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Bayesian Nonparametric Inference within Probabilistic Programming Languages

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Acknowledgments

First of all, I would like to express my indebtedness appreciation to my departmental supervisor Prof. Yee Whye Teh. His belief in me and his advices played a decisive role in making the execution of my work and thus this report.

I also express my deepest thanks to Benjamin Bloem-Reddy, who as a postdoc, oversaw me during this internship and with whom I frequently work.

Moreover, my gratitude goes to Guillaume Obozinski, my school training supervisor, whose guidance has continually shaped my career path since I have been at Ecole des Ponts ParisTech.

Abstract

On one side, Bayesian Nonparametric (BNP) models have gained attraction because of their flexibility. These models, which automatically adapt with the number and complexity of data, avoid having to define *a priori* the number of parameters of the model, such as the number of components for a mixture model. On the other side, Probabilistic Programming Languages (PPLs) allow practitioners to express probabilistic models in a universal way, and bring generic inference algorithms. These systems avoid designing specific inference schemes, which is error-prone and time consuming. Specific representations of BNP models must be used so as to denote such models in PPLs, since BNP models live in infinite dimensional space and machines only have finite memory and computational resources.

In this report, we review well-known BNP models with a focus on mixture models and discrete random probability measures, but we also give background on the design of PPLs and associated inference schemes. We utilize generative construction of BNPs and show that more generic BNP classes than the Dirichlet Process can be represented in PPLs. We prototype our approach by contributing to an existing PPL.

Keywords : Probabilistic Programming, Bayesian Non-parametric, Bayesian Inference, Generative process, Sampling methods.

Contents

Presentation of the Department of Statistics

1.1 Creation

The Department of Statistics [1] is part of the University of Oxford, along with the other departments and the 38 constituent colleges. The University of Oxford was founded in the 11th century, which makes it the oldest university in the English-speaking world and the world's second-oldest university in continuous operation.

The Department of Statistics was officially created in 1988, even though first moves in the development of Oxford statistics can be dated to the 19th century.

Indeed, In the 1870s, Florence Nightingale – the pioneer of modern nursing – discussed the possibility of endowing a Professorship of Statistics in Oxford, but the proposal eventually foundered. However, Oxford did appoint a statistician to a chair in 1891, although not to a chair in statistics.

The next significant moves in the development of Oxford statistics were by economists, who were increasingly keen to build economic theory on a foundation of sound data analysis. This led to the creation in 1935 of an Institute of Statistic, swhich was then renamed as the Institute of Economics and Statistics in 1962.

The sequence of events which led directly to the establishment of the present Department of Statistics began with the appointment in 1945 of David Finney as the universitys first Lecturer in the Design and Analysis of Scientific Experiment (LIDASE).

Then in the 1980s, after the Department of Biomathematics' head increasingly felt that Oxford was losing out in the face of developments in statistics, a working party appointed by the general board of the university to assess a careful analysis of the organisation of statistics in Oxford. They found fragmentation to be the dominant feature of Oxford statistics and concluded that fragmentation has serious disadvantages ..... The working partys report recommended the creation of a university statistics department, which were to include the former Department of Biomathematics, together with a new Professorship in

[1] https://www.stats.ox.ac.uk

Statistical Science and the two existing lecturerships in statistics within the Mathematical Institute.

These major recommendations were all accepted by the university and the new Department of Statistics was created in 1988.

1.2 Activities

The Department of Statistics at Oxford is a world leader in research including computational statistics and statistical methodology, applied probability, bioinformatics and mathematical genetics. The main research groups in the Department are Computational statistics and machine learning, Probability, Statistical genetics and bioinformatics, Protein Informatics and Statistical Genetics.

I am part of the Computational Statistics and Machine Learning Group (OxCSML) [2], which have research interests spanning Statistical Machine Learning, Monte Carlo Methods and Computational Statistics, Statistical Methodology and Applied Statistics.

The department offers an undergraduate degree (BA or MMath) in Mathematics and Statistics, jointly with the Mathematical Institute. At postgraduate level there is an MSc course in Applied Statistics (MSc in Statistical Science from 2017), as well as a lively and stimulating environment for postgraduate research (DPhil or MSc by Research). The department also has a consulting activity called *Oxford University Statistical Consulting*.

[2] `http://csml.stats.ox.ac.uk/people/mathieu/`

Mission

2.1 Themes of research

Prof. Yee Whye Teh [1] has worked for a long time on inference sampling schemes for BNP mixture models [27, 26, 53, 54], but also on stick-breaking constructions [81, 25]. He also has recently been interested in PPL and consequently in inference schemes within PPL for BNP models.

This theme requires knowledge in several fields – Probabilities, Computational Statistics, Programming Languages – which makes it deeply interesting. He proposed me working with him on this topic as part of a 3-years DPhil program, and to start earlier as an intern.

2.2 Context

In addition to inviting me to work with him, Prof. Yee Whye Teh also opened two postdoctoral positions for working on the same project, which have been filled by Tom Rainforth and Benjamin Bloem-Reddy.

Tom Rainforth [2] is finishing is third year of DPhil in the Dept. of Engineering Science in Oxford, supervised by Prof. Frank Wood. His interests include probabilistic programming, Bayesian optimization, probabilistic numerics, sequential Monte Carlo and particle Markov Chain Monte Carlo methods. He will join the group in October, but he has already attended several reading group meetings.

On the other hand, Benjamin Bloem-Reddy [3] arrived in May in Oxford and has already started working on the project. He was supervised by Peter Orbanz at Columbia University, and his research were focused on probabilistic and statistical analysis of networks and other discrete data.

[1] https://www.stats.ox.ac.uk/~teh
[2] http://www.robots.ox.ac.uk/~twgr
[3] http://www.stats.ox.ac.uk/~bloemred/

2.3 Reading group

Four reading groups are organised with a bi-weekly period: Kernel methods, Deep Learning, Bayesian Nonparametrics and Probabilistic Inference. I have been leading the Probabilistic Inference reading group [4] since July. Since, Ben and I have presented four papers [76, 84, 77, 17] with an emphasise on probabilist programming.

2.4 Organisation

In this section I develop my current organisation and workflow as a researcher. At first, I had much trouble to organise my workflow, I wrote my papers' review and new ideas on flying sheets, papers were saved in my computer's folders, citations for report was time-consuming, my code was locally saved, etc...

Thus, I worked on a better workflow and after trials and errors, I eventually arrived on what I describe below. I aim to modify this process with time, so as to continually enhance my productivity and be able to focus on the interesting part of the job.

2.4.1 Managing papers

My biggest trouble was keeping organised the dozens of new articles I read each week. I was saving them in a tree-like structure of folders, but with the number of articles saved growing, it became more and more difficult to find specific article. Moreover, this structure inherently prohibits cross-categories articles which is annoying for a project situated at the intersections of several fields. Furthermore, I had no fast way to cite an article, neither in plain format (for markdown [5] files for instance) nor in *BibTeX* format.

Then, I have heard of papers managing library such as Papers3 [6] or Mendeley [7]. I have eventually opted for Papers3 but Mendeley is also a popular choice in the academic community. These applications features many tools easing the life of a researcher, the main one being from my point of view:

- Synchronisation: between multiple computers or devices.
- Multi-labels: these are used in the search tool.
- Local search: search in titles, authors, labels and even papers' content.
- Online search: can import articles in a fast manner by being connected with online search engines such as *arXiv*.
- Collections: create a reading list, or group of papers which can be cited at once
- Citations: get *BibTeX* reference or *BibTeX* cite command in clipboard

[4] https://github.com/BigBayes/oxsml/wiki/Probabilistic-Inference-meetings
[5] https://en.wikipedia.org/wiki/Markdown
[6] https://www.readcube.com/papers/mac/
[7] https://www.mendeley.com

2.4.2 Managing research

Another of my organizational issue was keeping track of ideas. I happened to find that research is a result of a long chain of ideas which were continually iterated upon. I am now maintaining a single *master document* for keeping tracks of this chain of ideas.

It has a bulleted list of all ideas, problems, and topics that Id like to think more carefully about. This list is succinct but subsequent sections go in depth on particular entries. This list is sorted according to what Id like to work on next, but I continually revise my priorities according to whether I think the direction aligns with my broader research vision, and if I think the direction is necessarily impactful for the community at large.

2.4.3 Managing projects

Then, when an idea has matured enough and I have seriously started working on it, I create a Github [8] repository for the project. Each project has its separated repository. It contains a `/readme.md` file maintaining a list of todos, with also questions (and sometimes answers!) both for myself and collaborators. This makes it transparent how to keep moving forward and whats blocking the work.

There is also a `/doc/` folder for all the write-ups, usually in LaTeXformat. The `etc/` folder is used for everything not relevant to other directories such as pictures of whiteboards during conversations about the project. Finally, the `/src/` folder is where all code is written. Runnable scripts are written directly in `/src/` , and classes and utilities are written in `/src/codebase/`.

[8] `https://github.com`

Bayesian nonparametrics

3.1 Definition

A Bayesian nonparametric model is a model that (i) constitutes a Bayesian model (a statistical model with parameters being random variables) on an infinite-dimensional parameter space and (ii) can be evaluated on a finite sample in a manner that uses only a finite subset of the available parameters to explain the sample. The parameter space in (i) typically consists of functions or of measures, while (ii) is usually achieved by marginalizing out surplus dimensions over the prior. Random functions and measures, and more generally probability distributions on infinite-dimensional random objects, are called stochastic processes.

3.2 Motivation

Most scientists address the model selection problem by first fitting several models, with different numbers of clusters or factors, and then selecting one using model comparison metrics [15]. Model selection metrics usually include two terms. The first term measures how well the model fits the data. The second term, a complexity penalty, favors simpler models (i.e., ones with fewer components or factors).

BNP models provide a different approach to this problem. Rather than comparing models that vary in complexity, the BNP approach is to fit a single model that can adapt its complexity to the data. BNP models allow the complexity to grow as more data are observed, such as when using a model to perform prediction. This is an attractive property for many settings.

3.2.1 Exchangeability

The underlying assumption of all Bayesian methods is that the parameter specifying the observation model is a random variable. However, there is a very general type of so-called *exchangeable* observations for which the existence of such a random variable is a mathematical consequence of the data's properties. This is an important notion since all models we will be considering in Chapter 5 are assuming exchangeability.

Formally, a sequence of variables $X_1, \ldots, X_n$ over the same probability space $(\mathbb{X}, \Omega)$ is *exchangeable* if their joint distribution is invariant to permuting the variables. That is, if for any permutation σ of $\{1, \ldots, n\}$, then

$$\mathbb{P}(X_1 = x_1, \ldots, X_n = x_n) = \mathbb{P}(X_1 = x_{\sigma(1)}, \ldots, X_n = x_{\sigma(n)})$$

An infinite sequence $X_1, X_2, \ldots$ is *infinitely exchangeable* if $X_1, \ldots, X_n$ is *exchangeable* for every $n \geq 1$. Exchangeability reflects the assumption that the variables do not depend on their indices although they may be dependent among themselves. This is typically a reasonable assumption in machine learning and statistical applications, even if the variables are not themselves iid, since it is a much weaker assumption.

If θ parametrizes the underlying distribution, and one assumes a prior distribution over θ, then the resulting marginal distribution over $X_1, \ldots, X_n$ with θ marginalized out will still be exchangeable. A fundamental result credited to de Finetti [16] states that the converse is also true. That is, if $X_1, \ldots, X_n$ is (infinitely) exchangeable, then there is a random θ such that:

$$P(X_1, \ldots, X_n) = \int P(\theta) \prod_{i=1}^{n} P(X_i|\theta) d\theta \tag{3.1}$$

In other words, the seemingly innocuous assumption of exchangeability automatically implies the existence of a hierarchical Bayesian model with θ being the random latent parameter.

In de Finetti's Theorem it is important to stress that θ can be infinite dimensional (it is typically a random measure), thus the hierarchical Bayesian model 3.1 can be a nonparametric one.

3.3 Examples

Bayesian nonparametric models have recently been applied to a variety of machine learning problems, including regression, classification, clustering, latent variable modeling, sequential modeling, and others.

3.3.1 Dirichlet Process

The Dirichlet Process (DP) is a distribution over distributions. It is parameterized by a concentration parameter $\alpha > 0$ and a base distribution H_0, which is a distribution over a space $\mathbb{X}$. A random variable drawn from a Dirichlet Process (DP) is itself a distribution over $\mathbb{X}$. A random distribution P drawn from a DP is denoted $P \sim \mathrm{DP}(\alpha, H_0)$.

The DP was first developed in [30], who showed its existence by appealing to its finite dimensional distributions. Consider a measurable partition of $\mathbb{X}$, $\{A_1, \ldots, A_K\}$ If $P \sim \mathrm{DP}(\alpha, H_0)$ then every measurable partition of $\mathbb{X}$ is Dirichlet-distributed,

$$(P(A_1), \ldots, P(A_K)) \sim \mathrm{Dir}(\alpha H_0(A_1), \ldots, \alpha H_0(A_K)).$$

This means that if we draw a random distribution from the DP and add up the probability mass in a region $A \in \mathbb{X}$, then there will on average $H_0(A)$ mass in that region. The

concentration parameter plays the role of an inverse variance; for higher values of α, the random probability mass $P(A)$ will concentrate more tightly around $H_0(A)$.

[30] proved two properties of the Dirichlet process. The first property is that random distributions drawn from the Dirichlet process are discrete. They place their probability mass on a countably infinite collection of points, called atoms,

$$P = \sum_{k=1}^{\infty} p_k \delta_{X_k^\star}. \tag{3.2}$$

where p_k is the probability assigned to the kth atom and $X_k^\star$ is the location or value of that atom. Further, these atoms are drawn independently from the base distribution H_0.

The second property connects the Dirichlet process to the Chinese restaurant process. Consider a random distribution drawn from a DP followed by repeated draws from that random distribution,

$$P \sim \mathrm{DP}(\alpha, H_0) \tag{3.3}$$

$$X_i \sim P \quad \forall i = \{1, \ldots, n\} \tag{3.4}$$

Ferguson [30] examined the joint distribution of $X_{1:n}$, which is obtained by marginalizing out the random distribution P,

$$p(X_1, \ldots, X_n | \alpha, H_0) = \int \left(\prod_{i=1}^{n} p(X_i|P) \right) d\mathbb{P}(P|\alpha, H_0) \tag{3.5}$$

Ferguson showed that, under this joint distribution, the X_i will exhibit a *clustering property*–they will share repeated values with positive probability. The structure of shared values defines a partition of the integers from 1 to n, and the distribution of this partition is a Chinese restaurant process with parameter α. Finally, he showed that the unique values of X_i shared among the variables are independent draws from H_0.

The stick-breaking construction Ferguson [30] proved that the DP exists via its finite dimensional distributions. Sethuraman [80] provided a constructive definition based on the stick-breaking representation.

Consider a stick with unit length. We divide the stick into an infinite number of segments $\tilde{p}_k$ by the following process. First, choose a beta random variable $Z_1 \sim \mathrm{beta}(1, \alpha)$ and break off V_1 of the stick. For each remaining segment, choose another beta distributed random variable, and break off that proportion of the remainder of the stick. This gives us an infinite collection of weights

$$V_k \sim \mathrm{Beta}(1, \alpha) \tag{3.6}$$

$$\tilde{p}_k = V_k \prod_{j=1}^{k-1} (1 - V_j) \quad k = 1, 2, \ldots \tag{3.7}$$

Finally, we construct a random distribution using Equation 3.2, where we take an infinite number of draws from a base distribution H_0 and draw the weights as in Equation 3.7.

Sethuraman [80] showed that the distribution of this random distribution is a $DP(\alpha, H_0)$. He also showed that the sequence of weights $(\tilde{p}_k)_{k\geq 1}$ is a size-biased permutation of the DP's weights $(p_k)_{k\geq 1}$, i.e. the bigger is a weight p_k, the sooner it will be sampled by the previously described process.

Chinese Restaurant Process The Chinese Restaurant Process (CRP) is a distribution over infinite partitions of the integers [72, 2]. The CRP derives its name from the following metaphor. Imagine a restaurant with an infinite number of tables [1], and imagine a sequence of customers entering the restaurant and sitting down. The first customer enters and sits at the first table. The second customer enters and sits at the first table with probability $\frac{1}{1+\alpha}$, and the second table with probability $\frac{\alpha}{1+\alpha}$, where α is a positive real. When the nth customer enters the restaurant, he sits at each of the occupied tables with probability proportional to the number of previous customers sitting there, and at the next unoccupied table with probability proportional to α. At any point in this process, the assignment of customers to tables defines a random partition.

More formally, let z_n be the table assignment of the nth customer. A draw from this distribution

$$P(z_n = k|\mathbf{z}_{1:n-1}) \propto \begin{cases} \frac{m_k}{n-1+\alpha} \text{ if } k \leq K_+ \text{ (i.e., k is a previously occupied table)} \\ \frac{\alpha}{n-1+\alpha} \text{ otherwise (i.e., k is the next unoccupied table)} \end{cases}$$

where m_k is the number of customers sitting at table k, and K_+ is the number of tables for which $m_k > 0$. The CRP can also be obtained by marginalising out the random measure P.

Dirichlet process mixtures A DP mixture adds a third step to the model above: $Y_i \sim f(\cdot|X_i)$. Marginalizing out P reveals that the DP mixture is equivalent to a CRP mixture. Moreover, the stick-breaking representation is a generative process enabling to lazily sample according to the associated DP, in a *size-biased* order. We will talk more about this size-biased of the DP atoms in Proposition 1 and its discussion.

3.3.2 Nonlinear regression

The aim of regression is to infer a continuous function from a training set consisting of input-output pairs $\{(t_i, x_i)\}_{i=1}^n$. Parametric approaches parametrize the function using a finite number of parameters and attempt to infer these parameters from data. The prototypical Bayesian nonparametric approach to this problem is to define a prior distribution over continuous functions directly by means of a Gaussian Process (GP). As explained in [74], a GP is a distribution on an infinite collection of random variables X_t, such that the joint distribution of each finite subset $X_{t_1}, \ldots, X_{t_n}$ is a multivariate Gaussian. A value x_t taken by the variable X_t can be regarded as the value of a continuous function f at t, that is, $f(t) = x_t$. Given the training set, the Gaussian process posterior is again a distribution on functions, conditional on these functions taking values $f(t_1) = x_1, \ldots, f(t_n) = x_n$.

[1] The Chinese restaurant metaphor is due to Pitman and Dubins, who were inspired by the seemingly infinite seating capacity of Chinese restaurants in San Francisco.

3.3.3 Latent feature models

Latent feature models represent a set of objects in terms of a set of latent features, each of which represents an independent degree of variation exhibited by the data. Such a representation of data is sometimes referred to as a distributed representation. A Bayesian nonparametric approach to latent feature modeling allows for an unknown number of latent features. The canonical stochastic processes involved here are known as the Indian Buffet Process (IBP) [33, 81] and the Beta Process (BP). Draws from BPs are random discrete measures, where each of an infinite number of atoms has a mass in $(0, 1)$ but the masses of atoms need not sum to 1. Yet, their sum is finite almost surely. Each atom corresponds to a feature, with the mass corresponding to the probability that the feature is present for an object. We can visualize the occurrences of features among objects using a binary matrix, where the (i, k) entry is 1 if object i has feature k and 0 otherwise. The distribution over binary matrices induced by the BP is called the IBP. Thibaux and Jordan [82] showed that a particular subclass of Beta processes is to the IBP as the DP is to the CRP.

3.3.4 Hidden Markov models

Hidden Markov Models (HMMs) are popular models for sequential or temporal data, where each time step is associate with a state, with state transitions dependent on the previous state. An infinite HMM is a Bayesian nonparametric approach to HMMs, where the number of states is unbounded and allowed to grow with the sequence length. It is defined using one DP prior for the transition probabilities going out from each state. To ensure that the set of states reachable from each outgoing state is the same, the base distributions of the DPs are shared and given a DP prior recursively. The construction is called an Infinite Hierarchical Dirichlet Process (HDP) [5].

3.3.5 Density estimation

A nonparametric Bayesian approach to density estimation [23] requires a prior on densities or distributions. However, the DP is not useful in this context, since it generates discrete distributions. A useful density estimator should smooth the empirical density (such as a Parzen window estimator), which requires a prior that can generate smooth distributions. Priors applicable in density estimation problems include DP mixture models and Pólya trees.

3.4 Mixture models

3.4.1 Finite dimensional

Mixture models provide a statistical framework for modeling data where each observation is assumed to have arisen from one of k groups, with k possibly unknown, and each group being suitably modeled by a distribution function from some parametric family. We refer to the monographs by Titterington et al. [83] and McLachlan and Basford [60] for accounts on mixture models with a fixed number of components. The distribution function of each

group is referred to as a component of the mixture model and is weighted by the relative frequency of the group in the population. Specifically, assuming k being fixed, a collection of observations $Y_1, \ldots, Y_n$ is modeled as independent draws from a mixture distribution function with k components, that is,

$$Y_i \sim \sum_{j=1}^{k} p_j F(\cdot|X_j), \tag{3.8}$$

where $(X_1, \ldots, X_k)$ are parameters associated with component j, $F(\cdot|X)$ is a given parametric family of distribution functions indexed by a parameter X and $(p_1, \ldots, p_k)$ are the mixture proportions constrained to be nonnegative and sum to unity. Thus, finite mixture models define a density function over data items y of the form $p(y) = \sum_{k=1}^{k} p_j f(y|X_j)$, where f is the density of F. The density can be written in a non-standard manner as an integral: $p(y) = \int F(y|X)P(X)dX$, where $P = \sum_{j=1}^{k} p_j \delta_{X_j}$ is a discrete mixing distribution encapsulating all the parameters of the mixture model and δ_X is a Dirac distribution (atom) centered at X.

A convenient formulation of the mixture model (3.8) can be stated in terms of latent allocation random variables, namely, each observation Y_i is assumed to arise from a specific but unknown component Z_i of the mixture model. Accordingly, an augmented version of (3.8) can be written in terms of a collection of latent random variables $(Z_1, \ldots, Z_n)$, independent and identically distributed with probability mass function $\mathbb{P}[Z = j] = p_j$, such that the observations are modeled as

$$Y_i|Z_i \sim F(\cdot|X_{Z_i}). \tag{3.9}$$

Integrating out the random variables $(Z_1, \ldots, Z_n)$ then yields (3.8). In a Bayesian setting the formulation of the mixture model (3.9) is completed by specifying suitable prior distributions for the unknown quantities that are objects of the inferential analysis: the parameter $(X_1, \ldots, X_k)$ and the vector of proportions $(p_1, \ldots, p_k)$.

3.4.2 Infinite dimensional

Bayesian Nonparametric generalizations of finite mixture models provide an approach for estimating both the number of components in a mixture model and the parameters of the individual mixture components simultaneously from data [64]. As opposed to finite mixtures, BNP mixtures use mixing distributions consisting of a *countably infinite* number of atoms:

$$P = \sum_{j=1}^{\infty} p_j \delta_{X_j^\star} \tag{3.10}$$

This gives rise to mixture models with an infinite number of components. When applied to a finite training set, only a finite (but varying) number of components will be used to model the data, since each data item is associated with exactly one component but each component can be associated with multiple data items. Inference in the model then automatically recovers both the number of components to use and the parameters of the components. Being Bayesian, we need a prior over the mixing distribution P. Discrete Random Probability Measures are of the form of 3.10, defined on a suitable measurable space $\mathbb{X}$ with $X_i \in \mathbb{X}$ for $i = 1, \ldots$. The most common prior to use is a

DP. Consequently, the mixture components would be drawn accordingly to the base distribution of the DP.

We are therefore interested in hierarchical models of the form

$$\begin{gathered} P \text{ a Discrete Random Probability Measure,} \\ X_i|P \sim P, \\ Y_i|X_i \sim F(\cdot|X_i) \end{gathered}$$

3.5 Random probability measures

In this section, we explore classes of nonparametric priors for our previously defined mixture model. There are two possible random discrete distributions that can be obtained from a specific class of discrete random measures called Completely Random Measures (CRMs). Informally, a Completely Random Measure (CRM) is a discrete random measure with an independence property. One of them is the well known random discrete distributions called Normalised Random Measures with Independent Increments and the other is the class of Poisson-Kingman Random Probability Measures. Both are obtained from CRMs after a suitable normalisation operation. Poisson Kingman Process (PKP) specify a distribution for the total mass T, whereas Normalised Random Measures (NRMs) use the "natural" distribution of T induced by their Lévy measure ρ.

3.5.1 Normalised Random Measure

We start with a description of CRMs. See the monograph by Kingman [46] for a good reference on such a topic.

Definition 1 (Completely Random Measure)**.** *Let $\mathbb{X}$ be a complete and separable metric space endowed with the Borel σ-field $\mathcal{B}(\mathbb{X})$. A Completely Random Measure μ is a random element taking values on the space of boundedly finite measures on $\mathbb{X}$ such that, for any collection of measurable subsets, $A_1, \ldots, A_n$ in $\mathcal{B}(\mathbb{X})$, with $A_i \cap A_j = \emptyset \; \forall i \neq j$, the random variables $\mu(A_1), \ldots, \mu(A_n)$ are mutually independent.*

CRMs were first proposed and studied by Kingman [45], who showed that a CRM μ can always be decomposed into a sum of three independent parts

$$\mu = \mu_0 + \sum_{k \geq 1} J_k \delta_{X_k^\star} + \sum_{l=1}^{N} v_l \delta_{\psi_l}$$

where μ_0 is a (non-random) measure over $\mathbb{X}$, $\{\psi_l\}_{l \in [N]} \subset \mathbb{X}$ is a collection of N, $1 \leq N \leq \infty$, atoms at fixed locations and independent random masses $(v_l)_{l \in [N]}$, and $(J_k, X_k^\star)_{k \geq 1}$ is a collection of atoms with random masses and random locations.

In applications of Bayesian nonparametrics it is usually assumed that $\mu_0 = 0$ and $N = 0$, so that μ consists only of the atoms with random masses and locations. However, the posterior distribution of μ given data would typically contain atoms at fixed locations, hence, the usefulness of the larger class of CRMs.

The distribution of the random atoms $(X_k^\star)_{k\geq 1}$ and their masses $(J_k)_{k\geq 1}$ under a CRM is characterized by the Lévy-Khintchine representation of its Laplace functional transform [45]. Specifically,

$$\mathbb{E}\left[e^{-\int g(y)\mu(dy)}\right] = \exp\left\{-\int_{\mathbb{R}^+\times\mathbb{X}}\left(1-e^{-sg(y)}\right)\rho(ds)H_0(dy)\right\}, \tag{3.11}$$

for any measurable function $g:\mathbb{X}\to\mathbb{R}$ such that $\int_{\mathbb{X}}|g(x)|\mu(dx)<+\infty$ almost-surely. The underlying measure $\nu=\rho\times H_0$ uniquely characterises the random atoms in μ.

The only intensity measures that are considered herein are those that factorise $\nu(ds,dy)=\rho(ds)H_0(dy)$ for some measure ρ on $\mathbb{R}^+$ absolutely continuous with respect to the Lebesgue measure, and some non-atomic probability measure H_0 on $\mathbb{X}$. The corresponding CRM is said to be *homogeneous* and write $\mathrm{CRM}(\rho,H_0)$ for the law of μ. Successively, the measure ρ is referred to as the Lévy measure, while H_0 is the base distribution. Homogeneity implies independence between $(J_k)_{k\geq 1}$ and $(X_k^\star)_{k\geq 1}$, where $(X_k^\star)_{k\geq 1}$ is a sequence of random variables independent and identically distributed according to H_0 while the law of $(J_k)_{k\geq 1}$ is governed by ρ. Intuitively, the point process $(J_k,X_k^\star)_{k\geq 1}$ is described by a Poisson process over $\mathbb{R}^+\times\mathbb{X}$ with intensity measure $\nu=\rho\times H_0$, as illustrated in Figure 3.1.

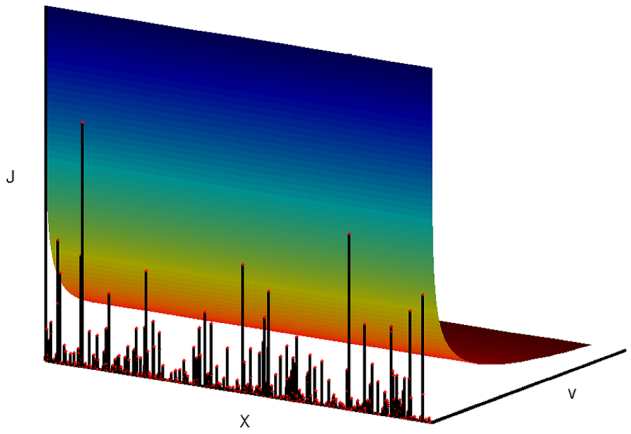

Figure 3.1: *A draw $\sum_{j\geq 1}J_j\delta_{X_j}$ from a* CRM*. Each stick denotes an atom in the* CRM*, with mass given by its height J_j and location given by X_j. Behind the* CRM *is the density of its Lévy intensity measure ν. Source: [27].*

It is required that μ has almost-surely finite total mass, Equation 3.11 with $g(y)=1$ shows that the Lévy measure is required to satisfy the property

$$\int_{\mathbb{R}^+\times\mathbb{X}}\left(1-e^{-s}\right)\rho(ds)H_0(dy)=\int_{\mathbb{R}^+}\left(1-e^{-s}\right)\rho(ds)<\infty$$

Furthermore, the expected number of random atoms in μ is obtained by Campbells Theorem to be the total mass of the Lévy measure $\rho(\mathbb{R}^+)$. In typical applications of Bayesian nonparametrics this is infinite, so we can work with mixture models with infinite number of components. This also guarantees that the total mass is positive almost-surely.

However, since $T\neq 1$ in general, CRMs cannot directly be used as priors for mixture models. One can normalize a CRM by its finite total mass to construct a BNP prior for

mixture models.

Definition 2 (Normalised Random Measure [75])**.** *Let μ be a homogeneous* CRM*, with Lévy measure ρ and base distribution H_0, with almost-surely positive and finite total mass. A* NRM *is an almost-surely discrete random probability measure P on $\mathbb{X}$ obtained by normalising μ*

$$P = \frac{\mu}{T} = \sum_{k \geq 1} p_k \delta_{X_k^\star}$$

with $T = \sum_{k \geq 1} J_k$ and $p_k = J_k/T$. Since μ is homogeneous, the law of $(p_k)_{k \geq 1}$ is governed by the Lévy measure ρ and the atoms $(X_k^\star)_{k \geq 1}$ are a sequence of random variables independent of $(p_k)_{k \geq 1}$, and independent and identically distributed according to H_0. We denote it by $P \sim NRM(\rho, H_0)$.

Let $\mu \sim \text{CRM}(\rho, H_0)$ with an almost-surely finite and positive total mass T, and $P = \mu/T$. Suppose that T is positive and finite almost-surely, and absolutely continuous with respect to Lebesgue measure with density $f_\rho(t)$. Let $(X_i)_{i \geq 1}$ be a sequence of random variables that, given P, are independent and identically distributed according to P. Since μ is almost-surely discrete, there is a positive probability that $X_i = X_j$ for each pair $i \neq j$, i.e. when both are assigned to the same atom in P. This induces a partition π on $\mathbb{N}$, where i and j are in the same block in Π if and only if $X_i = X_j$.

We can thus define a mixture model with an NRM acting as a BNP prior as following:

$$\begin{aligned} \mu &\sim \text{CRM}(\rho, H_0), \\ P &= \frac{\mu}{T}, \\ X_i | P &\sim P, \\ Y_i | X_i &\sim F(\cdot | X_i), \end{aligned}$$

An example of NRM is the Normalised Generalised Gamma Process (NGGP) [71, 50]. The Generalised Gamma Process (GGP) Lévy measure is

$$\rho(dy) = \frac{a}{\Gamma(1-\sigma)} y^{-\sigma-1} e^{-\tau y} dy, \tag{3.12}$$

where $\tau \in [0, \infty)$, $a \in (0, \infty)$ and $\sigma \in [0, 1)$. The NGGP is then obtained, as described above, by normalisation of the GGP. Notable special case of NGGP are $\sigma = 0$ where we obtain the DP, and $\sigma = 0.5$, where we obtain the inverse-Gaussian (IG) process.

3.5.2 Poisson-Kingman random probability measure

Poisson-Kingman Random Probability Measure (RPM) were introduced in [71] as a generalisation of homogeneous NRMs.

Definition 3 (Poisson-Kingman Random Probability Measure)**.** *Let $\mu \sim CRM(\rho, H_0)$ and let $T = \mu(\mathbb{X})$ be finite, positive almost-surely, and absolutely continuous with respect to Lebesgue measure. For any $t \in \mathbb{R}^+$, let us consider the conditional distribution of μ/t*

given that the total mass $T \in dt$. This distribution is denoted by $PK(\rho, \delta_t, H_0)$, were δ_t denotes the Dirac delta function. Poisson-Kingman RPMs *form a class of* RPMs *whose distributions are obtained by mixing $PK(\rho, \delta_t, H_0)$, over t, with respect to some distribution γ on the positive real line. Specifically, a Poisson-Kingman* RPM *has the hierarchical representation*

$$T \sim \gamma,$$
$$P|T = t \sim PK(\rho, \delta_t, H_0), \tag{3.13}$$

The RPM *P is referred to as the Poisson-Kingman* RPM *with Lévy measure ρ, base distribution H_0 and mixing distribution γ. The distribution of P is denoted by $PK(\rho, \gamma, H_0)$. If the density for the total mass equals the density obtained from its Lévy measure f_ρ, i.e. $\gamma(dt) = f_\rho(t)dt$, then the distribution $PK(\rho, f_\rho, H_0)$, coincides with $NRM(\rho, H_0)$.*

Since μ is homogeneous, the atoms $(X_k^\star)_{k\geq 1}$ of P are independent of their masses $(p_k)_{k\geq 1}$. They form a sequence of independent random variables identically distributed according to H_0. Finally, the masses of P have distribution governed by the Lévy measure ρ and the distribution γ.

Same as for NRMs, Poisson-Kingman RPMs can be used as BNP prior for mixture models. The associated hierarchical model is the following:

$$T \sim \gamma,$$
$$P|T = t \sim \mathrm{PK}(\rho, \delta_t, H_0),$$
$$X_i|P \sim P,$$
$$Y_i|X_i \sim F(\cdot|X_i),$$

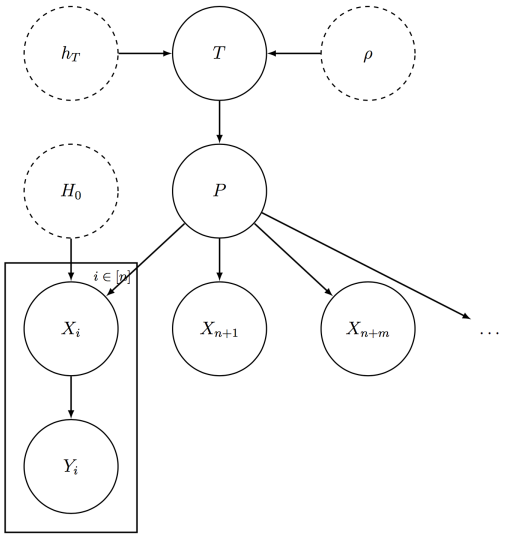

Figure 3.2: PKP *intractable graphical model: the latent variables are countably infinitely many which makes the model computationally intractable. Source: [52].*

Figure 3.2 represents the associated graphical model.

σ-Stable Poisson-Kingman RPMs One famous class of Poisson-Kingman RPM is the class σ-Stable Poisson-Kingman RPMs which encompasses most of the popular discrete RPMs used in Bayesian nonparametrics, for instance, the Pitman-Yor process and the normalised generalised Gamma process. For any $\sigma \in (0,1)$ the density function of a positive σ-Stable random variable is $f_\sigma(t) = \frac{1}{\pi}\sum_{j=0}^{\infty} \frac{(-1)^{j+1}}{j!} \sin(\pi\sigma j)\frac{\Gamma(\sigma j+1)}{t^{\sigma j+1}}$. A σ-Stable Poisson-Kingman RPM is a Poisson-Kingman RPM with Lévy measure given by

$$\rho(dy) := \rho_\sigma(dy) = \frac{a}{\Gamma(1-\sigma)} y^{-\sigma-1} dy, \tag{3.14}$$

and base distribution H_0. The mixing distribution for the total mass T takes the following factored form $\gamma(dt) \propto h(t) f_\sigma(t) dt$, for any non-negative measurable function h such that $\int_0^\infty h(t) f_\sigma(t) dt < \infty$. Accordingly, σ-Stable Poisson-Kingman RPMs form a class of discrete RPMs indexed by the parameters (ρ, h). The Dirichlet process can be recovered as a limiting case, if $\sigma \to 0$, for some choices of h. The following examples of σ-Stable Poisson-Kingman RPMs are obtained by specifying the tilting function h. See [52] for more examples and more details on those.

- Normalised σ-Stable process (NS): $h(t) = 1$
- Normalised Generalised Gamma Process (NGGP) : $h(t) = \exp\{\tau - \tau^{1/\sigma} t\}$, for any $\tau > 0$
- Pitman-Yor process (PY): $h(t) = \frac{\Gamma(\theta+1)}{\Gamma(\theta/\sigma+1)} t^{-\theta}$ with $\theta \geq -\sigma$
- Gamma-tilted process (GT): $h(t) = t^{-\theta}\exp\{-\eta t\}$ for any $\eta > 0$ or $\eta = 0$ and $\theta > -\sigma$
- Poisson-Gamma class (PG): $h(t) = \int_{\mathbb{R}^+} \exp\{\tau - \tau^{1/\sigma} t\} F(d\tau)$

Size-Biased Sampling process An important object induced by a Poisson-Kingman RPM is a size-biased permutation of its atoms. Specifically, order the blocks in the partition Π (induced by the RPM) by increasing order of the least element in each block, and for each $l \in \mathbb{N}$ let Z_l be the least element of the l-th block. Z_l is the index among $(X_i)_{i\geq 1}$ of the first appearance of the l-th unique value in the sequence. Let $\tilde{J}_l = \mu(\{X_{Z_l}\})$ be the mass of the corresponding atom in μ. Then $(\tilde{J}_l)_{l\geq 1}$ is a size-biased permutation of the masses of atoms in μ, with larger masses tending to appear earlier in the sequence. It is easy to see that $\sum_{l\geq 1} \tilde{J}_l = T$, and that the sequence can be understood as a stick-breaking construction: start with a stick of length $T_0 = T$; break off the first piece of length $\tilde{J}_1$; the surplus length of stick is $T_1 = T - \tilde{J}_1$; then the second piece with length $\tilde{J}_2$ is broken off, etc. This construction is called the Size-Biased Sampling (SBS) process.

The conditioning operation from the generative process from Equation 3.13 is not well defined a priori but the following proposition from [70] helps to bypass this difficulty. It also states an interesting Markovian property of the surplus masses, which will be of used to describe a Poisson Kingman (PK) generative process.

Proposition 1 (Perman et al. [70])**.** *The sequence of surplus masses $(T_k)_{k\geq 0}$ forms a Markov chain, where $T_k := T - \sum_{l=1}^{k} J_l$, with initial distribution and transition kernels*

given as follows

$$\begin{aligned}\mathbb{P}_{\rho,H_0}(T_0 \in dt_0) &= f_\rho(t_0)dt_0\\ \mathbb{P}_{\rho,H_0}(T_k \in dt_k | T_0 \in dt_0, \ldots, T_{k-1} \in dt_{k-1}) &= \mathbb{P}_{\rho,H_0}(T_{k-1} \in dt_{k-1})\\ &= \frac{(t_k - t_{k-1})\rho(d(t_k - t_{k-1}))}{t_{k-1}} \frac{f_\rho(t_k)}{f_\rho(t_{k-1})}\end{aligned}$$

Proposition 1 [70] states that the sequence of surplus masses $(T_l)_{l\geq 1}$ forms a Markov chain and gives the corresponding initial distribution and transition kernels. The density of T is denoted by $\gamma(t) \propto h(t)f_\rho(t)$. The PK generative process for the sequence $(X_i)_{i\geq 1}$ goes as follows, where parts of the PK random measure μ are simulated as required.

(i) Draw from the total mass from its distribution $\mathbb{P}_{\rho,H_0}(T \in dt) \propto h(t)f_\rho(t)$.

(ii) The first draw X_1 from μ/T is a size-biased pick from the masses of μ. The actual value of X_1 is simply $X_1^\star \sim H_0$, while the mass of the corresponding atom in μ is $\tilde{J}_1$, with conditional distribution given by

$$\mathbb{P}_{\rho,H_0}(\tilde{J}_1 \in ds_1 | T \in dt) = \frac{s_1}{t}\rho(ds_1)\frac{f_\rho(t - s_1)}{f_\rho(t)}$$

The leftover mass is $T_1 = T - \tilde{J}_1$.

(iii) For subsequent draws $i \geq 2$:

- Let k be the current number of distinct values among $X_1, \ldots, X_{i-1}$, and let $X_1^\star, \ldots, X_k^\star$ be the unique values, i.e., atoms in μ. The masses of these first k atoms are denoted by $\tilde{J}_1, \ldots, \tilde{J}_k$ and the leftover mass is $T_k = T - \sum_{l=1}^k \tilde{J}_l$.
- For each $l \leq k$, with probability $\tilde{J}_l/T$, we set $X_i = X_l^\star$.
- With probability T_k/T, X_i, takes on the value of an atom in μ besides the first k atoms. The actual value $X_{k+1}^\star$ is drawn from H_0, while its mass is drawn from
$$\mathbb{P}_{\rho,H_0}(\tilde{J}_{k+1} \in ds_{k+1} | T \in dt_k) = \frac{s_{k+1}}{t_k}\rho(ds_{k+1})\frac{f_\rho(t_k - s_{k+1})}{f_\rho(t_k)}$$
The leftover mass is again $T_{k+1} = T_k - \tilde{J}_{k+1}$.

By multiplying the above infinitesimal probabilities one obtains the joint distribution of the random elements T, Π, $(\tilde{J}_i)_{i\geq 1}$ and $(X_i^\star)_{i\geq 1}$.

Proposition 2 (Perman et al. [70])**.** *Let Π_n be the exchangeable random partition of $[n] := \{1, \ldots, n\}$ induced by a sample $(X_i)_{i\in[n]}$ from $P \sim PK(\rho, h, H_0)$. Let $(X_l^\star)_{l\in[k]}$ be the k distinct values in $(X_i)_{i\in[n]}$ with masses $(\tilde{J}_l)_{l\in[k]}$. Then*

$$\begin{aligned}&\mathbb{P}_{\rho,H_0}(T \in dt, \Pi_n = (c_l)_{l\in[k]}, X_l^\star \in dx_l^\star, \tilde{J}_l \in ds_l \text{ for } l \in [k])\\ &= h(t)t^{-n}f_\rho(t - \sum_{l=1}^k s_l)dt \prod_{l=1}^k s_l^{|c_l|}\rho(ds_l)H_0(dx_l^\star)\end{aligned}$$

where $(c_l)_{l\in[k]}$ denotes a particular partition of $[n]$ with k blocks, $c_1, \ldots, c_k$, ordered by increasing least element and $|c_l|$ is the cardinality of block c_l.

3.6 MCMC Inference

Constructing Markov chain Monte Carlo (MCMC) schemes for models with one or more Bayesian nonparametric components is an active research area since dealing with the infinite dimensional component P forbids the direct use of standard simulation-based methods. These methods usually require a finite-dimensional representation. The general idea for designing inference schemes is to find finite dimensional representations to be able to store the model in a computer with finite capacity.

There are two main sampling approaches to facilitate simulation in the case of Bayesian nonparametric models: random truncation and marginalisation. These two schemes are known in the literature as conditional and marginal, but hybrid samplers between these two also exist. Each sampler rely on a tailored, thus different, representation of the underlying process. Yet, these samplers are all instances of Gibbs sampler.

3.6.1 Marginal Samplers

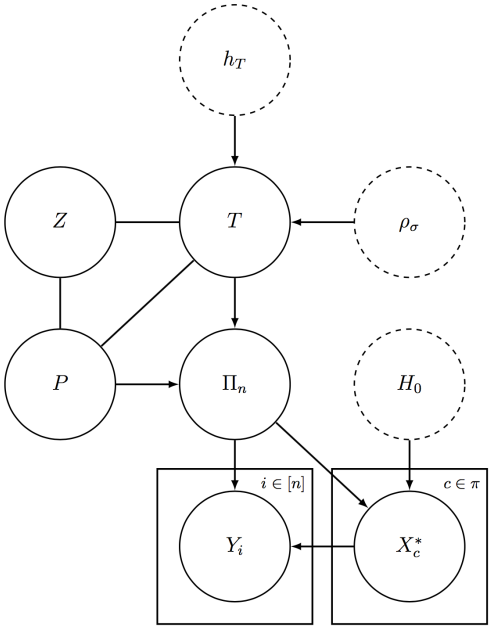

Figure 3.3: *Marginal samplers graphical model. Each node represents a variable used in the augmented representation for the joint distribution. The nodes with dashed lines represent the algorithmic inputs. Source: Maria Lomeli's thesis*

Marginal samplers bypass the need to represent the infinite-dimensional component by marginalising it out. These schemes have lower storage requirements than conditional samplers because they only store the induced partition, but could potentially have worse mixing properties [52].

With a conjugate model (H_0 and F are conjugate), both the RPM P and the cluster parameters $\{X_c^\star : c \in \pi\}$ can be marginalised out efficiently. Yet, for a more generic

nonconjugate marginalized sampler, the cluster parameters cannot be easily marginalised out and are thus included into the state of the MCMC algorithm. This yields the difficulty of the introduction of new clusters (along with their parameters) when Gibbs sampling the cluster assignments.

To tackle this issue, [65] conceptualizes the update in terms of an augmented state with additional temporarily existing variables, in a way that the marginal distribution of the permanent variables once the temporary ones are integrated out is still the appropriate posterior distribution. To do so, the state space is augmented as well to include both existing clusters and new empty clusters $[M] = \{1, \dots, M\}$, which parameters are independent of the existing ones and independent and identically distributed according to H_0. [27] extends this idea originally developed for DP mixtures, for all NRM mixture models.

For instance, if the σ-Stable Poisson-Kingman subclass is picked, then it is possible to obtain a tractable representation, given by Figure 3.2, in terms of some random variables and the partition induced by the RPM. This representation is based on an augmented version of its corresponding exchangeable partition probability function.

3.6.2 Conditional Samplers

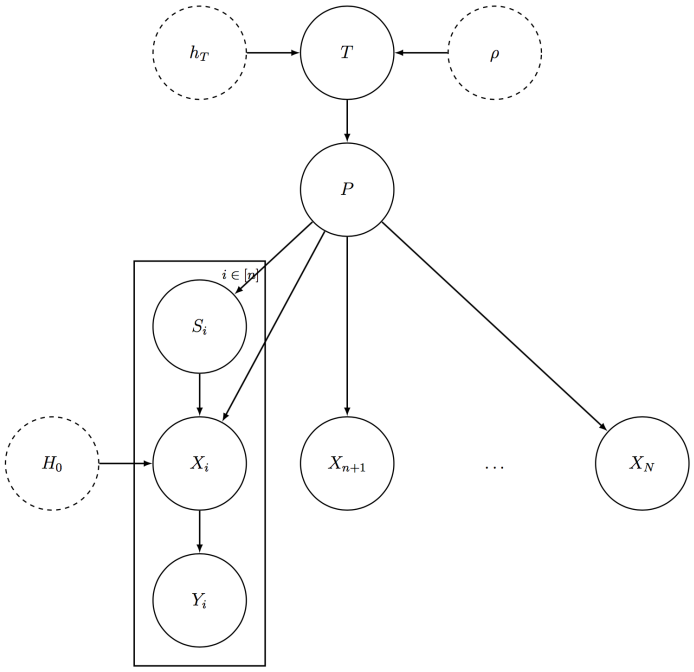

Figure 3.4: *Conditional samplers graphical model. Each node represents a variable used in the augmented representation for the joint distribution. The latent variables represent the number of occupied and unoccupied components. Source: [52].*

Conditional samplers replace the infinite-dimensional prior by a finite-dimensional representation chosen according to a truncation level. Since these samplers do not integrate

out the infinite-dimensional component, their output provides a more comprehensive representation of the random probability measure. Figure 3.4 shows such representation or the σ-Stable Poisson-Kingman family for the conditional slice MCMC sampler [28].

The truncation level needs to be randomised to have an exact MCMC scheme. A slice sampling step [66] within the Gibbs sampler is used in [27] so as to get an efficient sampler. It allows to represent a finite but random number of stick-breaking weights. These weights correspond to the ones that fall above the slice variables, sampled at every iteration. Then, the cluster assignment variable for each observation is chosen from a categorical distribution, where the number of categories given by the number of represented sticks. For this reason, both the number of occupied and empty clusters is stored at every iteration. These numbers could be potentially large.

The stick-breaking weights can be sampled either via a stick-breaking representation of the measure, or via thinning [27]. Unfortunately, only few models have a tractable stick-breaking representation, such as the DP, the Pitman-Yor process (PY) or a sub-class of σ-stable Poisson-Kingman models [25].

3.6.3 Hybrid Samplers

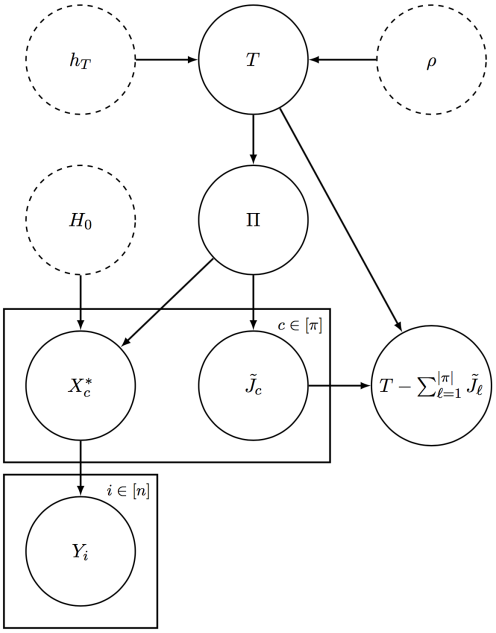

Figure 3.5: *PK hybrid samplers graphical model. Each node represents a variable used in the augmented representation for the joint distribution. The nodes with dashed lines represent the algorithmic inputs. Source: [52].*

An hybrid MCMC scheme has been developed [53], and combines the main strengths of both conditional and marginal MCMC samplers.

This hybrid scheme makes use of a representation of the model where only the size-biased weights associated to occupied clusters are needed to be explicitly represented along with

a surplus mass term, associated to the rest of the empty clusters. Figure 3.5 shows this tractable and compact representation for a Poisson-Kingman mixture model is based. The cluster reassignment step can be seen as a retrospective sampling scheme: we explicitly represent and update the weights associated to occupied clusters and create a new size-biased weight only when a new cluster appears.

This scheme has less memory requirements since it only represents the size-biased weights associated to occupied clusters as opposed to conditional samplers which represent both empty and occupied clusters. Also, since it does not integrate out all of the size-biased weights, we obtain a more comprehensive representation of the RPM.

3.6.4 Sequential Monte Carlo

Recently, various Sequential Monte Carlo (SMC) schemes (see Section 4.5.4 for more details on SMC) for Bayesian nonparametric models have been proposed. [29] and [90] propose an SMC scheme for Dirichlet process mixture models and [39] for NRM mixture models. These articles cast the marginal and conditional representations presented previously in a particle algorithm's setting.

3.7 Variational inference

To my knowledge, the first article tackling inference in a BNP setting is [10], where a truncated proposal is introduced to approximate a Dirichlet Process Mixture model.

Truncation-free variational inference methods have also been introduced [11]. These methods adapts model complexity on the fly by lazily representing clusters assignments. Yet, the sticks proportions and mixture components are marginalized out to obtain a closed form distribution for the mixture assignment hidden variables z_i. This marginalization is unfortunately only tractable for few models, such as the Dirichlet Process and the Pitman-Yor process.

Probabilistic programming

4.1 What is it ?

At a high level, PPLs are Programming Language (PL) techniques to abstract inference algorithms from statistics such that they apply automatically and correctly to the broadest possible set of model-based reasoning applications.

A bit more precisely, Probabilistic programming systems [35, 36, 58, 91] represent generative models as programs written in a specialized language that provides syntax for the definition and conditioning of random variables.

Indeed, "probabilistic programs are usual functional or imperative programs with two added constructs: (1) the ability to draw values at random from distributions, and (2) the ability to condition values of variables in a program via observations." [38]

Probabilistic programs define probability distributions over sequences of values, implicitly by means of program execution.

4.2 Why is it useful ?

For data science practitioners, statistical inference is typically just one step in a more elaborate analysis workflow. The first stage of this work involves data acquisition, preprocessing and cleaning. This is often followed by several iterations of exploratory model design and testing of inference algorithms. Once a sufficiently robust statistical model and a corresponding inference algorithm have been identified, analysis results must be post-processed, visualized, and in some cases integrated into a wider production system.

The main goal of PPLs is to increase productivity. The code for models written with these systems is generally concise, modular, and easy to modify or extend. Thus, one of the savings is to be found in the amount of code that needs to written in order to prototype and develop models.

Secondly, PPLs remove the burden of having to develop inference code for each new model which is error-prone and time consuming. This is done by providing a modeling language abstraction layer in which developers can denote their models. Once denoted, generic inference is provided for free.

4.3 Existing languages

The first generation of PPLs had limitation in the range of models that could be represented and in which inference could be performed. BUGS [55] and STAN [13] can only work with graphical models. Similarly, Factorie [59] and Infer.NET [62] only handle factor graphs. These so-called *First-Order* Probabilistic Programming Languages (PPLS), can only represent finite dimensional model and have bounded loops.

On the other hand, *High Order* PPLS which arrived a bit before the 2010s, are Turing complete, allow complex control flow, including stochastic recursion, thus can denote infinite dimensional objects. Anglican [91], Venture [58], Church [35] and WebPPL [36] are *High Order* PPLS.

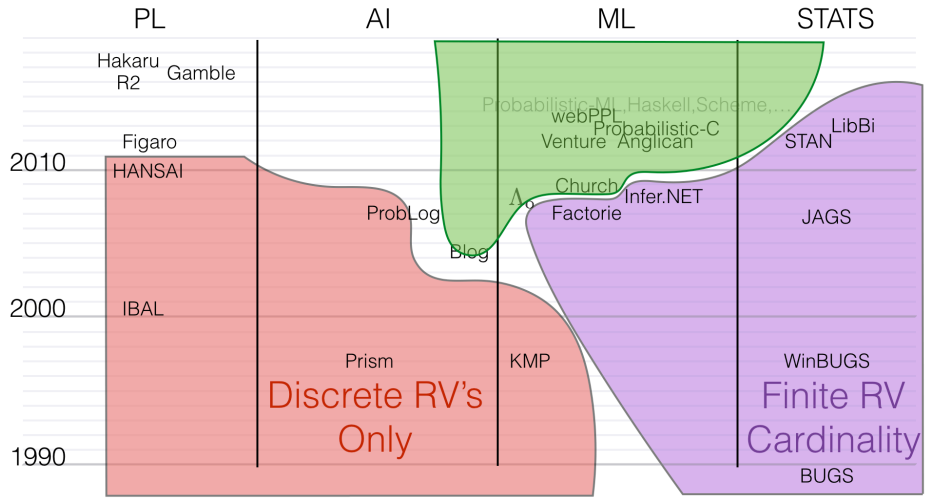

Figure 4.1: *First-order and high-order* PPLS. *Source: http://www.robots.ox.ac.uk/ fwood.*

Figure 4.1 shows a map of existing PPLs, with first-order ones being in red and purple (bottom left/right), and high-order ones in green (top). On one side, first-order PPLs are quite restrictive since the spectrum of models that can be represented is limited to finite dimensional models, but inference can be performed efficiently. On the other side, high-order PPLs are more flexible but the task of writing efficient inference algorithm is harder. There is therefore a trade-off between flexibility and efficiency, and the restrictions of first-order PPLs are a design choice.

Recently, a new PPL named Edward [84] has been developed. It is different from the classical PPLs since it focuses on variational inference (VI) and Hamiltonian methods.

4.4 Design

Probabilistic programs denote probabilistic generative models as programs that include `sample` and `observe` statements (see Listing 4.1). Both `sample` and `observe` are functions that specify random variables in this generative model using probability distribution

objects as an argument, while `observe`, in addition, specifies the conditioning of this random variable upon a particular observed value in a second argument. These observed values induce a conditional probability distribution over the execution traces whose approximations and expected values we aim to characterize by *performing inference*.

```
@model model(y) = begin
  x = sample(Bernoulli(.75))
  mu = x ? 2 : 0
  observe(Gaussian(mu, 1), y)
  return x
end

sample(model(0.5), SMC(100))
```

Listing 4.1: *Example of a Turing.jl model*

A good way to understand this is to imagine the following interpreter of probabilistic programs. Starting from a fixed initial state, the interpreter runs the deterministic parts of a program according to the standard semantics, executes the `sample` statement by generating a random sample, and treats the `observe` statement by skip. More importantly, the interpreter keeps a log that records information about all the `sample` and `observe` forms encountered during execution. The information recorded for `sample` is a triple (F, x, α) of (i) a primitive probability distribution F, such as the standard normal, for which we have the probability density f ; (ii) a value x sampled from the distribution F ; and (iii) an address α that uniquely and systematically identifies the random choice made. The information recorded for `observe` is a pair (G, y) where G is a primitive probability distribution with density g and y is an observed value.

An execution trace $\mathbf{x}$ is defined to be a sequence of triples (F, x, α) and $\mathbf{x}$ is said feasible if the trace is precisely the triple part of the log of some execution. The observed values are denoted by $\mathbf{y} := (y_j)_{j=1}^{N}$.

In most probabilistic programming systems any variable may be declared as being the output of a random procedure. Such variables can take different values in independent interpretations of the program. This leads to a "many-worlds" computational trace tree in which, at interpretation time, there is a branch at every random procedure application.

A (almost-surely terminating) probabilistic program defines a probability distribution over finite feasible traces $\mathbf{x}$ with probability density $\pi(\mathbf{x}) := \gamma(\mathbf{x})/Z$ where

$$\gamma(\mathbf{x}) := p(\mathbf{x}, \mathbf{y}) = \prod_{i=1}^{|\mathbf{x}|} f_i(x_i \mid x_{1:i-1}) \prod_{j=1}^{|\mathbf{y}|} g_j(y_j \mid x_{1:\tau(j)})$$

where Z is the normalizing constant $Z := \int \gamma(\mathbf{x}) d(\mathbf{x})$ and τ is a mapping from the index j of the `observe` statement to the index of the last `sample` statement encountered before this `observe` statement during the execution of the program. Without any `observe` statement, the probability distribution over traces $\mathbf{x}$ is simply the prior

$$p(\mathbf{x}) := \prod_{i=1}^{|\mathbf{x}|} f_i(x_i \mid x_{1:i-1})$$

4.5 Inference

Inference in probabilistic programming characterizes the conditional distribution of execution traces $\mathbf{x}$ given observed data $\mathbf{y}$ assumed to have been generated by executing the probabilistic program.

Concretely, using the `sample` statements, the PPL's model first defines a so called prior distribution on these execution traces, and then it adjusts this prior distribution based on observations in data using the `observe` statement. Samples from this conditioned distribution (also called posterior distribution) can be obtained by running the model under one of the PPLs inference algorithms.

The inference algorithms may make random choices that do not correspond to any statements in the program, and decide which parts of the program code are executed and how often. Some inference algorithms re-run the program multiple times partially, from a certain point on, while reusing random choices made in the previous runs as much as possible. Upon encountering a sample or observe record, the inference algorithm computes the updated program state and the value to be passed to the continuation. How the state is updated, the number of times the continuation is called, and the value passed to the continuation of sample depend on the inference algorithm executing the program. Implementing an inference algorithm in PPLs amounts to defining checkpoint handlers for `sample` and `observe`.

Typically inference can be performed for any probabilistic program using one or more generic inference techniques provided by the system back end, such as Metropolis-Hastings [88, 58], Hamiltonian Monte Carlo [13], expectation propagation [62], and extensions of Sequential Monte Carlo [85, 69, 92] methods.

4.5.1 Use-case

Even if as highlighted before, inference in PPLs should be able to deal with arbitrary series of targets, for simplicity we will focus on a non-Markovian State-Space Model (SSM).

SSMs are probabilistic models over a set of latent variables $X_t \in \mathcal{X}_t, \forall t = 1 : T$ and observed variables $Y_t \in \mathcal{Y}_t, \forall t = 1 : T$. We can further consider a model to be parameterized by $\theta \in \Theta$. The SSM is then characterized by an initial density $\mu_\theta(x_1)$, a series of transition densities $f_{t,\theta}(x_t|x_{1:t-1})$, and a series of emission densities $g_{t,\theta}(y_t|x_{1:t})$.

$$\begin{aligned} X_1 &\sim \mu_\theta(\cdot) \\ X_t|(X_{1:t-1} = x_{1:t-1}) &\sim f_{t,\theta}(\cdot|x_{1:t-1}) \\ Y_t|(X_{1:t} = x_{1:t}) &\sim g_{t,\theta}(\cdot|x_{1:t}) \end{aligned}$$

The joint density of the SSM is then as follows

$$\gamma_\theta(\mathbf{x}) := p_\theta(x_{1:T}, y_{1:T}) = \mu_\theta(x_1) \prod_{t=2}^{T} f_{t,\theta}(x_t|x_{1:t-1}) \prod_{t=1}^{T} g_{t,\theta}(y_t|x_{1:t})$$

We are free to choose any density for $\mu_\theta(x_1)$ and each $f_{t,\theta}(x_t|x_{1:t-1})$ and $g_{t,\theta}(y_t|x_{1:t})$. One is usually interested characterizing the posterior

$$p_\theta(x_{1:T}|y_{1:T}) \propto p_\theta(x_{1:T}, y_{1:T})$$

Or expectations of some function ϕ under this posterior

$$I(\phi) = \int \phi(x_{1:T}) p_\theta(x_{1:T}|y_{1:T}) dx_{1:T}$$

4.5.2 Enumeration

The easiest way one could think of to perform inference in a probabilistic program is via *rejection sampling*. An execution trace can be thought of a *path* in a *tree* implicitly defined by a discrete model. This tree could then be explored using depth-first search, breadth-first search, or a probability-based priority queue. Then only the paths matching the observations $\mathbf{x}$ are retained and the others are rejected. These retained execution traces form the targeted posterior distribution.

4.5.3 Markov Chain Monte Carlo

Yet, for many models with large state spaces, enumeration is infeasible. This is particularly clear for models with continuous random variables, where the state space is infinite. In the case of a large number of execution paths, one should avoid exploring all paths individually but only a subset of paths.

A popular way to estimate a difficult distribution is to sample from it by constructing a random walk that will visit each state in proportion to its probability. This class of algorithms are called MCMC. In our case, we are interested in random walk in the space of execution traces of a computation.

For discrete models, an easy way to a build random walk in the space of executions is to execute the probabilistic program by sampling variables at `sample` AND `observe` statements. The proposed execution trace $\mathbf{x}^\star$ shall then be rejected if at least one of the true observation y_k does not match the associated generated observation $y \sim G$. If accepted, that means that this trace is one of the trace that can lead to the observations $\mathbf{y}$, i.e. it belongs to the support of the targeted posterior distribution $p(\mathbf{x}|\mathbf{y})$. This method is called *rejection sampling*. Yet, for highly dimensional space, this method will accept quite rarely a proposed trace. What is more, for continuous models, it will almost-surely never be accepted.

A more complex Markov Chain needs to be built to have a reasonable acceptance rate. Given a current trace $\mathbf{x}$ and score $p(\mathbf{x})$, we proceed by reconsidering one random choice x_k. Each `sample` statement is equipped with a proposal kernel $\mathcal{K}_k(x^\star|x, \psi)$, which is used

to generate proposals to x_k. A random walk can the be built by (i) randomly choosing $k \in 1, \ldots, |\mathbf{x}|$, (ii) sample a new value $x_k^\star$ with $\mathcal{K}_k(x_k^\star|x_k, \psi)$ and (iii) re-run the program starting from x_k which generate a new trace $\mathbf{x}^\star$. This new execution trace is accepted with probability

$$1 \wedge \frac{\gamma(\mathbf{x}^\star)\mathcal{K}_k(x_k|x_k^\star, \psi)}{\gamma(\mathbf{x})\mathcal{K}_k(x_k^\star|x_k, \psi)}$$

This is better than our previous Metropolis-Hastings (MH) algorithm, but when the chosen k is close to 1, it is almost as sampling from the prior since we only reuse the random choices made before the point of regeneration. So as to avoid having a small acceptance rate, it is generally better to make smaller steps by reusing as many choices as possible. If we knew which sampled value was which, then we could look into the previous trace as the execution runs and reuse its values. That is, imagine that each call to sample was passed a (unique) name: `sample(name, dist)`. Then the `sample` function could try to look up and reuse values. Notice that, in addition to reusing existing sampled choices, we add the name and mark whether this choice has been resampled. We must account for this in the MH acceptance calculation. We now hope to reuse most of the choices from the old trace in making a proposal. This algorithm is called Lightweight MCMC [88], and has been improved in [77].

More generally, for an excellent introduction to MCMC and particle inference in PPLs, see [36].

4.5.4 Importance Sampling

Importance Sampling Importance sampling is an example of a Monte Carlo sampling scheme that provides approximately independent and identically distributed samples from a distribution of interest or target distribution, such as a posterior distribution, by generating a candidate sample from a proposal or importance distribution $q(\mathbf{x}|y_1, \ldots, y_T)$. The fact that the weights $w^k = \frac{p(\mathbf{x}, y_1, \ldots, y_T)}{q(\mathbf{x}|y_1, \ldots, y_T)} \propto \frac{p(\mathbf{x}|y_1, \ldots, y_T)}{q(\mathbf{x}|y_1, \ldots, y_T)}$, with $k \in 1, \ldots, K$ can be computed is exploited, and samples from the target are obtained by sampling from the following weighted empirical distribution

$$\hat{p}(\mathbf{x}|y_1, \ldots, y_T) = \sum_{k=1}^{K} \bar{w}^k \delta_{\tilde{\mathbf{x}}^k}(\mathbf{x})$$

where $\bar{w}^k = \frac{w^k}{\sum_{k=1}^K w^k}$ is the normalized weight and δ_z is a Dirac measure centered on z. The expectation $I(\phi)$ can also be approximated using

$$\hat{I}(\phi) = \sum_{k=1}^{K} \bar{w}^k \phi(\tilde{\mathbf{x}})$$

One problem with this method is that it is not easy to choose the proposal distribution q. A good proposal should share most of the support of the target distribution and have the same number of modes, i.e. it should be close to the target. A second problem is that it

is a batch estimation method. To tackle this latter issue, in the next section, an extension to a sequential scenario is described.

Sequential Importance Sampling Sequential Importance Sampling (SIS) exploits the structure of a model by breaking down the overall inference problem into a series of target distributions which get incrementally closer to the distribution of interest. These targets are then approximated by propagating a population of samples known as particles. If each intermediary target is kept similar to its predecessor, approximating one target given the last forms a significantly simpler problem than the overall inference. Breaking the overall inference problem into a series of intermediate distributions makes the design of proposals easier since they must now be of the form $q(x_t|x_{1:t-1}, y_{1:t})$ instead of $q(x_{1:T}|y_{1:T})$.

More formally, SIS performs approximate inference on a sequence of target distributions $(\pi_t(x_{1:t}))_{t=1}^T$ of increasing spaces $(\mathcal{X}_1 \times \cdots \times \mathcal{X}_t)_{t=1}^T$. In the context of SSMs, the target distributions are taken to be $(p_\theta(x_{1:t}|y_{1:t}))_{t=1}^T$. At each time step t, we have a set of K particles $\left(\tilde{x}_{1:t}^k\right)_{t=1}^T$, corresponding to samples of the latents, and respective particle weights $\left(w_t^k\right)_{t=1}^T$. Similarly to Importance Sampling (IS), using these weighted particles, one can approximate each posterior $p_\theta(x_{1:t}|y_{1:t})$. In particular, the posterior for the complete model $p_\theta(x_{1:T}|y_{1:T})$ and the expectation $I(\phi)$ can be approximated using the following estimators

$$\hat{p}(x_{1:T}|y_{1:T}) = \sum_{k=1}^{K} \bar{w}_T^k \delta_{\tilde{x}_{1:T}^k}(x_{1:T})$$

$$\hat{I}(\phi) = \sum_{k=1}^{K} \bar{w}_T^k \phi(\tilde{x}_{1:T})$$

where $\bar{w}_T^k = \frac{w_T^k}{\sum_{k=1}^K w_T^k}$ is the normalized weight.

Let's now focus on computing the particles' weights. The joint posterior can be written in the following factorised form

$$p(x_{1:T}|y_{1:T}) = p(x_1) \prod_{t=2}^{T} p(x_t|x_{1:t-1}, y_{1:t})$$

The corresponding importance weights are thus

$$\begin{aligned} w_t =& \frac{p(x_{1:T}|y_{1:T})}{q(x_{1:T}|y_{1:T})} \\ w_t =& \frac{\mu(x_1) \prod_{t=2}^{T} p(x_t|x_{1:t-1}, y_{1:t})}{q(x_1) \prod_{t=2}^{T} q(x_t|x_{1:t-1}, y_{1:t})} \end{aligned} \tag{4.1}$$

The target distribution is the posterior distribution up to time t, which changes sequentially as we observe more data. This posterior distribution can be estimated recursively

due to

$$p(x_{1:t+1}|y_{1:t+1}) = p(x_{1:t}|y_{1:t}) \times \frac{p(y_{t+1}|x_{1:t+1})p(x_{t+1}|x_{1:t})}{f(y_{t+1}|y_{1:t})} \tag{4.2}$$

Substituting the numerator of Equation 4.2 in 4.1 we obtain a recursive equation for the importance weight at time $t+1$

$$w_{t+1} = w_t \times \frac{p(y_{t+1}|x_{1:t+1})p(x_{t+1}|x_{1:t})}{q(x_{t+1}|x_{1:t}, y_{1:t+1})}$$

Even if we are not dealing with a SSM, SIS can be used as a general-purpose algorithm. The data are assumed to be observed sequentially so the observations index is the time index.

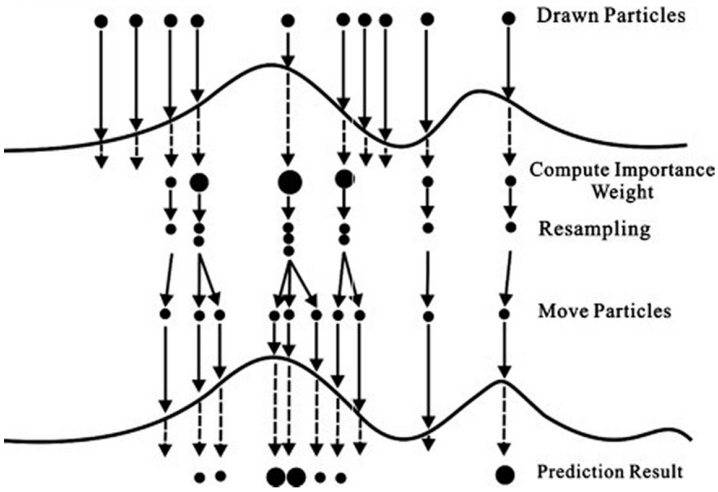

Figure 4.2: *Sequential Monte Carlo's algorithm main steps.*
Source: https://umbertopicchini.wordpress.com/2016/10/19/sequential-monte-carlo-bootstrap-filter.

Sequential Monte Carlo The main problem with SIS is that the weights become more skewed as the number of data points increases [20], after a few steps only one particle will have a significant weight. To remedy this, a resampling step can be introduced which allows to eliminate particles with small weights and replicate particles with high weights, as illustrated in Figure 4.2. The resampling step is achieved by, at each time step $t = 2, \ldots, T$, selecting the ancestor index a_{t-1}^k for the kth particle from a discrete distribution $\mathcal{F}(\cdot|\bar{w}_{t-1}^1, \ldots, \bar{w}_{t-1}^K)$ over parent indices $1, \ldots, K$ with probabilities equal to the normalized weights at the previous time step $(\bar{w}_{t-1}^1, \ldots, \bar{w}_{t-1}^K)$. The first resampling scheme introduced was the multinomial resampling for which $\mathbb{P}(a_{t-1}^k = i) \propto \bar{w}_{t-1}^i$. [19] provides a comparison of numerous different schemes for sampling from $\mathcal{F}(\cdot|\bar{w}_{t-1}^1, \ldots, \bar{w}_{t-1}^K)$ that reduce the variance of the SMC estimates compared with naïve multinomial resampling.

This selection step can be introduced only occasionally or at every step of the algorithm. If the selection step is to be performed occasionally, a possible criterion is when the Effective Sample Size (ESS) is below a given threshold, which is a function of the number of particles, a popular choice is $0.5T$. The ESS for the unnormalised weights is given by

$$ESS_t = \frac{\left(\sum_{k=1}^K w_t^k\right)^2}{\sum_{k=1}^K {w_t^k}^2}$$

At step t, after the ancestors indices $\{a_{t-1}^k\}_{k=1}^K$ have been sampled, new $\{x_t^k\}_{k=1}^K$ are proposed according to $q(\cdot|x_{1:t-1}, y_{1:t})$. Then, the particles' weights can be computed given

$$\begin{aligned} w_t^k :=& \frac{p(x_{1:t}^k, y_t)}{p(x_t^k|x_{1:t-1})q(x_t^k|x_{1:t-1}^k, y_{1:t})} \\ =& \frac{p(y_t|x_{1:t}^k)p(x_t^k|x_{1:t-1}^k)}{q(x_t^k|x_{1:t-1}^k, y_{1:t})} \end{aligned}$$

PPLs implementation of SMC One a practical point of view, so as to handle particle algorithms, PPLs must have the ability to stop the execution of the program at each time t (more generally at each `observe` statement). Indeed, these *chechpoints* are required by the SMC algorithm for the resampling step. Handling of checkpoints can be implemented through coroutines/co-operative multitasking (as in Turing [31]), and parallel execution/preemptive multitasking, as well as through explicit maintenance of program continuations (as in *Anglican* [91] and *WebPPL* [36]).

Moreover, the proposals $q(\cdot|x_{1:t-1}, y_{1:t})$ are generally implemented as being the prior $p(\cdot|x_{1:t-1})$ in PPLs, i.e. the program is simply ran until an `observe` statement is encountered. Yet, by overriding the `sampler` statements, different proposals can be implemented. In the former case, the weights simplify to the likelihood; $w_t^k = p(y_t|x_{1:t}^k)$, which can be computed at the `observe` statements.

4.5.5 Particle Markov Chain Monte Carlo

In a Bayesian setting, it is usual to consider the parameter θ in $p_\theta(x_{1:T}|y_{1:T})$ as a random variable by specifying a prior $p(\theta)$. In this subsection, we are therefore interested on algorithms targeting $p(\theta, x_{1:T}|y_{1:T})$. Let's think about MCMC algorithms targeting the distribution $p(\theta, x_{1:T}|y_{1:T})$ which rely on sampling exactly from $p_\theta(x_{1:T}|y_{1:T})$, called idealized algorithms. Such algorithms are purely conceptual but a natural idea consists of approximating these idealized algorithms by using the output of an SMC algorithm targeting $p_\theta(x_{1:T}|y_{1:T})$ using $K \geq 1$ particles as a proposal distribution for an MH update. Intuitively this could allow us to approximate with arbitrary precision such idealized algorithms while only requiring the design of low dimensional proposals for the SMC algorithm.

A direct implementation of this idea is impossible as the marginal density of a particle that is generated by an SMC algorithm is not available analytically but would be required for the calculation of the MH acceptance ratio. Yet the SMC algorithm yields an unbiased estimate of the marginal likelihood

$$\hat{p}(y_{1:T}) = \prod_{t=1}^{T} \frac{1}{K} \sum_{k=1}^{K} w_t^k$$

which can be used for the calculation of the MH acceptance ratio. These Particle Markov chain Monte Carlo (PMCMC) updates have been introduced in [3]. The key feature of PMCMC algorithms is that they are in fact exact approximations to idealized MCMC algorithms targeting either $p(\theta, x_{1:T}|y_{1:T})$ in the sense that for any fixed number $N \geq 1$ of particles their transition kernels leave the target density of interest invariant.

Particle Marginal Metropolis-Hastings Particle Marginal Metropolis-Hastings (PMMH) makes use of the standard decomposition $p(\theta, x_{1:T}|y_{1:T}) = p(\theta|y_{1:T})p_\theta(x_{1:T}|y_{1:T})$. It is natural to suggest the following form of proposal density for an MH update:

$$q\left(\theta^\star, x_{1:T}^\star|\theta, x_{1:T}\right) = q(\theta^\star|\theta)p_{\theta^\star}(x_{1:T}^\star|y_{1:T})$$

for which the proposed $x_{1:T}^\star$ is given by a SMC algorithm targeting $p_{\theta^\star}(x_{1:T}|y_{1:T})$. Thus, the only degree of freedom of the algorithm (which will affect its performance) is $q(\theta^\star|\theta)$. The resulting MH acceptance ratio is given by

$$1 \wedge \frac{p_{\theta^\star}(y_{1:T})p(\theta^\star)q(\theta|\theta^\star)}{p_\theta(y_{1:T})p(\theta)q(\theta^\star|\theta)}$$

PMMH uses $\hat{p}(y_{1:T})$ to compute the acceptance ratio. It has been proven [3] that the PMMH update leaves $p(\theta, x_{1:T}|y_{1:T})$ invariant and that under weak assumptions the PMMH sampler is ergodic.

Particle Gibbs An alternative to the previous algorithm to sample from $p(\theta, x_{1:T}|y_{1:T})$ consists of using the Gibbs sampler which samples iteratively from $p(\theta|x_{1:T}, y_{1:T})$ and $p_\theta(x_{1:T}|y_{1:T})$. It is often possible to sample from $p(\theta|x_{1:T}, y_{1:T})$ and thus the potentially tedious design of a proposal density for θ that is necessary in the PMMH update can be bypassed.

It has been shown [3] that the naïve particle approximation to the Gibbs sampler where sampling from $p_\theta(x_{1:T}|y_{1:T})$ is replaced by sampling from an SMC approximation $\hat{p}_\theta(x_{1:T}|y_{1:T})$ does not admit $p(\theta, x_{1:T}|y_{1:T})$ as invariant density.

A valid particle approximation to the Gibbs sampler requires the use of a special type of PMCMC update called the *conditional* SMC update. This update is similar to a standard SMC algorithm but is such that a prespecified path $x_{1:T}^\star$ is ensured to survive all the resampling steps, whereas the remaining $N - 1$ particles are generated as usual.

Particle Gibbs with Ancestor Sampling A drawback of Particle Gibbs (PG) is that it can be particularly adversely affected by path degeneracy in the Conditional Sequential Monte Carlo (CSMC) step. Conditioning on an existing trajectory means that whenever resampling of the trajectories results in a common ancestor, this ancestor must correspond to this trajectory. Consequently, the mixing of the Markov chain for the early steps in the

state sequence can become very slow when the particle set typically coalesces to a single ancestor during the CSMC sweep.

[51] introduces Particle Gibbs with Ancestor Sampling (PGAS), which alleviates the problem with path degeneracy by modifying the original PG kernel with a so-called Ancestor Sampling (AS) step. The idea is to sample a new value for the index variable a_t^N in an ancestor sampling step. While this is a small modification of the algorithm, the improvement in mixing can be quite considerable. The task is to artificially assign a history to the partial path $(x_{t:T}^\star)$ of the reference path. This is done by connecting $(x_{t:T}^\star)$ to one of the particles $(x_{1:t-1}^k)$. The ancestor index of the reference path $(x_{t:T}^\star)$ at time t $a_t^N \in \{1, \ldots, K\}$ encodes the ancestry of this particle.

To assign a history to this partial path, first the following weights are computed

$$\tilde{w}_{t-1|T}^k := w_{t-1}^k \frac{p((x_{1:t-1}^k, x_{t:T}^\star), y_{1:T})}{p(x_{1:t-1}^k, y_{1:t-1})}$$

for $k = 1, \ldots, K$. Then, a_t^K is sampled via $\mathbb{P}\left(a_t^K = k\right) \propto \tilde{w}_{t-1|T}^k$.

Interacting Particle Markov Chain Monte Carlo Interacting Particle Markov Chain Monte Carlo (IPMCMC) [73] is another way of tackling the path degeneracy issue. In IPMCMC, a pool of CSMC and unconditional SMC algorithms are ran as parallel processes (referred as nodes. After each run of this pool, successive Gibbs updates are applied to the indexes of the CSMC nodes, such that the indices of the CSMC nodes changes. Hence, the nodes from which retained particles are sampled can change from one MCMC iteration to the next. This lets us trade off exploration (SMC) and exploitation (CSMC) to achieve improved mixing of the Markov chains.

4.5.6 Hamiltonian samplers

Hamiltonian Monte Carlo In Hamiltonian Monte Carlo (HMC) [21, 67], a deterministic proposal process based on Hamiltonian dynamics is employed along with additional stochastic proposals that together provide an ergodic Markov chain capable of making large transitions that are accepted with high probability. The Hamiltonian makes use of the gradient of the joint distribution $p(\mathbf{x}, \mathbf{y})$ so as to construct better proposal.

No-U-Turn Sampler In [41], the authors address the issue of choosing the two hyperparameters of HMC: a step size ϵ and a desired number of steps L, since HMC's performance is highly sensitive on those.

First, No-U-Turn Sampler (NUTS) uses a recursive algorithm to build a set of likely candidate points that spans a wide swath of the target distribution, stopping automatically when it starts to double back and retrace its steps. The number of recursion calls is chosen to be the number of leapfrogs steps. Moreover, if α_t is the Metropolis acceptance probability for iteration t and δ is the desired average acceptance probability, we would like the statistic $H_t = \delta - \alpha_t$ to decreases towards 0. NUTS achieves that goal by adaptively computing the step size using the dual averaging scheme of Nesterov [68], an algorithm for nonsmooth and stochastic convex optimization.

Stochastic Gradient Markov Chain Monte Carlo A recent focus has been on devising scalable variants of MCMC algorithms that subsample the data and use stochastic gradients in place of full-data gradients in the dynamic simulations. Such algorithms are called Stochastic Gradient Markov chain Monte Carlo (SGMCMC) and a recipe has now been given [56] for deriving these schemes. SGMCMC algorithms are well suited for online setting and can scale to big datasets. Stochastic Gradient Langevin Dynamics (SGLD) [87] and Stochastic Gradient Hamiltonian Monte Carlo (SGHMC) [14] are examples of these schemes.

4.5.7 Variational Inference

MCMC methods can be slow to converge and their convergence can be difficult to diagnose. One class of alternative methods is provided by variational inference methods [44, 32]. The basic idea of variational inference is to formulate the computation of a marginal or conditional probability in terms of an optimization problem. This (generally intractable) problem is then "relaxed", yielding a simplified optimization problem that depends on a number of free parameters, known as variational parameters. Solving for the variational parameters gives an approximation to the marginal or conditional probabilities of interest.

To my knowledge, Edward [84] is the only PPL handling variational inference.

4.6 Contributions

During this internship I have taken the time to actually implement several inference algorithms, and by so, I contributed to two existing PPLs. Some only for the sake of learning more about sampling schemes and PPLs, but others as specifically part of the project.

First, I implemented [1] both the SGLD [2] and SGHMC inference algorithms in Turing.jl [31], a PPL based on Julia [7] and developed at the University of Cambridge. Then, I implemented [3] the Dual Averaging extension [41] of HMC for Edward [84], a PPL built on top of Tensorflow [1] by Blei's group [4] at Columbia University.

More recently, I have worked on PMCMC methods for Turing. PMMH [5] is implemented but not merged yet, and I am currently working on PGAS and IPMCMC. Consequently I became a *Collaborator* of the Turing's repository.

I have also written a stick-breaking representation of the Dirichlet Process which inherits the Distribution.jl [6] type so as to be easily used in Turing.

[1] See `https://github.com/yebai/Turing.jl/tree/master/src/samplers`

[2] See for instance, SGLD applied to a Bayesian logistic regression at `https://github.com/yebai/Turing.jl/blob/master/example-models/sgld-paper/lr_sgld.jl`

[3] See `https://github.com/blei-lab/edward/pull/728`

[4] `http://www.cs.columbia.edu/~blei/`

[5] `https://github.com/yebai/Turing.jl/pull/339`

[6] `https://github.com/JuliaStats/Distributions.jl`

BNP inference within PPLs

In this chapter we focus on the task of performing inference within a PPL for models with an infinite dimensional component, also called BNP models. For now we have restricted ourselves to infinite mixture models, but we hope that our framework will enable efficient sampling for other BNP models such as the infinite Hidden Markov Model [5]. We have also focused our study on sampling methods, but variational inference is considered in Section 6.3.

5.1 Recursion is key

In PPLs, to transform a variable in a random variable, one only needed to write `x = sample(Dist(parameters))`. Then the posterior distribution (given some observations) of `x` will automatically be performed during the inference scheme. The Bayesian setting thus naturally fits the framework of PPLs. Yet, we believe that there is more than just a connection between Bayesian inference and PPLs, but that there is also a connection between Bayesian Nonparametric and High-order PPL.

Working with BNP models can be impossible because of the constraints of computers. A NRM P can be written [45] as

$$P = \sum_{k \geq 1} \tilde{p}_k \delta_{X_k^\star}$$

where $(\tilde{p}_k, X_k^\star)_{k \geq 1}$ is an infinite collection of weights and atoms. Discrete probability measures with countable support such as Normalised Random Measures cannot be represented in a computer in a naïve manner since a machine has finite memory. Other representations of such objects must be used, if one hope to denote them in a program.

One key notion in programming languages which will be crucial is the concept of *lazy evaluation* (or *laziness*). It is an evaluation strategy which delays the evaluation of an expression until its value is needed and which also avoids repeated evaluations. Lazy evaluation is often combined with *memoization*, as described in [6]. After a function's value is computed for that parameter or set of parameters, the result is stored in a lookup table that is indexed by the values of those parameters; the next time the function is called, the table is consulted to determine whether the result for that combination of parameter values is already available. If so, the stored result is simply returned. If not, the function is evaluated and another entry is added to the lookup table for reuse.

Instead of hoping to construct the entire infinite sequence $(p_k, X_k^\star)_{k\geq 1}$, we will only "lazily" sample $(p_k, X_k^\star)$, i.e. when we need them. Since we work with homogeneous CRMs, the $\{X_k^\star\}_{k\geq 1}$ are independent and identically distributed according to the base distribution. Sampling the $(X_k^\star)_{k\geq 1}$ as we need them is therefore trivial. Yet, how could we lazily sample the $(p_k)_{k\geq 1}$? In Subsection 3.3.1, we presented the stick-breaking process, a generative process for constructing of a size-biased permutation of $(p_k)_{k\geq 1}$, denoted $(\tilde{p}_k)_{k\geq 1}$. In Section 5.2 we explore other generative processes, for more generic BNP classes. For now, Let us recall the construction given by [80] for the stick-breaking process:

$$
\begin{aligned}
V_1 &\sim \text{Beta}(1, \alpha) \\
V_2 &\sim \text{Beta}(1, \alpha) \\
&\vdots \\
V_j &\sim \text{Beta}(1, \alpha) \\
&\vdots \\
\tilde{p}_k = V_k \prod_{j=1}^{k-1} (1 - V_j) \quad & k = 1, 2, \dots
\end{aligned}
$$

Therefore, $\tilde{p}_k$ can be seen as the probability of the following sequence of outcomes: $k-1$ Bernouilli draws with respective probabilities V_j , $j = 1, \dots, k-1$, all yield failure, and one last Bernouilli draw with probability V_k yields success. How can this be interpreted as a generative process on an infinite set of discrete outcomes ? Imagine "walking" down the natural numbers in order, flipping a coin with weight V_k (also called stick) for each one; if the coin comes up `false`, we continue to the next natural number; if the coin comes up `true`, we stop and return the current natural number. The probability of getting the natural number k is given by $\tilde{p}_k$ defined above. This is formalised by the procedure `pickStick` in the code sample 5.1 below.

```
function pickStick(sticks, J) = begin
  return rand(Bernouilli(sticks(J))) ? J : pickStick(sticks, J+1)
end

function makeSticks(α) = begin
  sticks = @memoize (index) -> rand(Beta(1, α))
  return () -> pickStick(sticks, 1)
end
```

Listing 5.1: *Dirichlet Process stick-breaking representation written in Julia.*

The individual V_k are drawn lazily, only generating new ones when we have walked out further than furthest previous time. This is the role of the procedure `makeSticks` which uses memoization to enforce this property. Even though we started by imagining an infinite set of sticks we only ever construct a finite subset of them. The above construction of the DP defines a distribution over the infinite set of natural numbers.

Remark that the function `pickStick` is written in a special fashion: it is built via a *recursion*. A *recursive* function has one or more base cases for which the function produces

a result trivially (without recurring), and one or more recursive cases for which the program recurs (calls itself). For programming languages, allowing recursion means allowing a function to call itself within the program text. Moreover, before calling `pickStick`, no one knows the integer which will be returned, i.e. the number of recursion calls, since it is a random variable by construction.

Recall that high-order PPLs allow complex control flow, including stochastic recursion (stated in Section 4.3). *Stochastic* or *unbounded* recursion simply means that the number of recursive calls (also called *depth* of the recursion) is random or unbounded. Therefore, the DP stick-breaking process can be written and executed with such high-order PPLs.

PPLs are some sort of *simulators*, models need to be written as generative processes. Executing such a model – as is – via a PPL's interpreter, is sampling from its prior distribution. Once one can write a model as a generative process, (i.e can sample from the model's prior), the PPL can perform inference on the latent variables. Consequently, for BNP models, a representation similar to the stick-breaking process for the DP, seems to be necessary.

5.1.1 Implementation details

As highlighted, recursion is key to denote BNP models in a PPL. A function is called *tail-recursive* when the recursive call happens as the final action in a function (as for `pickStick`), in which case it can happen without the function call stack growing. In Continuation-Passing Style (CPS), there is no stack – all function calls are tail calls, hence all recursive functions are tail-recursive.

Clojure provides special forms *loop* and *recur* for writing tail-recursive programs. Anglican programs are CPS-converted and do not use the stack. Therefore recursive calls in the Anglican PPL cannot lead to stack overflow. Without such a specific *recur* operator, the call stack can exceed its maximum size and yields errors.

5.1.2 Existing work

Most high-order PPLs indeed already handle some BNP models [35, 91, 37]. See [1] for Anglican's examples of Hierarchical Dirichlet Process or Probabilistic Deterministic Infinite Automata. See also [2] for WebPPL's example of Infinite Hidden Markov Models or Infinite Relational Model. Yet, their experiments are mostly limited to Dirichlet Process, Pitman-Yor process or hierarchical versions of these processes, and often focused on sampling from priors. When performing inference, the used scheme is usually a particle algorithm such as Sequential Monte Carlo or Particle Gibbs.

5.2 Generative process construction

Previously, we recalled that to be able to denote a model in a PPL, one should know how to sample from its prior, i.e. know a generative construction. We also highlighted the fact

[1] `http://www.robots.ox.ac.uk/~fwood/anglican/examples/index.html`
[2] `https://probmods.org/chapters/12-non-parametric-models.html`

that such generative processes are implemented via stochastic recursion.

5.2.1 Stick-breaking processes

The first comprehensive treatment of stick-breaking priors dates back to the paper by Ishwaran and James [42]. There, they introduced a class of stick-breaking priors including as special cases the Dirichlet Process by Ferguson [30] and the two parameter Poisson-Dirichlet process by Perman et al. [70]. Specifically, let H_0 be a nonatomic probability measure on a complete and separable metric space $\mathbb{X}$. Also, let $(V_i)_{i\geq 1}$ be a sequence of independent random variables such that $\sum_{i\geq 1}\mathbb{E}[\log(1-V_i)] = -\infty$. Based on such V_i's, they define a sequence of random probabilities $(\tilde{p}_k)_{k\geq 1}$ as $\tilde{p}_1 = V_1$ and

$$\tilde{p}_k = V_k \prod_{j=1}^{k-1}(1-V_j)$$

for each $k > 1$, and let $(X_k^\star)_{k\geq 1}$ be a sequence of random variables, independent of $(\tilde{p}_k)_{k\geq 1}$, and independent and identically distributed according to H_0. Then,

$$P = \sum_{k\geq 1}\tilde{p}_k \delta_{X_k^\star}$$

is a stick-breaking prior in the class of Ishwaran and James [42].

For any $\sigma \in [0,1)$ and $\theta > -\sigma$, the stick-breaking representation of the two parameter Poisson-Dirichlet process is recovered by assuming the V_k's to be distributed according to the Beta distribution with parameter $(1-\sigma, \theta + k\sigma)$ for each $k \geq 1$. The stick-breaking representation of the DP, which was first derived by Sethuraman [80], is also recovered as special case, by setting $\sigma = 0$.

Apart from the two parameter Poisson-Dirichlet process, most of the discrete random probability measures do not admit a stick-breaking representation in terms of a collection of independent V_i's.

As an example, Favaro et al. [24] derived the stick-breaking representation of the normalized inverse Gaussian process introduced in Lijoi et al. [49]. Specifically, let $b > 0$ and let $(V_k)_{k\geq 1}$ be a sequence of dependent random variables such that, for each $k \geq 1$, the conditional distribution of V_k given $(V_1, \ldots, V_{k-1})$ coincides with the distribution of the random variable

$$\frac{X_k}{X_k + Y_k} \tag{5.1}$$

where X_k is distributed according to the generalized inverse Gaussian distribution and Y_k is distributed according to the positive $\frac{1}{2}$-stable distribution.

According to Favaro et al [25], the normalized inverse Gaussian process [24] is the first example of a prior admitting a stick-breaking representation in terms of dependent V_k's, and such that for any $k \geq 1$ the conditional distribution of V_k given $(V_1, \ldots, V_{k-1})$ is characterized by means of a straightforward transformation of random variables as in 5.1. Favaro et al [25] construct a similar transformation to build a stick-breaking process for a subclass of σ-stable Poisson-Kingman processes.

Similarly, James [43] builds a stick-breaking process for the class of PG(α, ζ)-Generalized Gamma Processes. The V_k's can be generated via the following process:

$$\zeta_0 \sim \zeta$$
$$\vdots$$
$$\zeta_k = \zeta_0 + \sum_{j=1}^{k-1} e_j, \; e_j \sim \text{Exp}(1)$$
$$R_k = \left(\frac{\zeta_{k-1}}{\zeta_k}\right)^{1/\alpha}$$
$$V_k = 1 - \beta_k(1 - R_k), \; \beta_k \sim \text{Beta}(1-\alpha, \alpha)$$
$$\vdots$$
$$\tilde{p}_k = V_k \prod_{j=1}^{k-1}(1 - V_j) \quad , k = 1, 2, \ldots$$

5.3 Models of interest

We focus our task on infinite mixture models. The stick-breaking construction of Subsection 5.2.1 defines a distribution over the infinite set of natural numbers. Ultimately we would like a distribution not over the natural numbers themselves, but over an infinite set of samples from some other distribution H_0 (called the base distribution) which will represent our mixture components. Using the homogeneous assumption, we can easily generalise the DP to this setting by using `@memoize` to associate to each natural number, a draw from the base distribution. This is what the code sample 5.2 formalises.

```
function DPmem(α,H0) = begin
  augmentedProc = @memoize (stickIndex) -> rand(H0)
  DP = makeSticks(α)
  return () -> augmentedProc(DP())
end
```

Listing 5.2: *Dirichlet Process with base distribution H_0 written in Julia.*

We uses this DP construction as a prior over mixture components so as to build an infinite mixture model (see code sample 5.3).

The code of the DP stick-breaking process and of the infinite mixture model which has been used for our experiments can be found on Github [3].

```
@model InfiniteMixutre(y) = begin
  N = length(y)
  α = 10.0
  m ~ Normal(meanMean, 1.0/sqrt(meanPrecision)) # Assume statement
  s ~ Gamma(precisionShape, 1.0/precisionInvScale) # Assume statement
  P = rand(DP(α, Normal(m, 1.0/sqrt(s)))) # Random probability measure
```

[3] https://github.com/emilemathieu/BNPMixPPL/blob/master/src/codebase/DPMixture2.jl

```
7
8     x = tzeros(N)
9     for i in 1:N
10      x[i] ~ P # Assume statement
11      y[i] ~ Normal(x[i], 1.0/sqrt(s)) # Observe statement
12    end
13
14    return x
15  end
```

Listing 5.3: *Nonconjugate infinite mixture model written in Turing.jl.*

Note the use of the `for-loop` above so as to express the model as State-Space Model. Such a formulation allow to make use of particle algorithms (described in Subsections 4.5.4 and 4.5.5) because of the sequence of `observe` statements. In the code sample 5.3 for the infinite mixture model, the `DP` Random Probability Measure could be replaced by another Normalised Random Measure of Poisson Kingman RPM.

Future Work

In this chapter we present several ideas which could be further developed. When matured enough, this ideas may become projects on themselves.

6.1 Learning parameters in PPL

6.1.1 Motivation

Since variational methods have arisen, ideas of mixing sampling with VI have emerged, including in the PPL literature.

In [89], the authors introduce the idea of automatically learning the parameters of proposals for SMC within a PPL. A lower bound on the KL divergence between the proposal and the true posterior distribution is optimize via gradient descent. In [76, 47], this idea is further developed using neural networks (such as LSTMs [40]) to parametrize these proposal distributions. These networks are fed with the previous latent and observed variables. In AESMC [48], FIVO [57] and VSMC [63], both the model and the SMC's proposal are learned by maximizing the marginal likelihood estimator given by the SMC.

The interest in learning parameters (for proposals and for the model) and performing inference on some random variables at once is thus great. PPLs allow to easily write probabilistic models and perform inference on latent variables. One may be interested in building a PPL with the capability of automatically optimizing some parameters given a loss/estimator.

Automatic Differentiation (AD) methods [4] enable the computation of gradients of some variables with respect to some parameters. The reverse differentiation is particularly popular in the machine learning community, where the history of each variable (how it has been constructed) is saved as a computational graph, and gradients can then be computed via the *chain rule*.

Some libraries such as TensorFlow [1] require the users to define static computation graphs within the syntactic and semantic constraints of a domain-specific mini language with limited support for control flow whereas the lineage of projects leading from autograd [1]

[1] https://github.com/HIPS/autograd

to PyTorch [2] provide truly general-purpose reverse mode AD capability. The latter mode is to be preferred for fully and easy support of control flow such as stochastic recursion which is needed for stick-breaking processes.

6.1.2 Choice of language/library

We this idea in mind, one can now think how to pragmatically build such a AD PPL.

Python: One of the most famous language for scientific computing is Python [78]. As *Edward* [84] is built on top of *Tensorflow*, one could build a PPL layer on top of PyTorch. *Edward* implements each MCMC step (specific for each algorithms) as a computational graph in *Tensorflow* which is thereafter run with the updated input so as to sample a new value. Similarly for VI, *Edward* implements a loss function as a computational graph, for which its gradient can be computed via auto-differentiation.

However, *Edward* focuses on VI and HMC-like schemes and does not handle particle algorithms. Indeed, so as to handle such algorithms, a PPL must have access to *breakpoints* at `assume` statement. This can be implemented via CPS [3] or coroutine [4] copying. Unfortunately implementing CPS is something non-trivial.

Julia: One could also think of using Julia [7], which has been specifically built for scientific usage. Julia has the advantage of natively handling coroutine copying, which is used in Turing [31] to implement particle methods.

Reverse mode AD libraries exist in Julia, *ReverseDiff.jl* [5] and *Knet.jl* [6] which respectively build a static and dynamic graph.

I am particularly interested in the perspective of adapting a AD library for Turing [31].

6.1.3 New models

With such as PPL in mind, one can think of new model or algorithms to be developed.

The idea of AESMC [48] might be extended to PG and PMMH so as to learn proposals' parameters for their SMC and for $p(\theta^\star|\theta)$ parameters (specific of PMMH).

6.1.4 Difficulties

Yet this is not a trivial task, one have to put proper care when computing unbiased gradient of a loss function defined by an expectation over a collection of random variables.

[2] `http://pytorch.org/`
[3] `http://matt.might.net/articles/by-example-continuation-passing-style/`
[4] `https://en.wikipedia.org/wiki/Coroutine`
[5] `https://github.com/JuliaDiff/ReverseDiff.jl`
[6] `https://github.com/denizyuret/Knet.jl`

Hopefully, a stochastic computation graph [79] can be converted into a deterministic computation graph, to which the backpropagation algorithm can then be applied on a surrogate loss function which results in an unbiased gradient estimator of the loss.

6.2 Piecewise Deterministic Markov Processes

A novel class of non-reversible Markov chain Monte Carlo schemes relying on continuous-time piecewise deterministic Markov Processes has recently emerged [86]. In these algorithms, the state of the Markov process evolves according to a deterministic dynamics which is modified using a Markov transition kernel at random event times. A general framework is presented in [8], and includes among others the Zig-Zag Process [9], the Bouncy Particle Sampler [12] and the Generalized Bouncy Particle Sampler [93].

It has been claimed [8] that the non-reversibility property of these algorithms enhances the mixing rate of the chain. I am consequently interested in understanding to what extent this class of MCMC schemes could fit the PPL's setting.

6.3 Variational Inference for BNP in PPL

As explained in Section 6.3, Truncation-free variational inference methods rely on a lazy representing of the clusters assignments. Yet, the marginalisation used seems to be only available for few models.

However, we may be able to use a similar approach for more flexible BNP models, by extending the latent space with the sticks proportions and mixture components (since they cannot be marginalized out). Moreover, there might be a deeper link between *Truncation-free* VI and stick-breaking processes.

6.4 Adversarial Inference for BNP in PPL

Adversarial inference methods [22, 18, 61] inspired by GANs [34] jointly learns a generation network and an inference network using an adversarial process.

The decoder/generator network $x' \sim p(x|z)$ maps samples from stochastic latent variables to the data space while the encoder/inference network $z' \sim q(z|x)$ maps training examples in data space to the space of latent variables.

An adversarial game is cast between these two networks and a discriminative network is trained to distinguish between joint latent/data-space samples (x', z) from the generative network and joint samples (x, z') from the inference network.

Adversarial inference seems to be closely related to VI. Yet, in adversarial inference the model can also be learned as opposed to VI where only the proposal is learned. Moreover, in VI the marginal likelihood is optimised via a lower bound (ELBO) whereas in adversarial inference, a classification loss is optimised.

This approach could be interesting in the BNP setting, if a tractable and tight lower bound on the marginal likelihood cannot be found.

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