Flexible Martingale Priors for Deep Hierarchies

Jacob Steinhardt Massachusetts Institute of Technology

Abstract

We present an infinitely exchangeable prior over discrete tree structures that allows the depth of the tree to grow with the data. We show that the depth of the tree under the prior increases with the amount of data, which distinguishes it from any existing model; we then implement the model for a hierarchical beta process. We also show that deep hierarchical models are in general intimately tied to a process called a *martingale*, and use Doob's martingale convergence theorem to demonstrate some unexpected properties of deep hierarchies.

1 Introduction

One of the most fundamental questions we face in machine learning is what structure we should use to interpret our data. Hierarchical modeling provides one answer to this question — by modeling data at multiple layers of abstraction, we can capture broad trends over the entire data set while also taking advantage of more specific patterns that only occur over small portions of the data. A hierarchical structure over a data set can thus provide a very powerful way of sharing statistical strength over different parts of the data. However, in most cases the hierarchical structure is not known in advance and must instead be learned. There are many heuristics for finding such structure, typically by iteratively merging together subtrees that are similar under some suitable metric (Duda et al., 2000; Heller and Ghahramani, 2005; Blundell et al., 2010). From a statistical perspective, these approaches are troublesome — there is no principled or consistent way to add new data to the tree, and it is unclear how to compare two different trees over the same data set if they have different numbers of internal nodes. Such heuristics

Zoubin Ghahramani University of Cambridge

also limit the potential scope of the model — for instance, it is not clear how to deal with hierarchies over latent parameters or with missing data. It is also unclear how to reconcile an ad hoc clustering algorithm with the eventual statistical model to be placed on the data.

The Bayesian solution to these problems is to specify a probability distribution over tree structures. In this way a hierarchical model has two components — a *prior* over the possible tree structures, including where the data lie in the tree, and a *likelihood* that specifies a distribution over latent parameters, and how those parameters affect the data. The task then is to find a suitable prior for trees. There are four general proposals for such a prior — Kingman coalescents (Kingman, 1982; Pitman, 1999; Teh et al., 2007), Dirichlet diffusion trees (Neal, 2003; Knowles and Ghahramani, 2011), tree-structured stick breaking (Adams et al., 2010), and nested Chinese restaurant processes (Blei et al., 2010).

Kingman coalescents and Dirichlet diffusion trees are both inherently continuous models, with paths either splitting or merging according to some arrival process, and the data corresponding to the final state of a diffusion process. In addition to being infinitely exchangeable, these models have the nice property that the complexity of the implied tree structure can grow to accomodate increasing amounts of data. Unfortunately, to use these models, one needs a time-indexed stochastic process (such as a Wiener process) to underlie the data. There is thus a distinction between discrete tree structures, where any likelihood may underlie the data, and continuous structures such as Dirichlet diffusion trees, where the likelihood must correspond to some continuous process. In some important cases, such as a hierarchical beta process (Thibaux and Jordan, 2007), no underlying continuous process is known to exist.

It is therefore important to also consider inherently discrete distributions over trees. This is the approach of tree-structured stick breaking (TSSB) as well as nested Chinese restaurant processes (nCRP). In both of these cases, the tree is fixed to be countably deep,

Preliminary work. Under review by AISTATS 2012. Do not distribute.

with every node having countably many children. The interesting structure then emerges in the locations of the data.

In TSSB a stick-breaking procedure is used to assign a probability distribution over nodes: the root node is given a constant portion of the probability mass (drawn from a beta distribution), and the rest of the mass is partitioned among subtrees of the root using a Dirichlet process (Teh et al., 2004). The mass in each subtree is then recursively divided in the same way. Finally, data are distributed throughout the tree according to the resulting probability distribution. While this model is infinitely exchangeable, the depth of the tree is fixed by the prior — all data occur with high probability at some finite collection of depths that does not increase with the size of the data. This constitutes an important way in which the complexity of the tree is unable to grow to accomodate the data.

Kingman coalescents, Dirichlet diffusion trees, and TSSB all separate out the prior over trees from the likelihood for the latent parameters and the data. The nCRP departs from this pattern. It associates each data point with a path down the tree: there is then an implicit tree structure based on where the different paths branch. Because the paths are infinitely long, care must be taken in choosing the likelihood to make sure that the model is well-defined. In (Blei et al., 2010), the likelihood is obtained by using a Dirichlet process (DP) to form a mixture over distributions given at each of the nodes in the path. This likelihood has the important property that the mass that the DP places on a tail of the path decays to zero; otherwise, the resulting mixture distribution would not be welldefined.

The nCRP makes the elegant decision to associate data with paths rather than nodes. By doing so, the depth of the CRP can grow to accomodate new data. The nCRP is therefore the only prior over trees that is fully Bayesian, infinitely exchangeable, grows to accomodate new data, and can handle inherently discrete processes. However, these properties come at a cost. Because of the convergence issues arising from the infinite paths, it is unclear how to construct a conditional distribution for a data point given its path, except by a model similar to (Blei et al., 2010), which in many cases does not accurately represent prior beliefs about the data.

The main contribution of this paper is to give a general approach for constructing likelihoods for the nCRP, or any similar path-based model. Our construction is universal for all path-based models (Theorem 2.3), and works by taking limits of latent parameters along paths down the tree, and using Doob's martingale convergence theorem to show that the limits exist with probability 1. We use this fact to construct a fully Bayesian hierarchical prior for both Dirichlet processes (Teh et al., 2004) and beta processes (Thibaux and Jordan, 2007). To show that inference is tractable in our model, we implement it for a hierarchical beta process (HBP).

It turns out that many existing hierarchical models already mimic our construction, except with finite rather than infinite trees. A second contribution of our paper is to use Doob's theorem to analyze the properties of these models for deep hierarchies. This analysis yields some surprising results about hierarchical models with an underlying gamma distribution, which includes both HBPs and HDPs (hierarchical Dirichlet processes).

The rest of the paper is organized as follows. In Section 2, we describe our construction, introduce Doob's theorem, and use it to analyze several examples of deep hierarchies, as well as to show that our proposed construction is both well-defined and universal. In Section 3, we derive the exact asymptotics of the depth of an nCRP as a function of the data size. Finally, in Section 4, we apply our model to a hierarchical beta process and use it to perform hierarchical clustering on a simple data set.

2 Model Description and Properties

In this section, we will present a general construction for hierarchical models that associate data with paths in the tree. For concreteness, we will use the nCRP as the prior over tree structures. We start with an informal description of the elements of our model, then formally state our model and show that it is well-defined. First, though, we need a bit of notation. Given a tree \mathcal{T} and a vertex $v \in \mathcal{T}$, let p(v) denote the parent of vand $\mathcal{A}(v)$ denote the ancestors of v. Also, let $\text{Root}(\mathcal{T})$ denote the root of \mathcal{T} , Subtree(v) denote the subtree of \mathcal{T} rooted at v, and Depth(v) denote the depth of v(with $\text{Depth}(\text{Root}(\mathcal{T})) = 0$).

2.1 Model Overview

We imagine that an infinite tree \mathcal{T} underlies our data. Eventually, each datum will be associated with an infinite path down the tree, and be defined in terms of a limiting process of the latent parameters. We ignore this aspect of the model for now, and merely assume that at each node v in the tree there is an associated latent parameter θ_v . Moreover, in order to even say that the tree underlies the data, we should assume that θ_v depends only on its ancestors $\mathcal{A}(v)$; more formally, we assume that $p(\{\theta_v\}_{v\in\mathcal{T}})$ factors as $\prod_{v \in \mathcal{T}} p(\theta_v \mid \theta_{\mathcal{A}(v)}).$ Note that p does not depend on v; this reflects the philosophy that the latent parameters, and not just the data itself, should satisfy an exchangeability property. We call models with this stronger property **completely exchangeable**.

By replacing θ_v with $\theta_{v \cup \mathcal{A}(v)}$ (i.e. by concatenating all the parameters on the path from $\text{Root}(\mathcal{T})$ to v), we can always obtain a model where θ_v depends only on its parent. In other words, the density can be assumed to factor as

$$p\left(\{\theta_v\}_{v\in\mathcal{T}}\right) = \prod_{v\in\mathcal{T}} p(\theta_v \mid \theta_{p(v)}).$$
(1)

We will therefore focus on this class of models for the remainder of the discussion, keeping in mind that we lose no generality in doing so.

It is often the case in models of the form given in (1) that some key quantity $f(\theta_v)$ is preserved in expectation as we walk down the tree – more formally,

$$\mathbb{E}[f(\theta_v) \mid \theta_{p(v)}] = f(\theta_{p(v)}). \tag{2}$$

For instance, in a hierarchical Dirichlet process, θ_v is a probability distribution over the space of possible data, and $\theta_v \mid \theta_{p(v)} \sim \text{DP}(c\theta_{p(v)})$ for some concentration parameter c, where $DP(\mu)$ is a Dirichlet process with base measure μ . In this case, $\mathbb{E}[\theta_v \mid \theta_{p(v)}] = \theta_{p(v)}$; that is, we can take $f(\theta) = \theta$.

If f satisfies (2), then f is said to be a **martingale**. The martingale property will be of importance in the sequel. It turns out that data living infinitely deep in the tree will have a well-defined distribution if they depend on a countable collection of L^1 -bounded martingales.

2.2 Formal Description

We now formally define our model. We have a tree \mathcal{T} of countable depth, such that every node v has a countable collection of children $\mathcal{C}(v)$. For each $v \in \mathcal{T}$ we have parameters θ_v (a latent parameter governing data in that subtree) and π_v (a probability distribution over $\mathcal{C}(v)$). For each datum X, we have an associated path $\{v_n(X)\}_{n=0}^{\infty}$ such that $v_0(X) = \operatorname{Root}(\mathcal{T})$ and the parent of $v_{n+1}(X)$ is $v_n(X)$. We also have a conditional distribution $G(\theta)$ representing $p(\theta_v \mid \theta_{p(v)})$ and a conditional distribution $H(\theta)$ representing $p(X \mid \theta)$ (this is elaborated on below). Finally, we have a single hyperparameter γ that roughly controls the branching factor of the tree.

The generative process for our model is as follows:

1.
$$\pi_v \sim \text{DP}(\mathcal{C}(v), \gamma)$$

2. $\theta_v \mid \theta_{p(v)} \sim G(\theta_{p(v)})$

For each X:

1.
$$v_0(X) = \operatorname{Root}(\mathcal{T})$$

2. $v_{n+1}(X) \mid v_n(X), \pi_{v_n(X)} \sim \operatorname{Multinomial}(\pi_{v_n(X)})$
3. $X \mid \{v_n(X)\}_{n=0}^{\infty} \sim H\left(\lim_{n \to \infty} f(\theta_{v_n(X)})\right)$

Thus a datum X is obtained by first sampling a path down the tree \mathcal{T} (using the distributions $\{\pi_v\}_{v\in\mathcal{T}}$ to choose which edge to follow at each point), then taking a limit of latent parameters along that path, and finally sampling X from a distribution indexed by that limit. (The skeptical reader may wonder whether the limit in the last step exists. This is established later, in Theorem 2.2.)

In the sequel, we will omit the dependence of v_n on Xwhen it is clear from context. We will also sometimes refer to θ_n and π_n instead of θ_{v_n} and π_{v_n} . Finally, we will abuse notation and say that $X \in \text{Subtree}(v)$ if $v_n(X) = v$ for some n.

2.3 Doob's Theorem

The potential problem with the procedure specified above is that $\lim_{n\to\infty} f\left(\theta_{v_n(X)}\right)$ need not exist. This issue is alleviated by the following theorem (Lamb, 1973):

Theorem 2.1 (Doob's martingale convergence theorem). Let $\{\theta_n\}_{n=0}^{\infty}$ be a Markov chain over a space Θ and let $f : \Theta \to \mathbb{R}$. Suppose that $\mathbb{E}[f(\theta_{n+1}) | \theta_n] = f(\theta_n)$ for each n. Furthermore, suppose that $\sup_n \mathbb{E}[|f(\theta_n)|] < \infty$. Then $\lim_{n\to\infty} f(\theta_n)$ exists with probability 1.

Before exploring the consequences of Theorem 2.1 for the model proposed in Section 2.2, we go over some examples of Doob's theorem applied to sequences of random variables.

Example 1: Suppose that $\theta_0 \sim \text{Beta}(1,1)$ and that $\theta_{n+1} \mid \theta_n \sim \text{Beta}(c\theta_n, c(1-\theta_n))$ for $n \geq 0$. If $f(\theta) = \theta$, then $\mathbb{E}[f(\theta_{n+1}) \mid \theta_n] = \mathbb{E}[\theta_{n+1} \mid \theta_n] = \mathbb{E}[\text{Beta}(c\theta_n, c(1-\theta_n))] = \theta_n$.¹ Furthermore, $0 \leq \theta_n \leq 1$, so $\sup_n \mathbb{E}[|f(\theta_n)|] \leq 1 < \infty$. Consequently, $\lim_{n \to \infty} \theta_n$ exists with probability 1.

In fact, the variance of $\text{Beta}(c\theta, c(1-\theta))$ is $\frac{\theta(1-\theta)}{c+1}$. Since this variance must converge to 0 in the limit (as

For each v:

¹We abuse notation here, using $\mathbb{E}[\text{Beta}(\alpha, \beta)]$ to refer to the expectation of a random variable who distribution is $\text{Beta}(\alpha, \beta)$. We will continue to use such notation throughout the paper.



Figure 1: Examples of Doob's martingale convergence theorem in action. Left: sequences of beta random variables from Example 1, with c = 50. Center: sequences of gamma random variables from Example 2, with $\lambda = 50$. Right: $\frac{\alpha}{\alpha+\beta}$ from Example 3.

otherwise $\lim_{n \to \infty} \theta_n$ would not exist), we can conclude that $\lim_{n\to\infty} \theta_n \in \{0,1\}$ with probability 1. Figure 1 illustrates this behavior.

Example 2: Suppose that $c_0 \sim \text{Gamma}(1, \lambda)$ and that $c_{n+1} \mid c_n \sim \text{Gamma}(c_n, 1)$. Then $\mathbb{E}[c_{n+1} \mid$ c_n] = c_n . Since $c_{n+1} \ge 0$, we also have $\mathbb{E}[|c_{n+1}|]$ c_n] = c_n . Consequently, $\sup_n \mathbb{E}[|c_n|] = \sup_n \mathbb{E}[c_0] =$ $\lambda < \infty$. Thus $\lim_{n \to \infty} c_n$ exists with probability 1. Since the variance of $\text{Gamma}(c_n, 1)$ is c_n , we see that $\lim_{n\to\infty} c_n = 0$ with probability 1. Note that this means that the process of iteratively sampling a gamma-distributed random variable with the mean of the previous one will always converge to 0 in the limit, which has interesting consequences for sequences of random variables based on a gamma variate; these include HBPs, hierarchical Dirichlet processes, and hierarchical gamma processes (Thibaux, 2008) as existing examples; one could also imagine an inverse-Wishart time series. The behavior of the sequence c_n is also illustrated in Figure 1.

Example 3: We now give an example of a martingale where f is not the identity function. Let $\alpha_0 \sim \text{Gamma}(1,1), \ \beta_0 \sim \text{Gamma}(1,1), \ d_n \mid \alpha_n \sim$ $\text{Gamma}(\alpha_n, 1), \ e_n \mid \beta_n \sim \text{Gamma}(\beta_n, 1), \ \text{and} \ \alpha_{n+1} =$ $\alpha_n + d_n, \beta_{n+1} = \beta_n + e_n$. Note that the sequences α_n and β_n are certainly not martingales. Indeed, since $\mathbb{E}[\alpha_{n+1} \mid \alpha_n] = \alpha_n + \mathbb{E}[\text{Gamma}(\alpha_n, 1)] = 2\alpha_n,$ and similarly for β_{n+1} , the sequences α_n and β_n both increase exponentially in expectation. However, if we let $f(\alpha_n, \beta_n) = \frac{\alpha_n}{\alpha_n + \beta_n}$, then (see Appendix B) $\mathbb{E}[f(\alpha_{n+1}, \beta_{n+1}) \mid \alpha_n, \beta_n] = \frac{\alpha_n}{\alpha_n + \beta_n}$. Therefore, $\lim_{n \to \infty} \frac{\alpha_n}{\alpha_n + \beta_n}$ exists with probability 1. This is again illustrated in Figure 1.

Example 4: Doob's theorem provides guarantees on the convergence of real-valued sequences satisfying the martingale condition. But there are many cases when we care about more than just a single real number. For instance, in a hierarchical Dirichlet process, we might care about a sequence $\{\mu_n\}_{n=0}^{\infty}$ where $\mu_{n+1} \mid \mu_n \sim \mathrm{DP}(\mu_n)$. Fortunately, we can still use Doob's theorem; since the output of a Dirichlet process consists of countably many atoms, we only need to worry about $\mu_n(\{p\})$ for the countably many points p that are atoms of μ_1 . Since $\mathbb{E}[\mu_{n+1} \mid \mu_n] = \mu_n$, we also have $\mathbb{E}[\mu_{n+1}(\{p\}) \mid \mu_n] = \mu_n(\{p\})$, hence $\lim_{n\to\infty} \mu_n(\{p\})$ exists almost surely for each p. Since there are only countably many such p, we then have that $\lim_{n\to\infty} \mu_n(\{p\})$ exists for all p almost surely. Also, by logic similar to example 1, each $\mu_n(\{p\})$ must converge to either 0 or 1, implying that the measure μ_n converges to a single atom in the infinite limit.²

Example 5: We finally go over an example of a martingale that does *not* converge. Let $x_0 = 0$ and let $x_{n+1} \mid x_n \sim \mathcal{N}(x_n, 1)$. In other words, x_{n+1} is equal to x_n perturbed by Gaussian noise with variance 1. Then $\mathbb{E}[x_{n+1} \mid x_n] = x_n$, so the sequence $\{x_n\}_{n=0}^{\infty}$ is a martingale. However, $\mathbb{E}[|x_n|] = \Theta(\sqrt{n})$, so $\sup_n \mathbb{E}[|x_n|] = \infty$. As a result, Theorem 2.1 does not apply, and indeed, the sequence $\{x_n\}$ clearly does not have a limit.

2.4 Constraints on the Likelihood

We hinted in Section 2.3 that Doob's theorem would give us conditions under which the process in Section 2.2 leads to a well-defined generative distribution. We now formalize this.

Theorem 2.2. Let $\theta_{n+1} \mid \theta_n \sim G(\theta_n)$, and suppose that $\mathbb{E}[f(\theta_{n+1}) \mid \theta_n] = f(\theta_n)$. Further suppose

²This actually requires a bit more of an argument than before, as the μ_n could converge in distribution but not almost surely; for instance we could have $\mu_n = \delta_{p_n}$ for a countable sequence of distinct points p_n , in which case $\lim_{n\to\infty} \mu_n(\{p\})$ would be identically zero for all p, but $\lim_{n\to\infty} \mu_n$ would not converge almost surely to any probability distribution. However, we will ignore these issues for this example.

that f is an at most countable collection $\{f_k\}_{k=1}^{\infty}$ of sufficient statistics for H, and that each f_k satisfies $\sup_n \mathbb{E}[|f_k(\theta_n)|] < \infty$. Then $\lim_{n \to \infty} f(\theta_n)$ exists with probability 1.

Proof. By Doob's theorem, $\lim_{n\to\infty} f_k(\theta_n)$ exists almost surely for each k individually. Since there are only countably many f_k , and the intersection of a countable collection of almost-sure events is still almost-sure, the theorem follows.

We thus end up with two constraints on the likelihood that we need in order to use our model — the martingale condition, and the boundedness of $\mathbb{E}[|f_k(\theta)|]$. Intuitively, we can think of a martingale sequence as revealing gradually more information about a random variable until it is completely determined. From this perspective, the parameter θ_v captures information that is true across all of Subtree(v), with the parameters at descendants containing more precise information about their specific subtrees. However, Example 5 shows that this intuition is not perfect, which is why we need the boundedness condition as well.

We next give a converse to Theorem 2.2, proved in Appendix A, showing that the martingale and boundedness conditions are both necessary:

Theorem 2.3. Consider any completely exchangeable model that associates a datum X with a path $\{v_n(X)\}_{n=0}^{\infty}$ down a tree \mathcal{T} , and that draws X from some distribution $p(X \mid \{v_n(X)\}_{n=0}^{\infty})$. Let θ_v be the de Finetti mixing distribution for $p(X \mid X \in \text{Subtree}(v))$. Then $\mathbb{E}[\theta_v \mid \theta_{p(v)}] = \theta_v$, and $\sup_n \mathbb{E}[|[\theta_n(X)](S)|] < \infty$ for all measurable sets S. If X lies in a Polish space³, then θ is determined by the value of $\{\theta(S)\}_{S \in \mathcal{C}}$ for a countable collection of sets C, and X $\mid \{v_n(X)\}_{n=0}^{\infty} \sim$ $\lim_{n \to \infty} \theta_n$, where the limit is in the topology of weak convergence.

Finally, we note that the conditions of Theorem 2.2 hold for any countable-dimensional martingale that is bounded either above or below (see Example 2 of Section 2.3). In particular, letting $f(\theta) = \theta$, they hold for hierarchical Dirichlet processes $(G(\theta) = \text{DP}(c\theta))$, hierarchical beta processes $(G(\theta) = \text{BP}(\theta, c))$, and hierarchical gamma processes $(G(\theta) = \text{GammaP}(\theta))$, since these are all non-negative and depend on only a countable collection of atoms.

3 Depth of an nCRP

The key property of an nCRP that makes it desirable over tree-structured stick breaking is the depth of the resulting tree. Note that in an nCRP, every data point is associated with an infinite path, and thus lies infinitely deep in the tree. However, we can talk about the *effective depth* of a data point as the smallest depth at which that point is the unique datum in its subtree.

Proposition 3.1. The effective depth of a data point is $\Theta_N\left(\frac{\log(N)}{\xi+\psi(1+\gamma)}\right)$ with high probability, where ξ is the Euler-Mascheroni constant and ψ is the digamma function.

To prove Proposition 3.1, we first need a basic lemma about Dirichlet processes:

Lemma 3.2. The posterior distribution of $\pi_{v_n}(v_{n+1}) \mid X \in \text{Subtree}(v_{n+1})$ is equal to $\text{Beta}(1, \gamma)$. In other words, the mass assigned to a child conditioned on a single datum having already been assigned to that child is distributed as $\text{Beta}(1, \gamma)$.

Proof. Note that $DP(\gamma)$ is actually obtained by drawing a sample from $DP(\gamma U)$, where U is uniform on [0, 1], and assigning the masses of the atoms to the children of v. Therefore, if we let $\mu \sim DP(\gamma U)$ and $q \sim \text{Multinomial}(\mu)$, then the posterior distribution of $\pi_{v_n}(v_{n+1})$ is equivalent to the distribution of $\mu(\{p\}) \mid q = p$. By conjugacy, $\mu \mid q = p \sim DP(\delta_p + \gamma U)$. Then, by the defining property of a Dirichlet process, $(\mu(\{p\}), \mu([0, 1] \setminus \{p\})) \sim \text{Dirichlet}(1, \gamma)$, hence $\mu(\{p\}) \sim \text{Beta}(1, \gamma)$.

Now we are ready to prove Proposition 3.1.

Proof of Proposition 3.1. Let X be a data point. The probability that $\operatorname{Depth}(X) \leq d$ is the probability that none of the other N-1 data points lie in $\operatorname{Subtree}(v_d(X))$, which is equal to $\left(1 - \prod_{i=0}^{d-1} \pi_{v_i}(v_{i+1}(X))\right)^{N-1}$. But $\prod_{i=0}^{d-1} \pi_{v_i}(v_{i+1}) = e^{\sum_{i=0}^{d-1} \log \pi_{v_i}(v_{i+1})}$. The $\log \pi_{v_i}(v_{i+1})$ are independent, and by Lemma 3.2 they are $\log \operatorname{Beta}(1, \gamma)$ -distributed. Since $\log \operatorname{Beta}(1, \gamma)$ has finite variance, it follows that $\sum_{i=0}^{d-1} \log \pi_{v_i}(v_{i+1}) = d\mathbb{E}[\log \operatorname{Beta}(1, \gamma)] + O(\sqrt{d})$ with high probability. One can show (see Appendix B) that $\mathbb{E}[\log \operatorname{Beta}(1, \gamma)] = \psi(1) - \psi(1 + \gamma) = -\xi - \psi(1 + \gamma)$. Then

$$\mathbb{P}[\operatorname{Depth}(X) \le d] = \left(1 - e^{-d(\xi + \psi(1+\gamma)) + O(\sqrt{d})}\right)^{N-1}.$$

If we let $d = \alpha \frac{\log(N)}{\xi + \psi(1+\gamma)}$, then the right-hand-side above becomes $\left(1 - N^{-\alpha + O\left(\frac{1}{\sqrt{\log(N)}}\right)}\right)^{N-1}$, which decays quickly from 1 to 0 as α passes the threshold value of 1. It follows that $\alpha = \Theta_N(1)$ with high prob-

ability, so $d = \Theta_N\left(\frac{\log(N)}{\xi+\psi(1+\gamma)}\right)$ with high probability, which completes the proposition.

³A Polish space is a completely metrizable separable space. All spaces of interest in statistics are Polish.



Figure 2: Trees drawn from the prior of the model with N = 100 data points. At the top is the tree generated by tree-structured stick breaking, and at the bottom is the tree generated by the nCRP. In both cases we used a hyper-parameter of $\gamma = 1$. For the stick breaking model, we further set $\alpha = 10$ and $\lambda = \frac{1}{2}$ (these are parameters that do not exist in our model). Note that the tree generated by TSSB is very wide and shallow. A larger value of α would fix this for N = 100, but increasing N would cause the problem to re-appear.



Figure 3: Tree depth versus number of data points. We drew a single tree from the prior for the nCRP as well as for tree-structured stick-breaking, and computed both the maximum and average depth as more data was added to the tree. The above plots show that the depth of the nCRP increases with the amount of data, whereas the depth of tree-structured stick-breaking (TSSB) quickly converges to a constant. The different curves for the TSSB model correspond to different settings of the hyperparameters α and λ .

In contrast to Proposition 3.1, the depth distribution of a datum is constant in the TSSB model, which leads to overly wide and shallow trees. This is illustrated in Figures 2 and 3, where we show samples from the prior over tree structures for both our model and the treestructured stick breaking model.

The TSSB model uses two extra hyperparameters (α and λ) that do not occur in the nCRP. By setting α to N^{ξ} and λ to $\frac{1}{\psi(1+\gamma)}$, it is possible to approximate the depth distribution of our model with tree-structured stick breaking. However, the models are still qualitatively different. While TSSB can mimic the marginal depth distribution as measured from the root of the entire tree, it cannot mimic the depth distribution as measured from an arbitrary subtree. Separately, setting α to N^{ξ} makes the prior data-dependent, which is problematic in itself.

4 Implementation for a Hierarchical Beta Process

We now show how our construction applies in the case of a hierarchical beta process (Thibaux and Jordan, 2007). Recall that an HBP is a model that generates an exchangeable sequence $\{X_n\}_{n=1}^{\infty}$, where each X_n is a finite collection of features. Typically a beta process is used when the feature set is not known a priori and is potentially infinite (Griffiths and Ghahramani, 2011). For simplicity, however, we will assume that the feature set is both finite and known in advance, so that each X_n can be represented as a binary vector of some length L. Then for each $v, \theta_v \in [0, 1]^L$, and our model is:

- 1. $\theta_{\text{Root}(\mathcal{T}),l} = 0.5$ for all $l \in \{1, ..., L\}$
- 2. $\theta_{v,l} \mid \theta_{p(v),l} \sim \text{Beta}(c\theta_{p(v),l}, c(1-\theta_{p(v),l}))$
- 3. $X_l \mid \{v_n(X), \theta_{n,l}(X)\}_{n=0}^{\infty} \sim \text{Bernoulli}(\theta_l)$, where $\theta_l = \left(\lim_{n \to \infty} \theta_{n,l}\right)$

Due to space constraints, we cannot give a full account of how to perform inference in this model. Our goal in the remainder of this section will be to give a high-level overview, showing in particular how to tractably deal with the infinitely long paths created by the nCRP. A more detailed description of inference is given in Appendices C and D.

Representing the tree The first issue is how to represent the tree. The prior specifies infinitely long paths for each datum, which is problematic for computation. We deal with this using Lemma 4.1, which implies that if a subtree contains only a single datum, then we can analytically marginalize out *all* of the parameters of that subtree:

Lemma 4.1. The marginal distribution of $X_l \mid (X \in \text{Subtree}(v), \theta_{p(v)})$ is equal to $\text{Bernoulli}(\theta_{p(v),l})$. Furthermore, $X \mid (X \in \text{Subtree}(v), \theta_{p(v)})$ is independent of Y for any $Y \notin \text{Subtree}(v)$.

We thus represent \mathcal{T} by a truncated tree \mathcal{T}' as follows: each internal node v of \mathcal{T}' corresponds to a node of \mathcal{T} with a non-empty subtree; v keeps track of its latent parameters θ_v as well as its size. Each leaf w of \mathcal{T}' corresponds to a data point X(w), which implicitly represents an entire subtree of \mathcal{T} that has been marginalized out using Lemma 4.1; w keeps track of just its associated data point. Finally, subtrees with no data are omitted altogether in \mathcal{T}' . As more data is added to a tree, a new datum Y might end up taking a path through X(w). In this case, X(w) is replaced with an internal node that then branches into new leafs containing X and Y (if the paths of X and Y share many vertices, then many new internal nodes will be created).

Incremental Gibbs Sampling Our specific approach to inference is incremental Gibbs sampling, although other MCMC variants could be used as well. There are three types of MCMC moves that we consider: adding a data point, removing a data point, and resampling the latent parameters. We outline each below.

Adding a data point We can add a new data point Y to \mathcal{T}' either by making it the child of an already existing internal node v, or by expanding an external node w. It is straightforward to calculate the conditional probability in the first case, as it is the probability that a datum would take the path to v, times the probability of creating a new table under the CRP at node v, times the probability of generating Y from Subtree(v) (which is given by Lemma 4.1). Expanding an external node is more complicated, as we need to create new internal nodes and sample their parameters conditioned on X(w) and Y. We also need to compute the conditional distribution over how deep X(w) and Y first branch. Both of these calculations can be made, and are given in Appendix C.

Removing a data point This step is trivial. We just need to remove the data point, decrement the sizes of all ancestor nodes, and delete any nodes that now have zero data points in their subtree.

Resampling the parameters An algorithm for resampling the latent parameters of an HBP was first proposed in (Thibaux and Jordan, 2007). Unfortunately, this algorithm is not suited to sampling deep



Figure 4: Part of a sample from the incremental Gibbs sampler for our model applied to a hierarchical beta process. The latent parameters at internal nodes are represented by gray lines with white = 0, black = 1. The nodes with thicker borders represent data. The complete tree is available in the supplementary material.

hierarchies due to general numerical issues with hierarchical Beta processes. The numerical issues occur when we are resampling the parameters of a node and one of the values of the children is very close to 0 or 1. If a child parameter is very close to 0, for instance, it actually matters for the likelihood whether the parameter is equal to 10^{-10} or 10^{-50} (or even 10^{-1000}). Since we cannot actually distinguish between these numbers with floating point arithmetic, this introduces innacuracies in the posterior that push all of the parameters closer to 0.5. To deal with this problem, we assume that we cannot distinguish between numbers that are less than some distance ϵ from 0 or 1. If we see such a number, we treat it as having a censored value (so it appears as $\mathbb{P}[\theta < \epsilon]$ or $\mathbb{P}[\theta > 1 - \epsilon]$ in the likelihood). We then obtain a log-concave conditional density, for which efficient sampling algorithms exist (Leydold, 2003).

Scalability If there are N data points, each with L features, and the tree has depth D, then the time it takes to add a data point is O(NL), the time it takes to remove a data point is O(L+D), and the time it takes to resample a single set of parameters is (amortized) O(L). The dominating operation is adding a node, so to make a Gibbs update for all data points will take total time $O(N^2L)$.

Results To demonstrate inference in our model, we created a data set of 53 stick figures determined by the presence or absence of a set of 29 lines. We then ran incremental Gibbs sampling for 100 iterations with hyperparameters of $\gamma = 1.0$, c = 20.0. The output of the final sample is given in Figure 4.

5 Conclusion

We have presented an exchangeable prior over discrete hierarchies that can flexibly increase its depth to accomodate new data. We have also implemented this prior for a hierarchical beta process. Along the way, we identified a common model property — the martingale property — that has interesting and unexpected consequences in deep hierarchies.

This paper has focused on a general theoretical characterization of infinitely exchangeable distributions over trees based on the Doob martingale convergence theorem, on elucidating properties of deep hierarchical beta processes as an example of such models, and on defining an efficient inference algorithm for such models, which was demonstrated on a small binary data set. A full experimental evaluation of nonparametric Bayesian models for hierarchices is outside the scope of this paper but clearly of interest.

References

- Ryan P. Adams, Zoubin Ghahramani, and Michael I. Jordan. Tree-structured stick breaking for hierarchical data. Advanced in Neural Information Processing Systems, 23, 2010.
- David M. Blei, Thomas L. Griffiths, and Michael I. Jordan. The nested chinese restaurant process and bayesian nonparametric inference of topic hierarchies. *Journal of the ACM*, 57(2), Jan 2010.
- Charles Blundell, Yee Whye Teh, and Katherine A. Heller. Bayesian rose trees. *Uncertainty in Artificial Intelligence*, 2010.
- R O Duda, P E Hart, and D G Stork. *Pattern classification*. Wiley Interscience, 2nd edition, 2000.
- Thomas L. Griffiths and Zoubin Ghahramani. The indian buffet process: An introduction and review. *Journal of Machine Learning Research*, 12:1185– 1224, Apr 2011.
- Katherine Heller and Zoubin Ghahramani. Bayesian hierarchical clustering. International Conference on Machine Learning, 22, 2005.
- John Kingman. The coalescent. Stochastic Processes and their Applications, 13(3):235–248, 1982.
- David Knowles and Zoubin Ghahramani. Pitman-yor diffusion trees. Uncertainty in Artificial Intelligence, 27, 2011.
- Charles W. Lamb. A short proof of the martingale convergence theorem. Proceedings of the American Mathematical Society, 38(1), Mar 1973.
- Josef Leydold. Short universal generators via generalized ratio-of-uniforms method. *Mathematics of Computation*, 72(243):1453–1471, Mar 2003.
- R M Neal. Density modeling and clustering using dirichlet diffusion trees. In *Bayesian Statistics* 7, pages 619–629, 2003.
- Jim Pitman. Coalescents with multiple collisions. Annals of Probability, 27(4):1870–1902, 1999.
- Y W Teh, M I Jordan, M J Beal, and D M Blei. Hierarchical dirichlet processes. Technical Report 653, 2004.
- Yee Whye Teh, Hal Daume III, and Dan M. Roy. Bayesian agglomerative clustering with coalescents. Advances in Neural Information Processing Systems, 2007.
- Romain Thibaux. Nonparametric Bayesian Models for Machine Learning. PhD thesis, University of California, Berkeley, 2008.
- Romain Thibaux and Michael I. Jordan. Hierarchical beta processes and the indian buffet process. *AIS*-*TATS*, 2007.

A Converse to Doob's Theorem

Proof of Theorem 2.3. We prove each of the parts of the theorem:

1. $\mathbb{E}[\theta_v \mid \theta_{p(v)}] = \theta_{p(v)}$: For any measurable set S of possibilities for X, we have

$$\mathbb{E}[\theta_v(S) \mid \theta_{p(v)}] = \mathbb{E}[\mathbb{P}[X \in S \mid X \in \text{Subtree}(v)] \mid \theta_{p(v)}]$$
$$= \mathbb{P}[X \in S \mid X \in \text{Subtree}(p(v))]$$
$$= \theta_v(S).$$

Since this holds for all S, we also have $\mathbb{E}[\theta_v \mid \theta_{p(v)}] = \theta_{p(v)}$.

- 2. $\sup_n \mathbb{E}[|[\theta_n(X)](S)|] < \infty$ for all S: this follows trivially from the fact that $\theta_n(X) \in [0, 1]$.
- 3. If X lies in a Polish space \mathcal{P} , then θ is determined by its value on a countable collection of sets: If \mathcal{P} is Polish, then the space \mathcal{D} of probability measures on \mathcal{P} is also Polish in the topology generated by sets of the form $U_{S,a,b} := \{\mu \mid a < \mu(S) < b\}$. In particular, since \mathcal{D} is a separable metric space, it is second-countable, and so its topology is generated by a countable subcollection \mathcal{C}_0 of the $U_{S,a,b}$. We then claim that $\mathcal{C} := \{S \mid U_{S,a,b} \in \mathcal{C}_0 \text{ for some } a, b\}$ is the desired collection for determining θ . Indeed, suppose that $\theta' \neq \theta \in \mathcal{D}$. Since \mathcal{D} is Hausdorff, there exists some $U_{S,a,b} \in \mathcal{C}_0$ with $\theta \in U_{S,a,b}$ and $\theta' \notin U_{S,a,b}$, which in particular implies that $\theta(S) \neq \theta'(S)$.
- 4. $\lim_{n\to\infty} \theta_n = \theta$ in the topology of weak convergence: Note that $\theta_n(S) = \mathbb{E}[\mathbb{P}[X \in S] \mid v_0, v_1, \ldots]$. Therefore, Lévy's zero-one law guarantees that $\lim_{n\to\infty} \theta_n(S) = \theta(S)$ almost surely for all $S \in \mathcal{C}$. Now suppose that $\lim_{n\to\infty} \theta_n(T) \neq \theta(T)$ for some set T. Take a_0, b_0 such that $\theta(T) \in (a_0, b_0)$ but $\lim_{n\to\infty} \theta_n(T) \notin a_0, b_0$. Thus $\theta \in U_{T,a_0,b_0}$ but $\theta_n \notin U_{T,a_0,b_0}$ for infinitely many n. Then by the previous part, there must be some $U_{S,a,b} \in \mathcal{C}_0$ such that $\theta \in U_{S,a,b}$ but $\theta_n \notin U_{S,a,b}$ for infinitely many n. But this would imply that $\lim_{n\to\infty} \theta_n(S) \neq \theta(S)$, which is a contradiction. Hence $\lim_{n\to\infty} \theta_n(T) = \theta(T)$ for all measurable sets T, as was to be shown.

B Statistics of Beta and Gamma Functions

Lemma B.1. Let $d_n \sim \text{Gamma}(\alpha_n, 1)$, $e_n \sim \text{Gamma}(\beta_n, 1)$, $\alpha_{n+1} = \alpha_n + d_n$, and $\beta_{n+1} = \beta_n + e_n$. Then $\mathbb{E}\left[\frac{\alpha_{n+1}}{\alpha_{n+1}+\beta_{n+1}}\right] = \frac{\alpha_n}{\alpha_n+\beta_n}$. Proof.

$$\mathbb{E}\left[\frac{\alpha_{n+1}}{\alpha_{n+1}+\beta_{n+1}}\right]$$

$$=\mathbb{E}_{d_n,e_n}\left[\frac{\alpha_n+d_n}{\alpha_n+\beta_n+d_n+e_n}\right]$$

$$=\mathbb{E}_s\left[\mathbb{E}_{d_n}\left[\frac{\alpha_n+d_n}{\alpha_n+\beta_n+s} \mid d_n+e_n=s\right]\right]$$

$$=\mathbb{E}_s\left[\mathbb{E}_{d_n}\left[\frac{\alpha_n+d_n}{\alpha_n+\beta_n+s}\mid d_n\sim s\operatorname{Beta}(\alpha_n,\beta_n)\right]\right]$$

$$=\mathbb{E}_s\left[\frac{\alpha_n+s\frac{\alpha_n}{\alpha_n+\beta_n}}{\alpha_n+\beta_n+s}\right]$$

$$=\mathbb{E}_s\left[\frac{\alpha_n}{\alpha_n+\beta_n}\right]$$

$$=\frac{\alpha_n}{\alpha_n+\beta_n}.$$

Lemma B.2. If $X \sim \text{Beta}(\alpha, \beta)$, then $\mathbb{E}[\log(X)] = \psi(\alpha) - \psi(\alpha + \beta)$, where ψ is the digamma function defined by $\psi(x) = \frac{d}{dx} \log \text{Gamma}(x)$.

Proof. Let $F(\alpha) = \int_{\infty}^{\alpha} \int_{0}^{1} x^{\tilde{\alpha}-1} (1-x)^{\beta-1} \log(x) dx d\tilde{\alpha}$. Then by the fundamental theorem of calculus, $\frac{dF}{d\alpha} = \text{Beta}(\alpha, \beta) \mathbb{E}[\log(X)]$. We claim that $F(\alpha) = \text{Beta}(\alpha, \beta)$. Indeed, we have

$$\begin{split} F(\alpha) &= \int_{\infty}^{\alpha} \int_{0}^{1} x^{\tilde{\alpha}-1} (1-x)^{\beta-1} \log(x) dx d\tilde{\alpha} \\ &= \int_{0}^{1} (1-x)^{\beta-1} \int_{\infty}^{\alpha} x^{\tilde{\alpha}-1} \log(x) d\tilde{\alpha} dx \\ &= \int_{0}^{1} (1-x)^{\beta-1} \left(x^{\tilde{\alpha}-1} \big|_{\infty}^{\alpha} \right) dx \\ &= \int_{0}^{1} (1-x)^{\beta-1} x^{\alpha-1} \\ &= \operatorname{Beta}(\alpha,\beta) \end{split}$$

Then it follows that

$$\mathbb{E}[\log(X)] = \frac{\frac{d}{d\alpha} \operatorname{Beta}(\alpha, \beta)}{\operatorname{Beta}(\alpha, \beta)}$$
$$= \frac{d}{d\alpha} \log \operatorname{Beta}(\alpha, \beta)$$
$$= \frac{d}{d\alpha} (\log \operatorname{Gamma}(\alpha) - \log \operatorname{Gamma}(\alpha + \beta))$$
$$= \psi(\alpha) - \psi(\alpha + \beta),$$

which proves the lemma.

C Properties of Hierarchical Beta Processes

In this section, we prove Lemma 4.1, and make some additional calculations regarding the hierarchical beta process model that will be useful for inference. We deal with inference itself in the next section.

Proof of Lemma 4.1. Since $X_l \in \{0,1\}$, we have $\mathbb{P}[X_l = 1 \mid \theta_v] = \mathbb{E}[X_l \mid \theta_v]$, hence $X_l \mid \theta_v \sim$ Bernoulli $(\mathbb{E}[X_l \mid \theta_v])$. But

$$\mathbb{E}[X_l \mid \theta_v] = \mathbb{E}\left[\text{Bernoulli}\left(\lim_{n \to \infty} \theta_{n,l}(X)\right) \mid \theta_v\right]$$
$$= \text{Bernoulli}\left(\mathbb{E}\left[\lim_{n \to \infty} \theta_{n,l}(X) \mid \theta_v\right]\right)$$
$$= \text{Bernoulli}(\theta_{v,l}),$$

where the last step uses the martingale property.⁴ This proves the first part of the lemma. The second part of the lemma follows from standard facts about directed graphical models. \Box

Lemma C.1. Let X be a data point with $X_l = 0$ for all l. Then $\mathbb{E}[\theta_{d_0+d}(X) \mid \theta_{d_0}(X)] = \left(\frac{c}{c+1}\right)^d \theta_{d_0}$. Furthermore, if $d = \max\{d' \mid v_{d_0+d'}(X) = v_{d_0+d'}(Y)\}$, then $\mathbb{P}[Y_l = 1 \mid d, \theta_{d_0}, X]$ is equal to $\left(\frac{c}{c+1}\right)^d \theta_{d_0}$ for $d \ge 0$.

Proof of Lemma C.1. By Lemma 4.1, $\mathbb{P}[X_l = 1 | \theta_e(X)] = \theta_{e,l}$. Then, by the conjugacy of the Beta distribution, $\theta_{e+1,l}(X) | \theta_{e,l}(X) \sim \text{Beta}(c\theta_{e,l} + 1, c(1 - \theta_{e,l}))$. It follows that $\mathbb{E}[\theta_{e+1,l}(X) | \theta_{e,l}(X)] = \frac{c}{c+1}\theta_{e,l}(X)$. Iteratively applying this relation yields the first part of the lemma. The second part of the lemma then follows by applying Lemma 4.1 with $v = v_{d_0+d}$.

Lemma C.2. As in Lemma C.1, let X be the allzeros vector, suppose that $v_{d_0}(X) = v_{d_0}(Y)$, and let $d = \max\{d' \mid v_{d_0+d'}(X) = v_{d_0+d'}(Y)\}$. Then

$$\theta_{d_0+1,l} \mid (\theta_{d_0}, X, Y_l = 1, d) \sim \text{Beta}(c\theta_{d_0,l} + 1, c(1 - \theta_{d_0,l}) + 1)$$

⁴In fact, we need something stronger, since the expectation of a limit does not necessarily equal the limit of the expectation, as can be seen in Example 2 of Section 2.3. However, if the random variables involved are uniformly integrable, then a stronger version of Theorem 2.1 implies that the limit of the expectation is indeed equal to the expectation of the limit. We then note that since the $\theta_{v,l}$ are bounded, they are trivially uniformly integrable.

and

$$\begin{aligned} \theta_{d_0+1,l} &| (\theta_{d_0}, X, Y_l = 0, d) \sim \\ \frac{\omega_1}{\omega_1 + \omega_2} \operatorname{Beta}(c\theta_{d_0,l} + 2, c(1 - \theta_{d_0,l})) \\ &+ \frac{\omega_2}{\omega_1 + \omega_2} \operatorname{Beta}(c\theta_{d_0,l} + 1, c(1 - \theta_{d_0,l}) + 1) \end{aligned}$$

where $\omega_1 = c(1 - \theta_{d_0,l}) + 1$ and $\omega_2 = c\theta_{d_0,l} \left(1 - \left(\frac{c}{c+1}\right)^{d-1}\right).$

Proof of Lemma C.2. For brevity, we will drop the subscript of l on θ , X, and Y. Also, we let $r := \left(\frac{c}{c+1}\right)^{d-1}$. Then by Bayes' rule, we have:

$$p(\theta_{d_0+1} | \theta_{d_0}, X, Y = 1, d) \propto p(Y = 1 | \theta_{d_0+1}, X, d) \times p(X | \theta_{d_0+1}) \times p(\theta_{d_0+1} | \theta_{d_0}) \propto r\theta_{d_0+1} \times (1 - \theta_{d_0+1}) \times \text{Beta}(\theta_{d_0+1}; c\theta_{d_0}, c(1 - \theta_{d_0})) \propto \text{Beta}(\theta_{d_0}; c\theta_{d_0} + 1, c(1 - \theta_{d_0}) + 1).$$

Where we applied Lemma C.1 to compute $p(Y = 1 | \theta_{d_0+1}, X, d)$, and we applied Lemma 4.1 to compute $p(X | \theta_{d_0+1})$. This proves the first part of the assertion. Similarly, we have

$$\begin{aligned} p(\theta_{d_0+1} \mid \theta_{d_0}, X, Y = 0, d) \\ \propto p(Y = 0 \mid \theta_{d_0+1}, X, d) &\times p(X \mid \theta_{d_0+1}) \times p(\theta_{d_0+1} \mid \theta_{d_0}) \\ \propto [1 - r\theta_{d_0+1}] &\times (1 - \theta_{d_0+1}) \\ &\times \text{Beta}(\theta_{d_0+1}; c\theta_{d_0}, c(1 - \theta_{d_0})) \\ \propto [(1 - \theta_{d_0+1}) + (1 - r) \theta_{d_0+1}] \\ &\times \text{Beta}(\theta_{d_0+1}; c\theta_{d_0}, c(1 - \theta_{d_0}) + 1) \\ \propto (c(1 - \theta_{d_0}) + 1) \text{Beta}(\theta_{d_0+1}; c\theta_{d_0}, c(1 - \theta_{d_0}) + 2) \\ &+ c\theta_{d_0} (1 - r) \text{Beta}(\theta_{d_0+1}; c\theta_{d_0} + 1, c(1 - \theta_{d_0}) + 1), \end{aligned}$$

where the extra terms in the last expression come from the fact that $\text{Beta}(\cdot; c\theta_{d_0}, c\theta_{d_0} + 2)$ and $\text{Beta}(\cdot; c\theta_{d_0} + 1, c(1-\theta_{d_0})+1)$ have different normalization constants. This completes the second part of the assertion. \Box

D Inference for Hierarchical Beta Processes

Adding a Data Point

When we add a data point Y, there are two cases to consider. First, we can add Y as a new child of an internal node v (this happens if the CRP at that node creates a new table), or we can add Y to a leaf w that implicitly represents the subtree containing X(w). Let Z(Y, v) denote the probability that a new node of \mathcal{T}' is generated as a child of v and creates the datum Y, and let Z(Y, w, d) denote the probability that a datum first branches from X(w) d levels below w, and that the resulting datum is Y.

It is straightforward to calculate Z(Y, v) — if the path to v is given by v_0, v_1, \ldots, v_d with $v_d = v$, and Size(v)denotes the number of data in Subtree(v), then we have

$$Z(Y, v) = \left(\frac{\gamma}{\gamma + \operatorname{Size}(v)} \prod_{e=0}^{d-1} \pi_{v_e}(v_{e+1})\right) \prod_{l:Y_l=1} \theta_l \prod_{l:Y_l=0} (1 - \theta_l).$$

Calculating Z(Y, w, d) is a bit trickier. We can easily compute the probability that the path of a datum goes through w. Then, in the case that $X_l = 0$ for all l, we can use Lemma C.1 to compute the probability that X and Y first split into unique subtrees at exactly dlevels deeper than w. The joint probability is given by

$$Z(Y, w, d) = \left(\frac{1}{\gamma + \operatorname{Size}(v)} \prod_{e=0}^{d-1} \pi_{v_e}(v_{e+1})\right) \left(\frac{1}{1+\gamma}\right)^d \frac{\gamma}{1+\gamma}$$
$$\times \prod_{l:Y_l=0} \left(1 - \left(\frac{c}{c+1}\right)^d \theta_l\right)$$
$$\times \prod_{l:Y_l=1} \left(\frac{c}{c+1}\right)^d \theta_l.$$

The cases where X_l is not identically zero can then be obtained by symmetry.

The function Z(Y, w, d) is a product of log-concave factors in d, and is therefore itself log-concave. We can thus find a rejection sampler with a constant acceptance rate (Leydold, 2003), and compute the normalization constant $\hat{Z}(Y, w)$ of the enveloping function.

Now, to perform incremental Gibbs sampling, we add a data point to an internal node with probability proportional to Z(Y, v), and we attempt to expand an external node with probability proportional to $\hat{Z}(Y, w)$. In the case that we try to expand an external node, we perform rejection sampling to determine what depth the two data points should branch at. If the sampler rejects, then we reject the Gibbs proposal, otherwise we insert the new data point at the given depth. We then need to sample all of the parameters at all of the newly created internal nodes, which can be done using Lemma C.2.

Resampling Parameters

As noted before, there exist numerical issues when parameters are too close to either 0 or 1. We deal with this problem by assuming that we cannot distinguish between numbers that are less than some distance ϵ from 0 or 1. If we see such a number, we treat it as

having a censored value (so it appears for instance as $\mathbb{P}[\theta < \epsilon]$ in the likelihood). A straightforward calculation shows that

$$\mathbb{P}[\theta_{v,l} < \epsilon \mid \theta_{p(v),l}] \approx \frac{\epsilon^{c\theta_{p(v),l}}}{c\theta_{p(v),l}},$$

and similarly

$$\mathbb{P}[\theta_{v,l} > 1 - \epsilon \mid \theta_{p(v),l}] \approx \frac{\epsilon^{c(1-\theta_{p(v),l})}}{c(1-\theta_{p(v),l})}.$$

With this strategy for dealing with the numerical issue, we now turn to the actual sampling algorithm.

The $\theta_{d,k}$ can be dealt with independently for different values of k, so we will restrict our attention to a fixed value of k. Suppose that θ is the parameter we want to sample, θ_0 is the value of its parent, $\theta_1, \ldots, \theta_m$ are the values of its children that are internal nodes, and X_1, \ldots, X_p are the values of its children that are external nodes. Let $a = \sum_{i=1}^p X_i$ and $b = \sum_{i=1}^p 1 - X_i$. Then the likelihood for θ is given by

$$p(\theta \mid \theta_0, \{\theta_1\}_{i=1}^m, a, b) \propto \theta^{c\theta_0 + a - 1} (1 - \theta)^{c(1 - \theta_0) + b - 1}$$

$$\times \prod_{i:\epsilon \le \theta_i \le 1 - \epsilon} \frac{\theta_i^{c\theta - 1} (1 - \theta_i)^{c(1 - \theta) - 1}}{\text{Beta}(c\theta, c(1 - \theta))}$$

$$\times \prod_{i:\theta_i < \epsilon} \frac{\epsilon^{c\theta}}{c\theta}$$

$$\times \prod_{i:\theta_i > 1 - \epsilon} \frac{\epsilon^{c(1 - \theta)}}{c(1 - \theta)}.$$

One can check that this function is either (i) logconcave, (ii) has infinite density at $\theta = 0$, or (iii) has infinite density at $\theta = 1$. In the first case, we can sample from it efficiently (Leydold, 2003). In the second case, θ is very likely to be less than ϵ ; since our sampler treats all numbers in the interval $[0, \epsilon)$ equivalently, we can arbitrarily set θ to 0. Similarly, in the third case, we can set θ to 1.