Stochastically Differentiable Probabilistic Programs

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Abstract

Probabilistic programs with mixed support (both continuous and discrete latent random variables) commonly appear in many probabilistic programming systems (PPSs). However, the existence of the discrete random variables prohibits many basic gradient-based inference engines, which makes the inference procedure on such models particularly challenging. Existing PPSs either require the user to manually marginalize out the discrete variables or to perform a composing inference by running inference separately on discrete and continuous variables. The former is infeasible in most cases whereas the latter has some fundamental shortcomings. We present a novel approach to run inference efficiently and robustly in such programs using stochastic gradient Markov Chain Monte Carlo family of algorithms. We compare our stochastic gradient-based inference algorithm against conventional baselines in several important cases of probabilistic programs with mixed support, and demonstrate that it outperforms existing composing inference baselines and works almost as well as inference in marginalized versions of the programs, but with less programming effort and at a lower computation cost.

1 Introduction

Probabilistic programming [8, 11, 26, 7] represents statistical models as programs written in an otherwise general programming language that provides syntax for the definition and conditioning of random variables. Inference can be performed on probabilistic programs to obtain the posterior distribution or point estimates of the variables. Inference algorithms are provided by the probabilistic programming framework, and each algorithm is usually applicable to a wide class of probabilistic programs in a black-box automated manner. The algorithms include Markov Chain Monte Carlo (MCMC) variants — Metropolis-Hastings [24, 11, 27], Hamiltonian Monte Carlo (HMC) [14, 2], as well as expectation propagation [12], extensions of Sequential Monte Carlo [26, 23, 15, 17, 13], variational inference [25, 9], and gradient-based optimization [2, 1].

A probabilistic program computes the (unnormalized) probability of its execution [26]. An execution is summarized as an instantiation of the program trace, and the probability is a function of the trace. Some probabilistic programming frameworks require that the trace shape be specified upfront, i.e. static [2, 21], while others allow introduction of trace components dynamically [8, 16, 7, 5, 22], in the course of a program execution.

Efficient inference methods for probabilistic programs, especially in the high-dimensional scenario, often involve computation of the gradient with respect to the latent variables [19, 2, 5, 21, 1]. This restricts gradient-based inference methods to differentiable programs with continuous variables only. Probabilistic programs with a mixture of continuous and discrete variables, such as mixture models, state space models, and factor models, must resort to alternatives which do not rely solely on differentiability, at the cost of lower performance and poorer scalability.

Take a standard Gaussian mixture model (GMM) as an example. In GMM, the continuous latent variables are usually the mean and variance of the Gaussian distribution of each mixture component, and the discrete variables are the assignments of each data point to a mixture component. Inference in GMM can be performed by either manually marginalizing out the discrete latent vari-
ables, or by combining conditional gradient-based inference on continuous variables, and conditional gradient-free (such as Gibbs sampling) inference on discrete variables. Manual marginalization is straightforward in the case of GMM, as suggested by Stan [19], but can be more complex in most other cases, and even intractable. Conditional inference on each group of variables is prone to slow mixing and poor robustness in the face of multimodality. A generic robust inference method which both exploits differentiability and is applicable to probabilistic programs with mixed support is highly desirable.

In this work, we focus on the probabilistic programs with a mixture of continuous and discrete variables, differentiable with respect to the continuous variables, and propose to treat them as stochastically differentiable. We derive an unbiased stochastic estimate of the gradient of the marginal log likelihood that can be efficiently computed. We then demonstrate how one can apply stochastic gradient-based inference methods [10], in particular stochastic gradient Hamiltonian Monte Carlo (sgHMC) [3], on stochastically differentiable models with this estimate. To show the potential usage, a reference implementation of the probabilistic programming facility that supports stochastically differentiable probabilistic programs is presented in Section 4. We compare our proposed adaptation of sgHMC on three stochastically differentiable models against manually marginalized inference and the state-of-the-art automated method in PPSs, composing inference, and empirically confirm the substantial improvements of our approach.

Contributions This work brings the following contributions:

- the notion of a stochastically differentiable probabilistic program;
- an unbiased stochastic estimator for the gradient of the marginal log likelihood of such a program;
- an adaptation of sgHMC with this estimator as the automated inference engine;
- a reference implementation of probabilistic programming with support for stochastically differentiable probabilistic programs in Go programming language [6].

Notation We denote by \( p(\mathbf{x}) \) the probability or probability density of random variable \( \mathbf{x} \), and by \( p(\mathbf{x}|\mathbf{y}) \) the conditional probability or probability density of \( \mathbf{x} \) given \( \mathbf{y} \), depending on the domain of \( \mathbf{x} \). We write \( \mathbf{z} \sim p(\cdot) \) when \( \mathbf{z} \) is a random variable with probability \( p(\cdot) \). We denote by \( \tilde{p}(\cdot) \) a probability known up to a normalization constant, i.e. the unnormalized probability.

2 Stochastically Differentiable Probabilistic Program

To define a stochastically differentiable probabilistic program, we begin with definitions of a deterministic and a stochastic probabilistic program. Different definitions of (deterministic) probabilistic programs are given in the literature and reflect different views and accents. For the purpose of this work, let us give the following broad definition:

**Definition 1.** A deterministic probabilistic program \( \Pi \) that defines a distribution over traces \( p(\mathbf{x}|\mathbf{y}) \) is a computer program that accepts a trace assignment \( \mathbf{x} \) as one of its arguments, and returns the unnormalized probability of \( \mathbf{x} \) conditioned on other arguments \( \mathbf{y} \):

\[
\Pi(\mathbf{x}, \mathbf{y}) \Rightarrow \tilde{p}(\mathbf{x}|\mathbf{y}).
\]  

The trace assignment \( \mathbf{x} \) may have the form of a vector, or of a list of address-value pairs, or any other form suitable for a particular implementation. Accordingly, let us define a stochastic probabilistic program:

**Definition 2.** A stochastic probabilistic program \( \Xi \) that defines a distribution over traces \( p(\mathbf{x}|\mathbf{y}) \) is a computer program that accepts a trace assignment \( \mathbf{x} \) as one of its arguments, and returns the unnormalized probability of \( \mathbf{x} \) conditioned on other arguments \( \mathbf{y} \) and random variable \( \mathbf{z} \) conditioned on \( \mathbf{y} \):

\[
z \sim p(\mathbf{z}|\mathbf{y}) \\
\Xi(\mathbf{x}, \mathbf{y}) \Rightarrow \tilde{p}(\mathbf{x}|\mathbf{y}, \mathbf{z}).
\]  

A rationale for this definition is that \( \mathbf{z} \) corresponds to the nuisance parameters or nondeterministic choices inside the program. Finally, let us define a stochastically differentiable probabilistic program:

**Definition 3.** A stochastically differentiable probabilistic program \( \Xi \) is a stochastic probabilistic program (Definition 2) with trace \( \mathbf{x} \in \mathbb{R}^n \) such that \( \tilde{p}(\mathbf{x}|\mathbf{y}, \mathbf{z}) \) is differentiable w.r.t. \( \mathbf{x} \) for any \( \mathbf{y} \) and \( \mathbf{z} \).

Let us illustrate a stochastic (and stochastically differentiable) probabilistic program on an example:

**Example 1.** A survey is conducted among a company’s employees. The survey contains a single question: “Are you satisfied with your compensation?” To preserve employees’ privacy, the employee flips a coin before answering the question. If the coin shows head, the employee answers honestly; otherwise, the employee flips a coin again, and answers ‘yes’ on head, ‘no’ on tail. Based on survey outcomes, we want to know how many of the employees are satisfied with their compensations.
of large data sets, where the gradient was estimated by a posterior inference was originally motivated by the handling of nuisance random variables coin representing coin flips which are sampled inside the program from their prior distribution, but are not included in the trace — this makes the probabilistic program stochastic. The unnormalized probability of the trace is accumulated in variable prob. First, a Beta prior is imposed on theta (line 2). Then, prob is multiplied by the probability of each answer given theta and coin (lines 5–9).

**Manual marginalization** Though not generally the case, the program in Figure 1a can be rewritten as a deterministic probabilistic program (Figure 1b). Instead of flipping a coin as in line 4 of the stochastic program in Figure 1a, the probability of observation \( y[i] \) is computed in lines 5–6 as the sum of probabilities given either head or tail, weighted by the probabilities of head and tail (both are 0.5). For case studies (Section 4), we chose probabilistic programs for which manual marginalization was possible, and compared inference in stochastic and marginalized versions.

### 3 Inference

Efficient posterior inference in probabilistic models for which a stochastic gradient estimate of the logarithm of the unnormalized posterior density is available can be performed using a stochastic gradient Markov Chain Monte Carlo method [10]. Stochastic gradient posterior inference was originally motivated by the handling of large data sets, where the gradient was estimated by subsampling — computing the gradient on a small part of the dataset [3], but stochastic gradient MCMC methods are agnostic to the way the gradient is estimated, given an unbiased estimate is available, and can as well be applied to stochastically differentiable probabilistic programs. However, a naive estimate of the gradient as

\[
\nabla_x \log \tilde{p}(x|y) = \frac{\int_z p(z|y) \tilde{p}(x|y,z)dz}{\tilde{p}(x|y)}
\]

In what follows, we derive an unbiased estimate of the stochastic gradient, and elaborate on the use of the estimate within the framework of stochastic gradient Hamiltonian Monte Carlo (sgHMC).

### 3.1 Unbiased Stochastic Gradient Estimate

The unnormalized probability density \( \tilde{p}(x|y) \) is a marginalization of \( \hat{p}(x|y,z) \) over \( z \):

\[
\hat{p}(x|y) = \int_z p(z|y) \hat{p}(x|y,z)dz
\]

Posterior inference and maximum a posteriori estimation require a stochastic estimate of \( \nabla_x \log \tilde{p}(x|y) \):

\[
\nabla_x \log \tilde{p}(x|y) = \frac{\int_z p(z|y) \hat{p}(x|y,z) \nabla_x \log \tilde{p}(x|y,z)dz}{\hat{p}(x|y)}
\]

\[
= \int_z p(z|y) \hat{p}(x|y,z) \nabla_x \log \tilde{p}(x|y,z)dz
\]

\[
= \int_z p(x|y,z) p(z|y) \nabla_x \log \hat{p}(x|y,z)dz
\]

\[
= \int_z p(z|x, y) \nabla_x \log \hat{p}(x|y,z)dz
\]
By Monte Carlo approximation,
\[ z_i \sim p(z|x, y) \]
\[ \nabla_x \log \tilde{p}(x|y) \approx \frac{1}{N} \sum_{i=1}^{N} \nabla_x \log \tilde{p}(x|y, z_i) \tag{5} \]

Draws of \( z_i \) are conditioned on \( x \) and can be approximated by a Monte Carlo method, such as Markov chain Monte Carlo; \( p(z|y) \) need not be known for the approximation. Note that there are two Monte Carlo approximations involved:

1. gradient \( \nabla_x \log \tilde{p}(x|y) \) is approximated by a finite sum of gradients \( \nabla_x \log \tilde{p}(x|y, z_i) \);
2. draws of \( z_i \) from \( p(z|x, y) \) are approximated.

An intuition behind estimate (5) is that for marginalization, assignments to nuisance parameters which make the trace assignment more likely contribute more to the gradient estimate.

### 3.2 Inference with Stochastic Gradient HMC

Stochastic gradient Hamiltonian Monte Carlo [3] does not involve Metropolis-Hastings correction and requires only that a routine that computes a stochastic estimate of the gradient of the unnormalized posterior probability density should be provided. We propose here to use a single-sample gradient estimate, where \( z \) is drawn using an MCMC method, such as a Gibbs sampler or a variant of Metropolis-Hastings:

**Algorithm 1:** Single-sample gradient estimate

1. Draw \( z \) from \( p(z|x, y) \) (MCMC).
2. Return \( \nabla_x \log \tilde{p}(x|y, z) \).

Note that \( z \) is freshly drawn for each estimation of the gradient. Hence, every step through \( z \) is performed using a gradient estimate based on a new sample of \( z \).

Variance of this stochastic gradient estimate can be reduced by computing and averaging multiple estimates, each for a new draw of \( z \). This is similar to the well-known mini-batch stochastic gradient descent in stochastic optimization. In the case studies (Section 4), we compare statistical efficiency and computation time of inference with the single-sample and multi-sample stochastic gradient estimates.

Compare inference with sgHMC, using Algorithm 1 as the gradient estimate, to alternating inference, with (non-stochastic) HMC on \( x \) and an MCMC variant on \( z \):

**Algorithm 2:** Baseline: alternating HMC on \( x \) and MCMC on \( z \)

1. Draw \( z \) from \( p(z|x, y) \) (MCMC).
2. Draw \( x \) from \( p(x|y, z) \) (HMC).

Despite apparent similarity between Algorithms 1 and 2, one HMC iteration of Algorithm 1 involves multiple computations of the gradient for each draw of \( x \), all for the same sample of \( z \), as in the Leapfrog steps. A new sample of \( z \) is only drawn between iterations of HMC. This results in poorer mixing and may lead the sampler to get stuck in one of the modes of a multimodal posterior distribution.

As an illustration, consider the probabilistic program in Figure 2. This program specifies a Gaussian mixture model, \( p(x) = 0.5p(x|\mu = -1, \sigma = 0.5) + 0.5p(x|\mu = 1, \sigma = 0.5) \). Nuisance variable \( z \) selects either component with equal probability. Figure 3 shows densities of each of the components and of the mixture. For Algorithm 1, it directly samples from the entire mixture density, i.e. it re-draws \( z \) before each gradient step of \( x \), which enables the posterior samples of \( x \) to cover both modes. However, the HMC step of Algorithm 2 will condition on a fixed \( z \), i.e. sample \( x \) for \( L \) leapfrog steps conditioned on \( z = 1 \) or 2, which makes the samples mainly concentrated around one mode. The estimates of \( x \) will only evolve to the other mode once \( z \) changes based on samples from the current mode, with potentially low mixing rate.

More evidence for poorer mixing and lower statistical efficiency is provided in the case studies. Compared to that, Algorithm 1 estimates the gradient for a new draw of \( z \) on each invocation.

### 4 Case Studies

We implemented inference in stochastically differentiable probabilistic programs using Infergo [21], a probabilistic programming facility for the Go programming language. Due to reliance of Infergo on pure Go code for probabilistic programs, no changes were necessary to the way probabilistic programs are represented. Implementation of sgHMC for the case studies in this paper will be made publicly available upon publication and proposed for inclusion into Infergo.

We evaluated inference in stochastically differentiable probabilistic programs on several models. In each evaluation, we created two probabilistic programs: the standard probabilistic program with a mixed support as
```python
func TwoNormals(x float) float {
  z := Bernoulli (0.5). sample()
  if z {
    return Normal(1, 0.5). pdf(x)
  } else {
    return Normal(-1, 0.5).pdf(x)
  }
}
```

(a) Mixture of two Gaussians: nuisance variable \( z \) selects either \( N(-1, 0.5) \) or \( 5N(1, 0.5) \).

(b) Mixture of two Gaussians: HMC conditioned on either \( z = \text{false} \) or \( z = \text{true} \) will alternate between exploring each of the components, while sgHMC will directly draw samples from the posterior.

Figure 2: An illustration example: sgHMC vs. MCMC + HMC

users may write (akin to Figure 1a) and a corresponding marginalized program (akin to Figure 1b). Additionally, for comparison, we implemented a marginalized program for each model in Stan \([2]\); we verified that the posterior distributions inferred by each of inference schemes on both mixed support and marginalized programs are consistent with the Stan version. We provide results for three models in this study: compensation survey (Section 4.1), Gaussian mixture model, and hidden Markov model. Details of each model are provided later in this section. The full source code, data, and evaluation scripts for the case studies will be made publicly available upon publication.

The purpose of these case studies is to compare statistical efficiency and computation time of sgHMC, combination of MCMC and HMC on mixed-support models, and HMC on marginalized models. For each model, we measured, and averaged over 10 independent runs, the effective sample size and the computation time. Four inference schemes were applied:

- (ours) sgHMC with a single-sample gradient estimate;
- (ours) sgHMC with 10-sample gradient estimate;
- a combination of MCMC (sitewise Metropolis-Hastings) on discrete variables and HMC on continuous variables;
- HMC on the marginalized model.

All inference schemes were run to produce 10 000 samples (sufficient for convergence on all models in the studies), with 10 steps (gradient estimates) between samples. The step resulting in the largest effective sample size for HMC on the marginalized model was chosen and fixed for all over schemes on the same model. This choice of the step size favors HMC in comparison, meaning that the actual comparative performance of sgHMC on stochastically differentiable probabilistic programs is at least as good, or better, as what follows from the evaluation.

The measurements are summarized in Tables 1 and 2 including empirical standard deviations over multiple runs. Table 1 shows effective sample sizes. Larger numbers are better. Effective sample size of HMC on marginalized program is 15%–20% larger than sgHMC with a single-sample gradient estimate and 5–7% larger than sgHMC with 10-sample estimate. The MH+HMC combination consistently produces sample sizes which are lower by 30–60%. Table 2 shows computation times. While 10-sample gradient estimate is computationally expensive and results in almost linear increase in the total computation time, cancelling the improvement due to a less noisy gradient estimate, sgHMC exhibits the shortest computation time for all models, 2.5–4.5 times shorter than HMC on the marginalized program. This is because the marginalized version has both a higher asymptotic complexity (more details are in descriptions of each of the case studies) and involves computationally expensive exponentiation (calls to LogSumExp in Figures 3b, 4b, and 5b).

Table 3 combines Tables 1 and 2 to show approximate effective sample size in seconds. Despite a slightly lower total effective sample size of sgHMC, the effective sample size of sgHMC with a single-sample gradient estimate is 2–4 times larger than that of HMC on the marginalized model. To summarize, sgHMC with a single-sample gradient estimate has the best performance on the mixed support probabilistic programs used in the case studies, outperforming HMC on marginalized models by a number of times even for parameters favoring...
Table 1: Effective sample size

| model       | sgHMC, 1 sample | sgHMC, 10 samples | MH+HMC    | HMC, marginalized |
|-------------|-----------------|-------------------|-----------|-------------------|
| Survey      | 4600 ± 180      | 5000 ± 160        | 2800 ± 300| 5200 ± 200        |
| GMM         | 5900 ± 240      | 6800 ± 200        | 1900 ± 200| 7200 ± 150        |
| HMM         | 6200 ± 280      | 6300 ± 220        | 4800 ± 190| 6700 ± 180        |

Table 2: Computation time, seconds

| model       | sgHMC, 1 sample | sgHMC, 10 samples | MH+HMC    | HMC, marginalized |
|-------------|-----------------|-------------------|-----------|-------------------|
| Survey      | 6.5 ± 0.1       | 40 ± 1            | 7.4 ± 0.1 | 21 ± 0.5          |
| GMM         | 35 ± 0.7        | 340 ± 5           | 38 ± 0.7  | 95 ± 2            |
| HMM         | 10 ± 0.3        | 98 ± 3            | 10 ± 0.3  | 46 ± 0.8          |

Table 3: Effective sample size per second

| model       | sgHMC | MH+HMC | HMC |
|-------------|-------|--------|-----|
| Survey      | 650   | 380    | 240 |
| GMM         | 170   | 50     | 75  |
| HMM         | 620   | 480    | 145 |

HMC in the comparison.

4.1 Compensation Survey

The compensation survey follows the description in Section 4.1. The mixed support program is shown in Figure 3a and the marginalized version in Figure 3b. For evaluation, a data set of 60 observations, corresponding to 67% satisfaction, was used. The marginalized version has the same asymptotic complexity as the mixed support version, but should take at least twice as long to run due to computation of the log probability for both coin flip outcomes (lines 5–7). This is consistent with the empirical measurements, 21 vs 6.5 seconds, (Table 2), with extra time spent in LogSumExp.

4.2 Gaussian Mixture Model

The Gaussian mixture model infers means and standard deviation of the components, given a set of samples from the mixture and the number of components. The mixed support program is shown in Figure 4a and the marginalized version in Figure 4b. For evaluation, a data set of 100 observations, corresponding to two components with equal probability of either component, was used. The computation time of the marginalized version is at least the computation time of the mixed support program times the number of components (at least twice longer for two components) due to the inner loop in lines 8–15. This is consistent with the empirical measurements, 95 vs. 35 seconds (Table 2), with extra time spent in LogSumExp.

4.3 Hidden Markov Model

The Hidden Markov model infers the transition matrix given the emission matrix and the observations. The mixed support program is shown in Figure 5a and the marginalized version in Figure 5b. For evaluation, a data set of 16 observations, corresponding to three distinct hidden states, was used. Following [20], the marginalized version implements the costly forward pass of the forward-backward algorithm. The computation time of the marginalized version, in a naive implementation, is at least the computation time of the mixed support program times the squared number of hidden states (at least nine times longer for three hidden states). This is due to the doubly-nested loop in lines 11–20. The forward pass also involves two distinct calls to LogSumExp, one in line 18, on each iteration of the inner loop, and the other in line 22. The marginalized version in Figure 5b optimizes the inner loop by reusing computations, but the computation time of the marginalized version is still five times longer than that of the mixed support version, 46 vs. 10 seconds (Table 2).

5 Related Work

Stochastically differentiable probabilistic programs as introduced in Section 2, though may be named differently, commonly appeared in many different probabilistic programming systems (PPSs). However, the mixture of continuous and discrete random variables substantially complicates the inference procedures in PPS as automated engines. Especially, the inference procedure...
1 func (m *StochasticModel)
2 Observe(x [] float64) float64 {
3 ll := 0.
4 theta := mathx.Sigm(x[0])
5 for i := 0; i < len(m.Y); i++ {
6 if m.Coin[i] {
7 ll += Flip.Logp(theta, m.Y[i])
8 } else {
9 ll += Flip.Logp(0.5, m.Y[i])
10 }
11 }
12 return ll
13 }

(a) Compensation survey

Figure 3: Code Example for the Compensation Survey

1 func (m *StochasticModel)
2 Observe(x [] float64) float64 {
3 ll := Normal.Logps(0, 10, x ...)
4 for j := range m.Mu {
5 m.Mu[j] = x[2*j]
6 m.Sigma[j] = math.Exp(x[2*j+1])
7 }
8 for i := 0; i < len(m.Data); i++ {
9 lj := Normal.Logp(m.Mu[j], m.Sigma[j], m.Data[i])
10 if j == 0 {
11 l = lj
12 } else {
13 l = mathx.LogSumExp(l, lj)
14 }
15 ll += l
16 }
17 return ll
18 }

(b) Gaussian mixture model

Figure 4: Code Example for the GMM

can become extremely challenging if the program trace is not static, i.e. the support of the program is dynamic.

To perform inference in such models in PPSs such as Stan [2], which are usually designed around one or two efficient gradient-based inference methods such as HMC, the user would need to manually marginalize out the discrete nuisance variables since they violate the prerequisite of the inference engines. Unfortunately, this is not feasible in most cases and also adds unnecessary burden for the user, which violates the principle of automation in PPS at the first place.

Alternative choices may be PPSs such as PyMC3 [19], Turing.jl [5], and Gen [4] where one can customize different kernels for different variables as composing inference. For example, one can use the Metropolis-within-Gibbs sampler for the nuisance variables and HMC for
1 func (m *StochasticModel)
2 Observe(x [] float64) float64 {
3 ll := Normal.Logps(0, 10, x ...)
4 for i := range m.logT {
5 D.SoftMax(x[i*m.NStat:(i+1)*m.NStat], m.logT[i])
6 for j := range m.logT[i] {
7 m.logT[i][j] = math.Log(m.logT[i][j])
8 }
9 }
10 noise := math.Exp(m.Noise)
11 for i := range m.Data {
12 ll += Normal.Logp(float64(m.States[i]), noise, m.Data[i])
13 if i != 0 {
14 for j := 0; j != m.NStat; j++ {
15 m.acc[j] = m.gamma[i-1][j] + m.logT[j][j]
16 m.gamma[i][j] += D.LogSumExp(m.acc)
17 }
18 }
19 return ll
20 }

(a) Hidden Markov model

1 func (m *DeterministicModel)
2 Observe(x [] float64) float64 {
3 ll := Normal.Logps(0, 10, x ...)
4 for i := range m.logT {
5 D.SoftMax(x[i+m.NStat:(i+1)*m.NStat], m.logT[i])
6 for j := range m.logT[i] {
7 m.logT[i][j] = math.Log(m.logT[i][j])
8 }
9 }
10 noise := math.Exp(m.Noise)
11 for i := range m.Data {
12 for j := 0; j != m.NStat; j++ {
13 m.gamma[i][j] = Normal.Logp(float64(m.States[i]), noise, m.Data[i])
14 if i != 0 {
15 for j_ := 0; j_ != m.NStat; j_++ {
16 m.gamma[i][j] += D.LogSumExp(m.gamma[i][j])
17 m.gamma[i][j] += D.LogSumExp(m.gamma[i][j])
18 }
19 return ll
20 }

(b) Hidden Markov model, marginalized

Figure 5: Code Example for the HMM

the remaining continuous ones. It is probably the state-of-the-art method for this type of models, especially in the PPSs oriented for the gradient-based inference engines. However, as we have discussed in Section 3 and empirically confirmed in Section 4 this method has some fundamental shortcomings and our approach provides substantial practical improvements.

There are also some other approaches for improving inference performance for this type of models. For example, LF-PPL [28] proposed a novel low-level language for PPS to incorporate more sophisticated inference techniques for piecewise differentiable models; Stochaskell [18] provided a way to perform reversible jump MCMC in PPS; [29] introduced a new sampling scheme, called Divide, Conquer and Combine, to perform inference in the general purpose PPS by dividing the program into sub-programs and conquering individual one before coming into an overall estimate. However, LF-PPL imposes some restrictions to the language of the PPS that are not required in our setup, whereas the latter two do not exploit gradient information at all. Therefore, they are less relevant to our approach and we leave the possible connection for future work.

6 Discussion

In this paper, we introduced the notion of a stochastically differentiable probabilistic program as well as an inference scheme for such programs. We provided a reference implementation of probabilistic programming with stochastically differentiable probabilistic programs. Stochastically differentiable probabilistic programs facilitate natural specification of probabilistic models and support efficient inference in the models, providing a viable alternative to explicit model marginalization, whether manual or algorithmic.

Our understanding of stochastically differentiable probabilistic programs, classes of models for which they are best suited, and inference schemes is still at an early stage and evolving. In particular, we are working towards future publications, on maximum a posteriori estimation in stochastically differentiable probabilistic programs. Another research direction would be selection and adaption of stochastic gradient-based inference al-
gorithms to probabilistic programming inference. Last
but not least, we are looking into introducing support for
stochastically differentiable probabilistic programs into
existing probabilistic programming frameworks.

References

[1] Eli Bingham, Jonathan P. Chen, Martin Jankowiak,
Fritz Obermeyer, Neeraj Pradhan, Theofanis Kar-
aletsos, Rohit Singh, Paul Szerlip, Paul Horsfall,
and Noah D. Goodman. Pyro: deep universal prob-
abilistic programming. *Journal of Machine Learn-
ing Research*, 20(28):1–6, 2019.

[2] Bob Carpenter, Andrew Gelman, Matthew Hoff-
mant, Daniel Lee, Ben Goodrich, Michael Betan-
court, Marcus Brubaker, Jiqiang Guo, Peter Li,
and Allen Riddell. Stan: a probabilistic programming
language. *Journal of Statistical Software, Articles*,
76(1):1–32, 2017.

[3] Tianqi Chen, Emily B. Fox, and Carlos Guestrin.
Stochastic gradient Hamiltonian Monte Carlo. In *Proceedings of the 31st International Conference on
International Conference on Machine Learn-
ing, ICML’14*, pages II–1683–II–1691. JMLR.org,
2014.

[4] Marco F Cusumano-Towner, Feras A Saad,
Alexander K Lew, and Vikash K Mansinghka. Gen:
a general-purpose probabilistic programming system with programmable inference. In *Proceedings of
the 40th ACM SIGPLAN Conference on Programming Language Design and Implementation*, pages 221–236, 2019.

[5] Hong Ge, Kai Xu, and Zoubin Ghahramani. Turing:
composable inference for probabilistic programming.
In *International Conference on Artificial
Intelligence and Statistics, AISTATS 2018*, 9–11 April 2018, Playa Blanca, Lanzarote, Canary
Islands, Spain, pages 1682–1690, 2018.

[6] The Go team. The Go programming language.
[http://golang.org/](http://golang.org/), 2009.

[7] N. D. Goodman and A. Stuhlmüller. *The Design
and Implementation of Probabilistic Programming Languages*. 2014. electronic; retrieved 2019/3/29.

[8] Noah D. Goodman, Vikash K. Mansinghka,
Daniel M. Roy, Keith Bonawitz, and Joshua B.
Tenenbaum. Church: a language for generative
models. In *Proc. of Uncertainty in Artificial Intel-
lence*, 2008.

[9] Alp Kucukelbir, Dustin Tran, Rajesh Ranganath,
Andrew Gelman, and David M. Blei. Automatic
differentiation variational inference. *J. Mach.
Learn. Res.*, 18(1):430–474, January 2017.

[10] Yi-An Ma, Tianqi Chen, and Emily Fox. A
complete recipe for stochastic gradient MCMC.
In C. Cortes, N. D. Lawrence, D. D. Lee,
M. Sugiyama, and R. Garnett, editors, *Advances in
Neural Information Processing Systems 28*, pages
2917–2925. Curran Associates, Inc., 2015.

[11] Vikash K. Mansinghka, Daniel Selsam, and Yura N.
Perov. Venture: a higher-order probabilistic
programming platform with programmable inference,
2014.

[12] T Minka, J Winn, J Guiver, and D Knowles. Infer
.net 2.4. Microsoft research Cambridge, 2010.

[13] Lawrence M. Murray and Thomas B. Schön.
Automated learning with a probabilistic programming
language: Birch. *Annual Reviews in Control*, 46:29 – 43, 2018.

[14] Radford M. Neal. MCMC using Hamiltonian dy-
namics. Published as Chapter 5 of the Handbook of
Markov Chain Monte Carlo, 2011, 2012.

[15] B. Paige, F. Wood, A. Doucet, and Y.W. Teh. Asyn-
chronous anytime sequential Monte Carlo. In *Adv-
ances in Neural Information Processing Systems*,
2014.

[16] Avi Pfeffer. Figaro: An object-oriented probabilis-
tic programming language. In *Charles River Ana-
litics Technical Report (2009)*, 2009.

[17] Tom Rainforth, Christian A Naesseth, Fredrik
Lindestroem, Brooks Paige, Jan-Willem van de Meent,
Arnaud Doucet, and Frank Wood. Interacting par-
ticle Markov chain Monte Carlo. In *Proceedings of
the 33rd International Conference on Machine
Learning*, volume 48 of *JMLR: W&CP*, 2016.

[18] David A Roberts, Marcus Gallagher, and Thomas
Taimre. Reversible jump probabilistic programming.
In *The 22nd International Conference on Ar-
tificial Intelligence and Statistics*, pages 634–643,
2019.

[19] John Salvatier, Thomas V. Wiecki, and Christopher
Fonnesbeck. Probabilistic programming in Python
using PyMC3. *PeerJ Computer Science*, 2:e55, apr
2016.

[20] Stan Development Team. *Stan Modeling Lan-
guage User’s Guide and Reference Manual, Ver-
sion 2.18.0*. 2018.
[21] David Tolpin. Deployable probabilistic programming. In Proceedings of the 2019 ACM SIGPLAN International Symposium on New Ideas, New Paradigms, and Reflections on Programming and Software, Onward! 2019, pages 1–16, New York, NY, USA, 2019. ACM.

[22] David Tolpin, Jan-Willem van de Meent, Hongseok Yang, and Frank Wood. Design and implementation of probabilistic programming language Anglican. In Proceedings of the 28th Symposium on the Implementation and Application of Functional Programming Languages, IFL 2016, pages 6:1–6:12, New York, NY, USA, 2016. ACM.

[23] Jan-Willem van de Meent, Hongseok Yang, Vikash Mansinghka, and Frank Wood. Particle Gibbs with ancestor sampling for probabilistic programs. In Artificial Intelligence and Statistics, 2015.

[24] David Wingate, Andreas Stuhlmüller, and Noah D. Goodman. Lightweight implementations of probabilistic programming languages via transformational compilation. In Proceedings of the 14th Artificial Intelligence and Statistics, 2011.

[25] David Wingate and Theophane Weber. Automated variational inference in probabilistic programming, 2013.

[26] Frank Wood, Jan-Willem van de Meent, and Vikash Mansinghka. A new approach to probabilistic programming inference. In Artificial Intelligence and Statistics, 2014.

[27] Lingfeng Yang, Pat Hanrahan, and Noah D Goodman. Generating efficient MCMC kernels from probabilistic programs. In Proceedings of the Seventeenth International Conference on Artificial Intelligence and Statistics, pages 1068–1076, 2014.

[28] Yuan Zhou, Bradley J Gram-Hansen, Tobias Kohn, Tom Rainforth, Hongseok Yang, and Frank Wood. LF-PPL: A Low-Level First Order Probabilistic Programming Language for Non-Differentiable Models. In The 22nd International Conference on Artificial Intelligence and Statistics, pages 148–157, 2019.

[29] Yuan Zhou, Hongseok Yang, Yee Whye Teh, and Tom Rainforth. Divide, conquer, and combine: a new inference strategy for probabilistic programs with stochastic support, 2019.
A Stan versions of the programs in the case studies

A.1 Compensation Survey

```stan
data {
  int<lower=0> N;
  int<lower=0,upper=1> y[N];
}
parameters {
  real<lower=0,upper=1> theta;
}
model {
  for (n in 1:N) {
    target += log_mix(0.5, bernoulli_lpmf(y[n] | theta), bernoulli_lpmf(y[n] | 0.5));
  }
}
```

A.2 Gaussian Mixture Model

```stan
data {
  int<lower = 0> N;
  vector[N] y;
}
parameters {
  vector[2] mu;
  real<lower=0> sigma[2];
}
model {
  mu ~ normal(0, 10);
  sigma ~ lognormal(0, 10);
  for (n in 1:N)
    target += log_mix(0.5, normal_lpdf(y[n] | mu[1], sigma[1]),
                      normal_lpdf(y[n] | mu[2], sigma[2]));
}
```

A.3 Hidden Markov model

```stan
```
data {
  real<lower=0> noise;
  int<lower=1> K; // number of states
  int<lower=1> N;
  real y[N];
}

parameters {
  simplex[K] theta[K];
}

model {
  real acc[K];
  real gamma[N,K];
  for (k in 1:K)
    gamma[1,k] = normal_lpdf(y[0]|k−1, noise);
  for (t in 2:N) {
    for (k in 1:K) {
      for (j in 1:K)
        acc[j] = gamma[t−1,j] + log(theta[j,k])
            + normal_lpdf(y[t]|k−1, noise);
    gamma[t,k] = log_sum_exp(acc);
    }
  }
  target += log_sum_exp(gamma[N]);
}