat{\phi}_n = (\hat{\alpha}_n, \hat{\theta}_n)$ is a maximizer of $\ell_n$, by a Taylor expansion of $\ell_n$ near $\hat{\phi}_n$ for all $\phi$ there is $u \in (0, 1)$ such that

$$
\ell_n(\phi) - \sup \ell_n = \frac{1}{2} (\phi - \hat{\phi}_n)^T H(u\phi + (1 - u)\hat{\phi}_n)(\phi - \hat{\phi}_n).
$$

In particular if $\phi = (\hat{\alpha}_n, \theta)$,

$$
\ell_n(\phi) - \sup \ell_n = \frac{(\theta - \hat{\theta}_n)^2}{2} H(\phi + (1 - u)\hat{\phi}_n)_{2,2}.
$$

But by equation (S7.1)

$$
\partial_\theta \ell_n(\alpha, \theta) = \psi(\theta + 1) + \alpha^{-1}\psi(\theta/\alpha + K_n) - \alpha^{-1}\psi(\theta/\alpha + 1) - \psi(\theta + n),
$$

and,

$$
\partial_\theta^2 \ell_n(\alpha, \theta) = \psi'(\theta + 1) + \alpha^{-2}\psi'(\theta/\alpha + K_n) - \alpha^{-2}\psi'(\theta/\alpha + 1) - \psi'(\theta + n).
$$

Furthermore, $\psi(z) = z^{-1} + o(z^{-2})$ as $z \to \infty$ [Olver et al., 2010], so whenever $\alpha$ is bounded away from zero

$$
H(\phi)_{2,2} = \psi'(\theta + 1) - \alpha^{-2}\psi'(\theta/\alpha + 1) + O(K_n^{-1})
$$

$$
= \sum_{k=1}^\infty \left[ \frac{1}{(k + \theta)^2} - \frac{1}{(\alpha k + \theta)^2} \right] + O(K_n^{-1})
$$

$$
= -\sum_{k=1}^\infty \frac{(1 - \alpha^2)k^2 + 2(1 - \alpha)\theta k}{(k + \theta)^2(\alpha k + \theta)^2} + O(K_n^{-1})
$$

where the second line follows from equation (S7.8). Now we observe that if $\phi = (\hat{\alpha}_n, \theta)$ then $u\phi + (1 - u)\hat{\phi}_n \in B$ for all $u \in (0, 1)$ with probability $1 + o(1)$ and we can find a constant $C > 0$ such that $H(u\phi + (1 - u)\hat{\phi}_n)_{2,2} \geq -C + O(K_n^{-1})$. Consequently $\inf_{\phi \in B} \{\ell_n(\phi) - \sup \ell_n\} \geq -C\eta^2/2 + O(K_n^{-1})$.

### S7.6 Proof of Theorem 2

In the whole proof we let $Z_{n,\alpha} = \hat{Y}_{n,\alpha}^{1/2}(\alpha - \hat{\alpha}_n)$ for simplicity. We define $A_n = \{x \in \mathbb{R} : x^2 \leq C \log(n)\}$ and $B_n = \{x \in \mathbb{R} : r_n^{-1} \leq x \leq r_n\}$, with $C > 0$ a constant and $(r_n)$ a slowly increasing sequence to be chosen accordingly later. We also let $C_n = A_n \times B_n$. Then, we decompose

$$
\sup_{A,B} |G(Z_{n,\alpha} \in A, \gamma \in B \mid \Pi_n) - \phi(A)H_s(B)| \leq R_1 + R_2 + R_3,
$$

with

$$
R_1 = \sup_{A,B} \left\{ \frac{G(Z_{n,\alpha} \in A \cap A_n, \gamma \in B \cap B_n \mid \Pi_n) - \phi(A \cap A_n)H_s(B \cap B_n)}{\phi(A_n)H_s(B_n)} \right\},
$$

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\[ R_2 = \sup_{A,B} \left| \frac{G(Z_{n,\alpha} \in A \cap A_n, \gamma \in B \cap B_n | \Pi_n)}{G(Z_{n,\alpha} \in A_n, \gamma \in B_n | \Pi_n)} - G(Z_{n,\alpha} \in A, \gamma \in B | \Pi_n) \right|, \]
\[ R_3 = \sup_{A,B} \left| \frac{\phi(A \cap A_n)H_*(B \cap B_n)}{\phi(A_n)H_*(B_n)} - \phi(A)H_*(B) \right|. \]

We bound each of the terms \( R_1, R_2 \) and \( R_3 \) in the following subsections.

**Bound on \( R_1 \).**

We let for simplicity \( \tilde{G}_n(A, B) = \frac{G(Z_{n,\alpha} \in A \cap A_n, \gamma \in B \cap B_n | \Pi_n)}{G(Z_{n,\alpha} \in A_n, \gamma \in B_n | \Pi_n)} \) and we write \( h_* \) the density of \( H_* \), \( \tilde{g}_n \) the density of \( \tilde{G}_n \), and \( f \) the density of \( \phi \). Then,

\[ R_1 = \sup_{A,B} \left| \int_{A \cap A_n} \int_{B \cap B_n} \left( 1 - \frac{f(x)h_*(y)}{\phi(A_n)H_*(B_n)\tilde{g}_n(x, y)} \right) \tilde{g}_n(x, y) \, dx \, dy \right| \]
\[ \leq \int_{C_n} \left| 1 - \frac{f(x)h_*(y)}{\phi(A_n)H_*(B_n)\tilde{g}_n(x, y)} \right| \tilde{g}_n(x, y) \, dx \, dy, \]

Introducing the shorthand notation \( \hat{x}_n \equiv \hat{V}_n^{-1/2}x \) to ease the reading, we have by Bayes’ rule that

\[ \tilde{g}_n(x, y) = \frac{e^{\mathcal{L}_n(x,y)\alpha}g_\alpha(\hat{x}_n + \hat{x}_n')g_\gamma(y)1_{A_n}(x)1_{B_n}(y)}{\int_{C_n} e^{\mathcal{L}_n(x',y')\alpha}g_\alpha(\hat{x}_n + \hat{x}_n')g_\gamma(y')dx'dy'} \]

with \( \mathcal{L}_n(x,y) = \ell_n(\hat{\alpha}_n + \hat{x}_n, y - \hat{\alpha}_n - \hat{x}_n) \). Here we note that on an event of probability \( 1+o(1) \) we always have \( \hat{\alpha}_n + \hat{x}_n \in (0,1) \) so \( \tilde{g}_n(x, y) \) is well-defined on this event. We assume without loss of generality that \( \tilde{g}_n \) is always well-defined. Then,

\[ R_1 \leq \int_{C_n} \left| 1 - \frac{f(x)h_*(y)e^{\mathcal{L}_n(x',y')\alpha}g_\alpha(\hat{x}_n + \hat{x}_n')g_\gamma(y')dx'dy'}{\phi(A_n)H_*(B_n)} \right| \tilde{g}_n(x, y) \, dx \, dy \]
\[ = \int_{C_n} \left| 1 - \frac{f(x)h_*(y)e^{\mathcal{L}_n(x',y')\alpha}g_\alpha(\hat{x}_n + \hat{x}_n')g_\gamma(y')f(x')h_*(y')dx'dy'}{\phi(A_n)H_*(B_n)\tilde{g}_n(x, y)} \right| \tilde{g}_n(x, y) \, dx \, dy \]
\[ \leq \int_{C_n} \left| 1 - \frac{f(x)h_*(y)e^{\mathcal{L}_n(x',y')\alpha}g_\alpha(\hat{x}_n + \hat{x}_n')g_\gamma(y')f(x')h_*(y')dx'dy'}{\phi(A_n)H_*(B_n)\tilde{g}_n(x, y)} \right| \tilde{g}_n(x, y) \, dx \, dy \]
\[ \leq \sup_{x,x',y,y' \in A_n, B_n} \left| 1 - \frac{f(x)h_*(y)e^{\mathcal{L}_n(x',y')\alpha}g_\alpha(\hat{x}_n + \hat{x}_n')g_\gamma(y')}{f(x')h_*(y')e^{\mathcal{L}_n(x',y')\alpha}g_\alpha(\hat{x}_n + \hat{x}_n')g_\gamma(y')} \right|. \]

Let define \( H(y) = \log \Gamma(1 - \alpha_* + y) - \log \Gamma(y/\alpha_*) + \frac{y}{\alpha_*} \log [\Gamma(1 - \alpha_*)], \) so that \( h_*(y) \propto e^{H(y)}g_\gamma(y) \). Since \( f(x) \propto e^{-x^2/2} \), we obtain from the last display that

\[ R_1 \leq \sup_{x,x',y,y' \in A_n, B_n} \left| 1 - \frac{e^{-\frac{1}{2}x^2 - \mathcal{L}_n(x,y) + H(y)}g_\alpha(\hat{x}_n + \hat{x}_n')}{e^{-\frac{1}{2}(x')^2 - \mathcal{L}_n(x',y') + H(y')}g_\alpha(\hat{x}_n + \hat{x}_n')} \right|. \]
Since \( \sup_{x \in A_n} \hat{x}_n = o_p(1) \), since \( \hat{\alpha}_n = \alpha_* + o_p(1) \), and since \( g_o \) has a continuous and positive density in a neighborhood of \( \alpha_* \), it is enough to establish that there exists a sequence \( (E_n) \) [not depending on \( x \) or \( y \)] such that

\[
\sup_{x \in \mathbb{A}_n, \ y \in B_n} \left| \frac{x^2}{2} + \mathcal{L}_n(x, y) - \mathcal{H}(y) + E_n \right| = o_p(1) \tag{S7.9}
\]

to obtain that \( R_1 = o_p(1) \). We dedicate the rest of this section to prove that equation (S7.9) holds true. First, we note that by Stirling’s formula [see also the computations above the equation (S7.6)]

\[
\sup_{x \in \mathbb{A}_n, \ y \in B_n} \left| \mathcal{L}_n(x, y) - \Psi_n(\hat{\alpha}_n + \hat{x}_n, y - \hat{\alpha}_n - \hat{x}_n) - \log \frac{\Gamma(K_n)}{\Gamma(n)} + \log(\hat{\alpha}_n) - \ell_n(\hat{\alpha}_n + \hat{x}_n, 0) \right| = o_p(1).
\]

Also,

\[
\Psi_n(\hat{\alpha}_n + \hat{x}_n, y - \hat{\alpha}_n - \hat{x}_n) - \mathcal{H}(y) = \log \Gamma(y - \hat{\alpha}_n - \hat{x}_n + 1) - \log \Gamma(y - \alpha_* + 1)
- \log \Gamma\left(\frac{y}{\hat{\alpha}_n + \hat{x}_n}\right) + \log \Gamma\left(\frac{y}{\alpha_*}\right)
+ \frac{y - \hat{\alpha}_n - \hat{x}_n}{\hat{\alpha}_n + \hat{x}_n} \log \frac{K_n}{n^{\hat{\alpha}_n + \hat{x}_n}} - \frac{y}{\alpha_*} \log \Gamma(1 - \alpha_*).
\]

Since \( \sup_{x \in \mathbb{A}_n} \log(n)\hat{x}_n = o_p(1) \), \( \log(n)\|\hat{\alpha}_n - \alpha_*\| = o_p(1) \) by Theorem 1, and \( K_n/n^{\alpha_*} = L\Gamma(1 - \alpha_*) + o_p(1) \) [see for instance the proof of Theorem 1], if the sequence \( (r_n) \) increases slowly enough, it must be that

\[
\sup_{x \in \mathbb{A}_n, \ y \in B_n} \left| \frac{y}{\hat{\alpha}_n + \hat{x}_n} \log \frac{K_n}{n^{\hat{\alpha}_n + \hat{x}_n}} - \frac{y}{\alpha_*} \log \Gamma(1 - \alpha_*) \right| = o_p(1).
\]

Next, \( \hat{\alpha}_n + \hat{x}_n \) are in a small neighborhood of \( \alpha_* \) with probability \( 1 + o(1) \) and \( y - \alpha_* \) is bounded away from 1 for all \( y > 0 \). Hence, by a suitable Taylor expansion

\[
\sup_{x \in \mathbb{A}_n, \ y \in B_n} \left| \log \Gamma(y - \hat{\alpha}_n - \hat{x}_n + 1) - \log \Gamma(y - \alpha_* + 1) \right|
\leq \sup_{x \in \mathbb{A}_n} \sup_{|\delta| \leq \|\hat{\alpha}_n + \hat{x}_n - \alpha_*\|} \left| \psi(y - \alpha_* + 1 + \delta)(\hat{\alpha}_n + \hat{x}_n - \alpha_*\right| = o_p(1)
\]

because \( y - \alpha_* + 1 + \delta \) remains bounded away from zero and is never more than \( \lesssim r_n \), so the last display is indeed a \( o_p(1) \) is the sequence \( (r_n) \) grows slowly enough [recall \( \psi(z) \sim \log(z) \) as \( z \to \infty \) and \( \psi(z) \sim -1/z \) as \( z \to 0 \)]. With a similar reasoning, there is \( u \) between \( y/(\hat{\alpha}_n + \hat{x}_n) \) and \( y/\alpha_* \) such that

\[
\log \Gamma\left(\frac{y}{\hat{\alpha}_n + \hat{x}_n}\right) - \log \Gamma\left(\frac{y}{\alpha_*}\right) = \psi(u) \left[ \frac{y}{\hat{\alpha}_n + \hat{x}_n} - \frac{y}{\alpha_*}\right]
\]
and thus provided \((r_n)\) grows slowly enough

\[
\sup_{x \in A_n, y \in B_n} \left| \log \Gamma \left( \frac{y}{\alpha_n + x_n} \right) - \log \Gamma \left( \frac{y}{\alpha_*} \right) \right| = o_p(1).
\]

Finally, \(\hat{\alpha}_n^0\) is the maximizer of \(\ell_n(\cdot, 0)\), so there is \(\bar{\alpha}\) in a neighborhood of \(\hat{\alpha}_n^0\) [hence in a neighborhood of \(\hat{\alpha}_n\) and \(\alpha_*\) too] such that

\[
\ell_n(\hat{\alpha}_n + \hat{x}_n, 0) = \ell_n(\hat{\alpha}_n^0, 0) + \frac{1}{2} \partial^2 \ell_n(\hat{\alpha}_n^0, 0)(\hat{\alpha}_n - \hat{\alpha}_n^0 + \hat{x}_n)^2 + \frac{1}{6} \partial^3 \ell_n(\hat{\alpha}_n^0, 0)(\hat{\alpha}_n - \hat{\alpha}_n^0 + \hat{x}_n)^3.
\]

Thus, by Theorem 1, by definition of \(\bar{V}_n\), and because \(\partial^2 \ell_n(\hat{\alpha}_n^0, 0) = O_p(n^{\alpha_*})\) and \(\partial^3 \ell_n(\hat{\alpha}_n^0, 0) = O_p(n^{\alpha_*})\) (this follows by direct computations, see for instance in Favaro and Naulet [2021]), it follows

\[
\sup_{x \in A_n, y \in B_n} \left| \ell_n(\hat{\alpha}_n + \hat{x}_n, 0) - \ell_n(\hat{\alpha}_n^0, 0) + \frac{x^2}{2} \right| = o_p(1).
\]

Combining all the estimates, we have shown that if \((r_n)\) grows slowly enough, then equation (S7.9) is proved with

\[
E_n = \log(\hat{\alpha}_n) - \ell_n(\hat{\alpha}_n^0, 0) - \log \frac{\Gamma(K_n)}{\Gamma(n)} + \log \frac{K_n}{n^{\alpha_*}}.
\]

**Bound on \(R_2\).**

To prove that \(R_2 = o_p(1)\) it is enough to show that \(G(Z_n, \alpha \notin A_n \mid \Pi_n) = o_p(1)\) and \(G(\gamma \notin B_n \mid \Pi_n) = o_p(1)\). We have to be careful enough to ensure that these results hold for any slowly increasing sequence \((r_n)\). First, following the same steps as in the proofs of Proposition 7 and 9, for every \(c > 0\) we can choose \(C > 0\) such that

\[
\sup_{\gamma > 0} \left\{ \ell_n(\alpha, \gamma - \alpha) - \sup_{\gamma > 0} \ell_n \right\} \leq -c \log(n).
\]

We deduce that (with \(\hat{\gamma}_n = \hat{\theta}_n + \hat{\alpha}_n\))

\[
G(Z_n, \alpha \notin A_n \mid \Pi_n) = \frac{\iiint 1_{V_n(a - \hat{\alpha}_n)^2 > C \log(n)} e^{\ell_n(a, \gamma - \alpha) - \sup_{\gamma > 0} \ell_n} G_\alpha(da) G_\gamma(d\gamma)}{\iiint e^{\ell_n(a, \gamma - \alpha) - \sup_{\gamma > 0} \ell_n} G_\alpha(da) G_\gamma(d\gamma)} \leq n^{-c} \left( \iiint 1_{V_n(a - \hat{\alpha}_n)^2 \leq 1, |\gamma - \hat{\gamma}_n| \leq 1} e^{\ell_n(a, \gamma - \alpha) - \sup_{\gamma > 0} \ell_n} G_\alpha(da) G_\gamma(d\gamma) \right)^{-1} \leq G_\alpha(V_n(a - \hat{\alpha}_n)^2 \leq 1) G_\gamma((\gamma - \hat{\gamma}_n)^2 \leq 1) \, n^{-C}.
\]
where the last line follows by a trivial extension of the arguments in the proof of Proposition 3. Next, $G_\alpha$ has a positive density in a neighborhood of $\alpha_*$ and $\hat{\alpha}_n = \alpha_* + o_p(1)$ by Theorem 1; and similarly $G_\gamma$ has a positive density in a neighborhood of $\gamma_* = \theta_* + \alpha_*$ and $\hat{\gamma}_n = \gamma_* + o_p(1)$.

By standard arguments and by taking $c$ sufficiently large, we find that

$$G(Z_{n, \alpha} \notin A_n | \Pi_n) = o_p(1).$$

We now prove that $G(\gamma \notin B_n | \Pi_n) = o_p(1)$. In fact, in view of the previous, it is enough to consider $G(Z_{n, \alpha} \in A_n, \gamma \notin B_n | \Pi_n)$. We start with a rough concentration result. We let $D_n = \{ \gamma > 0 : n^{-a} \leq \gamma \leq a \log(n) \}$ for an arbitrarily large constant $a > 0$. Then, in view of Proposition 7, for every $c > 0$ we can choose $a$ such that

$$\sup_{Z_{n, \alpha} \in A_n, \gamma \notin D_n} \{ \ell_n(\alpha, \gamma - \alpha) - \sup \ell_n \} \leq -c \log(n).$$

Hence, with the same reasoning as before, we deduce that $G(Z_{n, \alpha} \in A_n, \gamma \notin D_n | \Pi_n) = o_p(1)$. It is now enough to consider $G(Z_{n, \alpha} \in A_n, \gamma \in B_n^c \cap D_n | \Pi_n)$. Consider the function $f_\gamma(\alpha) = \ell_n(\alpha, \gamma - \alpha) + \log(\alpha) - \ell_n(\alpha, 0)$. By a Taylor expansion, for all $\alpha \in (0, 1)$ there exists $\bar{\alpha}$ between $\alpha$ and $\hat{\alpha}_n^0$ such that for all $\gamma > 0$

$$f_\gamma(\alpha) - f_\gamma(\hat{\alpha}_n^0) = f'_\gamma(\bar{\alpha})(\alpha - \hat{\alpha}_n^0) = \frac{f'_\gamma(\bar{\alpha})Z_{n, \alpha}}{\bar{\gamma}^{1/2}} + f_\gamma(\bar{\alpha})(\hat{\alpha}_n - \hat{\alpha}_n^0).$$

Observe that,

$$f'_\gamma(\alpha) = -\psi(\gamma + 1 - \alpha) + \frac{\gamma \psi(\gamma/\alpha)}{\alpha^2} - \frac{\gamma \psi(\gamma/\alpha + K_n - 1)}{\alpha^2} + \psi(\gamma - \alpha + n).$$

By classical properties of the digamma function $\gamma \psi(\gamma/\alpha) \to \alpha$ as $\gamma \to 0$ and $\psi(z) \sim \log(z)$ as $z \to \infty$ [Olver et al., 2010]. Furthermore $\hat{\alpha}_n - \hat{\alpha}_n^0 = O_p[n^{-a} \cdot \log(n)]$ by Theorem 1, so we deduce that

$$\sup_{Z_{n, \alpha} \in A_n, \gamma \in D_n} |f_\gamma(\alpha) - f_\gamma(\hat{\alpha}_n^0)| = o_p(1).$$

Since $\log(\alpha/\hat{\alpha}_n^0) = o_p(1)$ uniformly over $Z_{n, \alpha} \in A_n$, we have shown that

$$\sup_{Z_{n, \alpha} \in A_n, \gamma \in D_n} |\ell_n(\alpha, \gamma - \alpha) - \ell_n(\hat{\alpha}_n^0, \gamma - \hat{\alpha}_n^0) - \{ \ell_n(\alpha, 0) - \ell_n(\hat{\alpha}_n^0, 0) \}| = o_p(1).$$

It follows that

$$G(Z_{n, \alpha} \in A_n, \gamma \in B_n^c \cap D_n | \Pi_n)$$

$$= \int \int 1_{A_n}(Z_{n, \alpha})1_{B_n^c \cap D_n}(\gamma)e^{\ell_n(\alpha, \gamma - \alpha)}G_\alpha(\alpha)G_\gamma(\gamma)$$

$$\int \int e^{\ell_n(\alpha, \gamma - \alpha)}G_\alpha(\alpha)G_\gamma(\gamma).$$
\[
\frac{\int 1_{A_n}(Z_n, \alpha) \mathbf{1}_{B_n^c \cap D_n}(\gamma) e^{t_n(\alpha, \gamma - \alpha)} G_\alpha(d\alpha) G_\gamma(d\gamma)}{\int 1_{A_n}(Z_n, \alpha) \mathbf{1}_{D_n}(\gamma) e^{t_n(\alpha, \gamma - \alpha)} G_\alpha(d\alpha) G_\gamma(d\gamma)}
= \frac{(1 + o_p(1)) \int_{\{Z_n, \alpha \in A_n\}} e^{t_n(\alpha, 0) - t_n(\alpha_n^0, 0)} G_\alpha(d\alpha) \int_{B_n^c \cap D_n} e^{t_n(\alpha_n^0, \gamma - \alpha_n^0)} G_\gamma(d\gamma)}{\int_{\{Z_n, \alpha \in A_n\}} e^{t_n(\alpha, 0) - t_n(\alpha_n^0, 0)} G_\alpha(d\alpha) \int_{D_n} e^{t_n(\alpha_n^0, \gamma - \alpha_n^0)} G_\gamma(d\gamma)}
= (1 + o_p(1)) \frac{\int_{B_n^c \cap D_n} e^{t_n(\alpha_n^0, \gamma - \alpha_n^0)} G_\gamma(d\gamma)}{\int_{D_n} e^{t_n(\alpha_n^0, \gamma - \alpha_n^0)} G_\gamma(d\gamma)}.
\]

Thus,

\[G(Z_n, \alpha \in A_n, \gamma \in B_n^c \cap D_n \mid \Pi_n) \leq (1 + o_p(1)) \frac{\int_{B_n^c \cap D_n} e^{t_n(\alpha_n^0, \gamma - \alpha_n^0)} G_\gamma(d\gamma)}{\int_{\gamma - \hat{\gamma}_n \leq 1} e^{t_n(\alpha_n^0, \gamma - \alpha_n^0)} - \sup G_\gamma(d\gamma)} \leq 1.
\]

By the arguments in Proposition 3, the denominator in the previous expression is always greater than a constant with probability \(1 + o(1)\), while the numerator goes to zero because by the same arguments that we used for instance in the proof of Proposition 9. In summary, we have shown that for every sequence \((r_n)\) going to infinity

\[G(\gamma \notin B_n \mid \Pi_n) = o_p(1).
\]

**Bound on \(R_3\).**

It is enough to show that \(\phi(A_n^c) = o_p(1)\) and \(H_*(B_n^c) = o_p(1)\). Both facts are immediate.

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