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# Automatically Marginalized MCMC in Probabilistic Programming

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## Abstract

Hamiltonian Monte Carlo (HMC) is a powerful algorithm to sample latent variables from Bayesian models. The advent of probabilistic programming languages (PPLs) frees users from writing inference algorithms and lets users focus on modeling. However, many models are difficult for HMC to solve directly, which often require tricks like model reparameterization. We are motivated by the fact that many of those models could be simplified by marginalization. We propose to use automatic marginalization as part of the sampling process using HMC in a graphical model extracted from a PPL, which substantially improves sampling from real-world hierarchical models.

## 1. Introduction

Probabilistic programming languages (PPLs) promise to automate Bayesian reasoning. A user specifies a probabilistic model and provides data, and the PPL automatically performs inference to approximate the posterior distribution. The user derives scientific insights without highly specialized expertise in probabilistic inference (van de Meent et al., 2018). Through tools like BUGS (Lunn et al., 2009), JAGS (Hornik et al., 2003), and Stan (Carpenter et al., 2017), this paradigm has had tremendous impact in the applied sciences, and there has been considerable research in computer science to advance the foundations of PPLs (Goodman et al., 2008; Wood et al., 2014; Goodman & Stuhlmüller, 2014; Cusumano-Towner et al., 2019; Minka et al., 2018).

PPLs vary in many dimensions, including the distributions they can represent and their primary inference approach. We focus on a setting that has had large impact in practice, where a model is compiled to a differentiable log-density function for inference by a variant of Hamiltonian Monte Carlo (HMC) (Duane et al., 1987; Neal, 1996). Our methods would likely benefit other Markov chain Monte Carlo (MCMC) inference approaches as well. We focus in par-

ticular on (1) *generative* PPLs, where a model is expressed by writing a sampling procedure, and (2) on programs that correspond to a (directed) graphical model, which means that random variables are generated according to a fixed sequence of conditional distributions in each program execution. This includes most applied statistical models written in generative PPLs such as Pyro (Bingham et al., 2018), NumPyro (Phan et al., 2019), PyMC (Patil et al., 2010), Edward (Tran et al., 2017) and TensorFlow Probability (Piponi et al., 2020). It does not directly include Stan programs, which do not always specify a sampling procedure, though most can be converted to do so (Baudart et al., 2021).

Despite their promise, the barrier between users and inference in PPLs is often blurred. There may be different ways to write a model, with inference performance depending critically on the specific choice, such that users again need specialized knowledge. One issue is the main focus of this paper: it is often possible to reformulate a generative model so that some latent variables are generated *after* all observed variables, which allows them to be dropped during MCMC and then reconstructed afterward. An example is shown in Figure 1: the well known eight schools model is reformulated so latent variables  $x_{1:8}$  are generated last; they can then be dropped during MCMC and reconstructed given samples of  $\mu$  and  $\tau$  by sampling from  $p(x_{1:8} | \mu, \tau, y_{1:8})$ . We refer to this as *marginalization*, because the variables are marginalized while running MCMC, but it is important that they are later reconstructed. By reducing the number of variables for MCMC, marginalization can lead to substantial performance gains. We also find that marginalization applies in several hierarchical model settings that are known to be difficult for HMC and is an even better remedy than an existing approach of *reparameterization* (Betancourt & Girolami, 2015; Gorinova et al., 2020). However, it places a significant burden on the user to reformulate the model.

We develop a method to automatically marginalize variables in a user-specified probabilistic program for inference with HMC. Our work builds on prior research on automatic marginalization (see Section 4) and shares technical underpinnings with work to automatically Rao-Blackwellize particle filters for evaluation-based PPLs (Murray et al., 2018; Atkinson et al., 2022). A key difference is we focus on graphical models and HMC, which leads to different technical considerations. Our method works by first compiling

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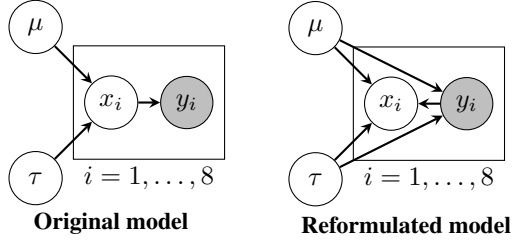


Figure 1. Graphical models of original and reformulated eight schools models. We use a plate to represent shared substructure of different branches. Gray variables are observed.

a probabilistic program into a graphical model. Although most HMC-based PPLs compile directly to a log-density, we use the program-tracing features of JAX (Bradbury et al., 2018) to extract a graphical-model representation of programs written in NumPyro. In the graphical model, we identify conjugacy relationships that allow some variables to be marginalized, then manipulate the graphical model to marginalize those variables. HMC is run on the reduced model, and the marginalized variables are recovered by direct sampling conditional on the variables sampled by HMC. Importantly, the interface between the user and the PPL does not change. Experiments show that our methods can substantially improve the effectiveness of samples from hierarchical partial pooling models and hierarchical linear regression models and significantly outperforms reparameterization in those models where both apply. Our implementation is limited to scalar and elementwise array operations and may require user input to avoid excessive JAX compilation times, though these limitations are not fundamental.

## 2. Motivating examples

We first present example models where marginalization can significantly benefit HMC-based inference.

**The eight schools model** (Gelman et al., 1995) is an important demonstration model for PPLs (Gorinova, 2022) and reparameterization (Papaspiliopoulos et al., 2007). It is a hierarchical model to study the effect of coaching on SAT performance in eight schools. An example probabilistic program for eight schools with NumPyro-like syntax is:

```
def eight_schools(sigma, y):
    mu = sample(normal(0, 5))
    tau = sample(half_cauchy(5))
    with plate(8):
        x = sample(normal(mu, tau))
        observe(normal(x, sigma), y)
```

Mathematically, the model is

$$\begin{aligned} \mu &\sim \mathcal{N}(0, 5^2), \quad \tau \sim \text{HalfCauchy}(5), \\ x_i &\sim \mathcal{N}(\mu, \tau^2), \quad y_i \sim \mathcal{N}(x_i, \sigma_i^2), \end{aligned}$$

where  $i \in \{1, \dots, 8\}$  and  $(\sigma_{1:8}, y_{1:8})$  are given as data. We want to reason about all latent variables,  $\mu$ ,  $\tau$  and  $x_{1:8}$ . A PPL will compile the model code to a log joint density  $\log p(\mu, \tau, x_{1:8}, y_{1:8})$  and then run HMC over the latent variables  $\mu$ ,  $\tau$  and  $x_{1:8}$ .<sup>1</sup> However, there is another model with the same joint density:

$$\begin{aligned} \mu &\sim \mathcal{N}(0, 5^2), \quad \tau \sim \text{HalfCauchy}(5), \\ y_i &\sim \mathcal{N}(\mu, \tau^2 + \sigma_i^2), \quad x_i \sim \mathcal{N}\left(\frac{y_i \tau^2 + \mu \sigma_i^2}{\tau^2 + \sigma_i^2}, \frac{\tau^2 \sigma_i^2}{\tau^2 + \sigma_i^2}\right). \end{aligned}$$

Both models are shown as graphical models in Figure 1: they have different causal interpretations but identical joint distributions and are therefore the same for performing inference. Importantly, in the reformulated model, we no longer need to run HMC over all latent variables. Since only  $y_{1:8}$  are observed, it is possible to marginalize  $x_{1:8}$  to obtain the reduced model  $p(\mu, \tau, y_{1:8}) = p(\mu)p(\tau) \prod_{i=1}^8 p(y_i | \mu, \tau)$ . We can sample  $\mu$  and  $\tau$  by running HMC on the reduced model then sample  $x_{1:8}$  directly from  $p(x_{1:8} | \mu, \tau, y_{1:8})$  given  $\mu$  and  $\tau$ . With this strategy, HMC samples 2 variables instead of 10, which significantly speeds up inference.

The principle that allows us to transform the model is conjugacy. In a Bayesian model  $p(x, y) = p(x)p(y | x)$  the prior  $p(x)$  is conjugate to the likelihood  $p(y | x)$  if the posterior  $p(x | y)$  is in the same parametric family as  $p(x)$  for all  $y$ . For our working definition, we assume the parametric families of the prior and likelihood have a tractable density function and sampling procedure and that there is an analytical formula for the parameters of the posterior in terms of  $y$ . Given these assumptions, it is also possible to sample from the marginal  $p(y)$  and compute its density efficiently.<sup>2</sup> Conjugacy is formally a property of distribution families, but we will also say “ $x$  is conjugate to  $y$ ” when the meaning is clear from context.

In the eight schools model,  $x_i$  is conjugate to  $y_i$  given  $\mu$  and  $\tau$ , which leads to analytical expressions for the distributions  $p(x_i | \mu, \tau, y_i)$  and  $p(y_i | \mu, \tau)$  in the reformulated model and ensures they have tractable densities and samplers.

**Hierarchical linear regression.** The eight schools model is very simple, but already requires user effort to reformulate. To emphasize the complexity of reformulating larger models, in Figure 2 we present a simplified version of the electric company model (Gelman & Hill, 2006). The full model appears in Section 5.2. The observed variables are  $y_1$  and  $y_2$ . One can guess that the model can be reformulated because, conditioned on  $\sigma$ , all variables are normal with means that are affine functions of other variables. However, the calculations are complex: the right side of Figure 2

<sup>1</sup>In practice, latent variables are transformed to have real support (Kucukelbir et al., 2017).

<sup>2</sup>To sample, draw  $x \sim p(x)$ ,  $y \sim p(y | x)$  and ignore  $x$ ; for the density, use  $p(y) = \frac{p(x_0)p(y | x_0)}{p(x_0 | y)}$  for a reference value  $x_0$ .

Original model	Distributions of $a$ , $b_1$ , and $b_2$ , in the reformulated model
$\log \sigma \sim \mathcal{N}(0, 1)$ ,	$a \sim \mathcal{N}\left(\frac{y_1 + 100\sigma^2\mu_a - b_1t_1 - \sigma^2b_1t_1}{(1 + \sigma^2)(2 + \sigma^2)} + \frac{1 + \sigma^2}{2 + \sigma^2}(y_2 - b_2t_2), \frac{\sigma^2}{(1 + \sigma^2)(2 + \sigma^2)}\right)$ ,
$\mu_a \sim \mathcal{N}(0, 1)$ ,	
$a \sim \mathcal{N}(100\mu_a, 1)$ ,	$b_1 \sim \mathcal{N}\left(\frac{100^2t_1(y_1 - 100\mu_a)}{1 + 100^2t_1^2 + \sigma^2}, \frac{100^2 + 100^2\sigma^2}{1 + 100^2t_1^2 + \sigma^2}\right)$ ,
$b_{1:2} \sim \mathcal{N}(0, 100^2)$ ,	
$y_i \sim \mathcal{N}(a + b_it_i, \sigma^2)$ .	$b_2 \sim \mathcal{N}\left(\frac{100^2t_2(y_2 + \sigma^2y_2 - y_1 - 100\sigma^2\mu_a + b_1t_1 + \sigma^2b_1t_1)}{100^2t_2^2 + 100^2\sigma^2t_2^2 + 2\sigma^2 + \sigma^4}, \frac{2 * 100^2\sigma^2 + 100^2\sigma^4}{100^2t_2^2 + 100^2\sigma^2t_2^2 + 2\sigma^2 + \sigma^4}\right)$ .

Figure 2. The original model and the reformulated model of the simplified electric company model.  $(t_1, y_1), (t_2, y_2)$  are given as data.

shows a portion of the reformulated model. In this version, HMC is run to sample  $\mu_a$  and  $\sigma$  (distributions not shown) conditioned on  $y_1$  and  $y_2$ . Then  $a$ ,  $b_1$ , and  $b_2$  are reconstructed conditioned on  $\mu_a, \sigma, y_1, y_2$  by sampling from the shown distributions. By reducing the number of variables from 5 to 2, HMC inference can be accelerated. However, it is extremely cumbersome for the user to derive the new model, which no longer corresponds to the originally conceived data generating process. We wish to automate this procedure so users only write the original model and our framework reformulates it.

### 3. Automatically marginalized MCMC

Given a program written by a user, our method will construct a graphical model and then manipulate it into a reformulated model for which MCMC samples fewer variables. The key operation will be *reversing* certain edges (based on conjugacy) to create unobserved leaf nodes that can be marginalized. For example, in the eight schools model of Figure 1, the edge from  $x_i$  to  $y_i$  is reversed (which has the side effect of creating edges from  $\mu$  and  $\tau$  to  $y_i$ ), after which  $x_i$  is a leaf. In this section, we first develop the algorithm assuming a suitable graphical model representation. Then, in Section 3.7, we describe how we obtain such a representation in our implementation using JAX and NumPyro.

#### 3.1. Graphical model representation

Assume there are  $M$  random variables  $x_1, x_2, \dots, x_M$  where  $x_i$  belongs to domain  $\mathcal{X}_i$ . The full domain is  $\mathcal{X} = \prod_i \mathcal{X}_i$ . For a set of indices  $A$ , we write  $\mathbf{x}_A = (x_i)_{i \in A}$  and  $\mathcal{X}_A = \prod_{i \in A} \mathcal{X}_i$ . A graphical model  $G$  is defined by specifying a distribution family for each node together with a mapping from parents to parameters. Specifically, for node  $i$ , let  $D_i$  represent its distribution family from a finite set of options (e.g., “Normal”, “Beta”, etc.), let  $\text{pa}(i) \subseteq \{1, \dots, M\}$  be its parents, and let  $f_i: \mathcal{X}_{\text{pa}(i)} \rightarrow \Theta_i$  be a mapping such that  $x_i$  has distribution  $D_i(\theta_i)$  with parameters  $\theta_i = f(\mathbf{x}_{\text{pa}(i)})$ . For example, if  $x_2 \sim \mathcal{N}(x_1, 1)$ , then  $D_2 = \text{“Normal”}$ ,  $\text{pa}(2) = \{1\}$ , and  $f_2(x_1) = (x_1, 1)$ . Furthermore, for each distribution family, assume a density function and sampling routine are available. Let  $p_i(x_i | \theta_i)$

be the density function for node  $i$  and  $h_i(u | \theta_i)$  be the sampling function, which maps a random seed  $u$  to a sample from  $D_i(\theta_i)$ . The parent relationship is required to be acyclic. Initially, nodes will be ordered topologically so that  $\text{pa}(i) \subseteq \{1, \dots, i - 1\}$ . Our algorithms will manipulate the graphical model to maintain acyclicity but will not preserve the invariant that nodes are numbered topologically. In our example models we use standard notation for hierarchical models with variable names such as  $\mu, \tau, x_i, y_i$ ; in these cases, the mapping to a generic sequence of random variables  $x_1, \dots, x_M$ , the parent relationship, and the distribution families are clear from context.

With this representation, given concrete values of all variables, the log density can be computed easily as  $\sum_{i=1}^M \log p_i(x_i | f_i(\mathbf{x}_{\text{pa}(i)}))$ , assuming nodes are ordered topologically. Generating a joint sample is similar: iterate through nodes and sample  $x_i \sim h_i(\cdot | f_i(\mathbf{x}_{\text{pa}(i)}))$ . A key idea of our approach is that by factoring the log-density computation into the sequence of conditional functions  $f_i$  for each random variable, we can manipulate the conditional distributions to achieve automatic marginalization.

#### 3.2. Computation graph representation

Our operations to transform the graphical model will require examining and manipulating the functions  $f_i(\mathbf{x}_{\text{pa}(i)})$  mapping parents to distribution parameters. For example, in the electric company model of Figure 2, we need to detect from the symbolic expression  $y_2 \sim \mathcal{N}(a + b_2t_2, \sigma^2)$  that the mean parameter is an affine function of  $b_2$ , which is required to reverse the edge  $b_2 \rightarrow y_2$ . Similarly, we must manipulate symbolic expressions to obtain ones like those in the reformulated model. For this purpose we assume functions are represented as computation graphs.

Consider an arbitrary function  $f(x_{i_1}, x_{i_2}, \dots, x_{i_k})$  for  $i_1, \dots, i_k \in \{1, \dots, m\}$ . We assume the computation graph of  $f$  is specified as a sequence of  $N_f$  primitive operations that each write one value (Griewank & Walther, 2008), which is similar to the JAX expression (Jaxpr) representation we can obtain from JAX. Specifically, the sequence of values  $w_1, w_2, w_3, \dots, w_{k+N_f}$  are computed as follows: (1) the first  $k$  values are the inputs to the function, i.e.,  $w_j = x_{i_j}$

for  $j = 1$  to  $k$ , and (2) each subsequent value is computed from the preceding ones as  $w_j = \phi_j(\mathbf{w}_{\text{pred}(j)})$ , where  $\phi_j$  is a primitive operation (e.g., “ADD”, “MUL”, “SQUARE”) on values  $\mathbf{w}_{\text{pred}(j)}$  and  $\text{pred}(j) \subseteq \{1, \dots, j-1\}$  is the set of predecessors of  $j$ . The predecessor relationship defines a DAG for the variables in a computation graph.

We will also need to algorithmically manipulate computation graphs. In the text, we will denote manipulations symbolically as follows. Suppose  $f(x_A)$  and  $g(x_B)$  are two functions represented by computation graphs with potentially overlapping sets of input variables. We use expressions such as  $f * g$  or  $f + g$  to mean the new computation graph representing this symbolic expression. For example the computation graph for  $f + g$  has input variables  $x_{A \cup B}$  and consists of the graphs for  $f$  and  $g$  together with one additional node (primitive operation) for the final addition.

### 3.3. Marginalizing unobserved leaf nodes

As a first useful transformation of the graphical model, we consider how to improve HMC if there is an unobserved leaf node. Without loss of generality, assume the leaf is numbered  $M$ . Then we can factor the joint distribution as

$$p(\mathbf{x}_{1:M}) = p(\mathbf{x}_{1:M-1})p(x_M | \mathbf{x}_{1:M-1}), \quad (1)$$

and run HMC on the marginalized model  $p(\mathbf{x}_{1:M-1})$ , then sample  $x_M$  directly from  $p(x_M | \mathbf{x}_{1:M-1})$  by executing  $h_M(\cdot | f_M(\mathbf{x}_{\text{pa}(M)}))$ . Importantly, the marginal  $p(\mathbf{x}_{1:M-1}) = \prod_{i=1}^{M-1} p_i(x_i | f_i(\mathbf{x}_{\text{pa}(i)}))$  is simply the original graphical model with the leaf node deleted, so it is tractable. More generally, the argument is easily extended by repeatedly stripping leaves to marginalize all variables with no path to an observed variable for HMC, then to reconstruct those variables by *forward sampling* (sometimes called *ancestral sampling*) from the graphical model (Koller & Friedman, 2009).

### 3.4. Marginalizing non-leaf nodes by edge reversals

Generative models such as the eight schools and electric company models do not have unobserved leaf nodes in their original forms, since these nodes would play no useful role in the data-generating process. Instead, our goal will be to transform the model by a sequence of *edge reversals* to create unobserved leaf nodes. Each edge reversal will preserve the joint distribution of the graphical model, so it is the same for performing inference. However, it will not preserve the causal semantics of the data-generating process (which is not required for inference), so it is reasonable for the transformed model to have unobserved leaf nodes.

**Reversing a single edge.** The process of reversing a single parent-child edge  $v \rightarrow c$  is illustrated in Figure 3. There must be no other path from  $v$  to  $c$ ; otherwise reversing

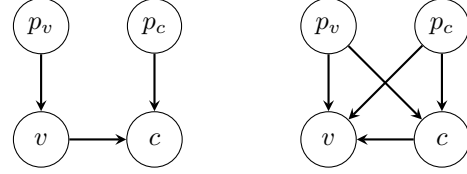


Figure 3. Reversing edge  $v \rightarrow c$ . Nodes  $p_v \in \text{pa}(v)$  and  $p_c \in \text{pa}(c) \setminus \{v\}$  are representative parents to demonstrate the transformation. Left: the graphical model before reversing  $v \rightarrow c$ . Right: the graphical model after reversing  $v \rightarrow c$ .

the edge would create a cycle. In the example, there is no other path because  $v$  has only one child. Let us define the “local distribution” of  $x_v$  and  $x_c$  as the product of the conditional distributions of those two variables given their parents, which looks like  $p(x_v | \dots)p(x_c | x_v, \dots)$ . If these distributions satisfy the appropriate conjugacy relationship, we can derive replacement factors that look like  $p(x_c | \dots)p(x_v | x_c, \dots)$  to “reverse” the  $v \rightarrow c$  edge while preserving the local distribution. Formally, the operation is:

**Definition 1** (Edge reversal). Assume  $G$  is a graphical model where node  $v$  is a parent of  $c$  and there is no other path from  $v$  to  $c$ . Reversing edge  $v \rightarrow c$  replaces factors  $p(x_v | \mathbf{x}_{\text{pa}(v)})p(x_c | x_v, \mathbf{x}_{\text{pa}(c) \setminus \{v\}})$  by  $p(x_c | \mathbf{x}_U)p(x_v | x_c, \mathbf{x}_U)$  and updates the parent sets as  $\text{pa}'(c) = U$ ,  $\text{pa}'(v) = U \cup \{c\}$  for  $U = \text{pa}(v) \cup \text{pa}(c) \setminus \{v\}$ .

It is easy to show that edge reversal yields a graphical model with the same joint distribution as the original. To understand the utility of this operation, observe in Figure 3 that node  $v$  becomes a leaf and can be marginalized after reversing  $v \rightarrow c$ . In principle, any edge can be reversed, but it is only tractable when one can derive the replacement factors. We can do so if the distributions are *locally conjugate*:

**Definition 2** (Local conjugacy). Let  $G$  be a graphical model where node  $v$  is a parent of  $c$ . We say the distribution of  $x_v$  is locally conjugate to the distribution of  $x_c$  if  $\hat{p}(x_v) := p(x_v | \mathbf{x}_{\text{pa}(v)})$  is conjugate to  $\hat{p}(x_c | x_v) := p(x_c | x_v, \mathbf{x}_{\text{pa}(c) \setminus \{v\}})$  for all values of  $\mathbf{x}_{\text{pa}(v)}$  and  $\mathbf{x}_{\text{pa}(c) \setminus \{v\}}$ .

For example, in the model  $x_1 \sim \mathcal{N}(0, 1)$ ,  $x_2 \sim \mathcal{N}(x_1, 1)$ ,  $x_3 \sim \mathcal{N}(x_1 x_2, 1)$ , the random variable  $x_1$  is conjugate to  $x_2$ , and also conjugate to  $x_3$  for fixed  $x_2$ . So it is locally conjugate to both  $x_2$  and  $x_3$ . Section 3.6 will describe the details of edge reversal using our graphical model representation and specific conjugate pairs of distribution families.

#### Creating a leaf by reversing all outgoing edges of a node.

We next consider how, if possible, to convert an arbitrary node  $v$  to a leaf by reversing all of its outgoing edges. Suppose  $v$  has  $H$  children  $c_1, \dots, c_H$ . For an arbitrary child  $c$  it may not be safe to reverse  $v \rightarrow c$  even if  $x_v$  is locally conjugate to  $x_c$  because there may be another path from  $v$  to  $c$ , which would lead to a cycle. See Figure 4 for an example.

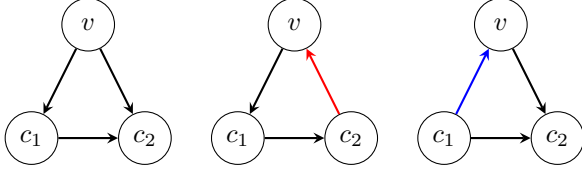


Figure 4. Challenges of reversing multiple outgoing edges. Left: the local structure. Middle: A loop is formed after reversing  $v \rightarrow c_2$ , which is invalid. Right: The model is still valid after reversing  $v \rightarrow c_1$ , and now  $v \rightarrow c_2$  can also be reversed.

However, if  $c$  is minimal among  $c_1, \dots, c_H$  in a topological ordering of  $G$ , then there can be no other  $v \rightarrow c$  path, so it is safe to reverse  $v \rightarrow c$ . Further, after reversing the edge,  $v$  will move in the topological ordering to appear after  $c$  but before the other children, and the relative ordering of the other children will remain unchanged. Then another child will be minimal in the topological ordering. Therefore, if it is possible to convert  $v$  to a leaf, we should reverse the edges from  $v$  to each of its children following their topological ordering. This reasoning is summarized in the following theorem, which is proved in the appendix.

**Theorem 1.** *Let  $G$  be a graphical model where node  $v$  has children  $c_1, \dots, c_H$ . If  $x_v$  is locally conjugate to each of  $x_{c_1}, \dots, x_{c_H}$ , then  $v$  can be turned into a leaf by reversing the edges from  $v$  to each child sequentially in the order of a topological ordering of the children.*

**Marginalizing many non-leaf nodes.** Theorem 1 describes how to modify a graphical model, while preserving the joint distribution, to convert one non-leaf node to a leaf so it can be marginalized. We now wish to use this operation to marginalize as many nodes as possible. The MARGINALIZE function in Algorithm 1 presents our heuristic for doing so: it simply applies the operation of Theorem 1 to attempt to marginalize every node  $v$  in *reverse* topological order. This is convenient because it automatically strips all nodes with no path to an observed variable at the same time. If  $v$  can be marginalized, the reversal operations are executed and  $v$  is removed from  $G$  and pushed onto a stack  $S$  that determines the recovery order. The RECOVER function augments a sample of the non-marginalized variables with direct samples of the marginalized variables. The next sections discuss the implementations of CONJUGATE and REVERSE.

### 3.5. Conjugacy detection

Detecting when  $x_a$  is locally conjugate to  $x_b$  uses the patterns listed in Table 1, where (1)  $\text{AFFINE}(u, v)$  means that  $u$  can be written as  $u = pv + q$  for expressions  $p$  and  $q$  that do not contain  $v$ , (2)  $\text{DEPENDENT}(u, v)$  means that there exists a path from  $v$  to  $u$  in the computation graph, and (3)  $\text{LINEAR}(u, v)$  means that  $u$  can be written as  $u = pv$ ,

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#### Algorithm 1 Marginalize and recover unobserved nodes

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```

1: function MARGINALIZE ( $G$ )
2:   Initialize stack  $S$  and sort nodes so they are numbered
   in topological order
3:   for each unobserved node  $v$  in descending order do
4:     if CONJUGATE( $G, v, c$ ) for all children  $c$  then
5:       // Marginalize  $v$ 
6:       for each child  $c$  in ascending order do
7:          $G = \text{REVERSE}(G, v, c)$ 
8:       Remove  $v$  from  $G$ 
9:       Add  $v$  to top of  $S$ 
10:  return  $G, S$ 

11: function RECOVER ( $S, x_v$  for nodes  $v$  not removed)
12:  while  $S$  is not empty do
13:     $v = \text{pop}(S)$ 
14:    Sample  $x_v$  given  $x_{\text{pa}(v)}$ 
15:  return  $x_{1:M}$ 

```

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for an expression  $p$  that does not contain  $v$ . For example, the pattern in the first matches the case when  $x_a$  and  $x_b$  both have normal distributions, in which case we can extract expressions (computation graphs) for the parameters  $\mu_b$  and  $\sigma_b^2$  as the two outputs of the expression  $f_b(\mathbf{x}_{\text{pa}(b)})$ . The pattern further implies that if  $\text{AFFINE}(\mu_b, x_a)$  is true and  $\text{DEPENDENT}(\sigma_b^2, x_a)$  is false, then  $x_a$  is locally conjugate to  $x_b$ . The functions  $\text{AFFINE}$ ,  $\text{LINEAR}$  and  $\text{DEPENDENT}$  require examining computation graphs; details and pseudocode can be found in appendix C.

### 3.6. Edge reversal details

If conjugacy is detected, Algorithm 1 will call the REVERSE operation to reverse an edge. Algorithm 2 shows the portion of the REVERSE algorithm for normal-normal conjugacy. We emphasize that operations like  $+$ ,  $-$  and  $*$  are symbolic operations on computation graphs. The algorithm implements well known Gaussian marginalization and conditioning formulas. Line 5 extracts the symbolic expressions for the parameters of the normal distributions. Line 6 extracts expressions  $p$  and  $q$  such that  $\mu_c = px_v + q$ ; conjugacy detection has already determined that such expressions exist. Lines 7–13 compute symbolic expressions for parameters of the marginal  $p(x_c | \dots)$  and conditional  $p(x_v | x_c, \dots)$  and write them to  $f_c$  and  $f_v$ . Finally, Lines 15–16 update the DAG to reflect the new dependencies.

### 3.7. Implementation

We have assembled the pieces for automatically marginalized HMC. The full pipeline is to: (1) extract a graphical model  $G$  from the user's program, (2) call the MARGINALIZE function to get a marginalized model  $G'$  and recovery stack  $S$ , (3) run HMC on  $G'$ , (4) for each HMC sample  $\mathbf{x}$ ,

Table 1. Patterns of conjugacy. If conditions of a row are satisfied, then the distribution of  $x_a$  is locally conjugate to the distribution of  $x_b$ .

DISTRIBUTION OF $x_a$	DISTRIBUTION OF $x_b$	CONDITION 1	CONDITION 2
$\mathcal{N}(\mu_a, \sigma_a^2)$	$\mathcal{N}(\mu_b, \sigma_b^2)$	AFFINE( $\mu_b, x_a$ )	NOT DEPENDENT( $\sigma_b, x_a$ )
$\Gamma(\alpha_a, \beta_a)$	$\Gamma(\alpha_b, \beta_b)$	LINEAR( $\beta_b, x_a$ )	NOT DEPENDENT( $\alpha_b, x_a$ )
$\Gamma(\alpha_a, \beta_a)$	EXPONENTIAL( $\lambda_b$ )	LINEAR( $\lambda_b, x_a$ )	-
BETA( $\alpha_a, \beta_a$ )	BINOMIAL( $n_b, p_b$ )	$p_b = x_a$	NOT DEPENDENT( $n_b, x_a$ )
BETA( $\alpha_a, \beta_a$ )	BERNOULLI( $\lambda_b$ )	$\lambda_b = x_a$	-

**Algorithm 2** Reversing an edge (normal-normal case)

```

1: function REVERSE ( $G = (D_i, \text{pa}(i), f_i)_{i=1}^M, v, c$ )
2:   //  $\text{pa}(v), \text{pa}(c), f_v, f_c, D_c$  updated in place
3:   // all variables represent symbolic expressions
4:   if  $D_c$  is normal and  $D_v$  is normal then
5:     Let  $\mu_v$  and  $\sigma_v^2$  be the two output expressions  $f_v$ ,
       and  $\mu_c$  and  $\sigma_c^2$  be the output expressions of  $f_c$ .
6:      $p, q = \text{AFFINE\_COEFF}(\mu_c, x_v)$ 
7:      $k = \sigma_v^2 p / (p^2 \sigma_v^2 + \sigma_c^2)$ 
8:      $\mu'_c = p\mu_v + q$ 
9:      $\sigma'^2_c = p^2 \sigma_v^2 + \sigma_c^2$ 
10:     $\mu'_v = \mu_v + k(x_c - \mu'_c)$ 
11:     $\sigma'^2_v = (1 - kp)\sigma_v^2$ 
12:     $f_c = (\mu'_c, \sigma'^2_c), f_v = (\mu'_v, \sigma'^2_v)$ 
13:   else
14:      $\vdots$  (see full algorithm in appendix)
15:    $\text{pa}(c) = (\text{pa}(c) \setminus \{v\}) \cup \text{pa}(v)$ 
16:    $\text{pa}(v) = \text{pa}(v) \cup \{c\} \cup \text{pa}(c)$ 
17:   return  $G$ 

```

call RECOVER( $S, \mathbf{x}$ ) to sample the marginalized variables.

Our implementation uses JAX (Bradbury et al., 2018) and NumPyro (Bingham et al., 2018; Phan et al., 2019) to extract a graphical model  $G$ . We use JAX tracing utilities to convert the NumPyro program to a JAX expression (Jaxpr), i.e., computation graph, for the entire sampling procedure. The NumPyro program must use a thin wrapper around NumPyro’s sample statement to register the model’s random variables in the Jaxpr. We extract the distribution families from the NumPyro trace stack and obtain the parameter functions  $f_i$  by parsing the Jaxpr to extract the partial computation mapping from parent random variables to distribution parameters. As stated earlier, our approach is limited to programs that map to a graphical model, which means they sample from a fixed sequence of conditional distributions. This closely matches those programs for which NumPyro can currently perform inference, because the JIT-compilation step of NumPyro inference requires construction of a static computation graph. NumPyro’s experimental control flow primitives (“scan” and “cond”) are not supported, and it may be difficult to do so. Our current implementation is limited to Jaxprs with scalar operations and elementwise array

operations, though this restriction is not fundamental. We expect our approach is compatible with other PPLs that use computation graphs, with similar restrictions on programs.

## 4. Related work

Conjugacy and marginalization have long been important topics in probabilistic programming. In BUGS (Lunn et al., 2000) and JAGS (Hornik et al., 2003), conjugacy was used to improve automatic Gibbs sampling. Hakaru (Narayanan et al., 2016) and PSI (Gehr et al., 2016; 2020) use symbolic integrators to perform marginalization for the purposes of exact inference. We make use of information provided by graphical models to identify certain patterns, which is more efficient in large scale models. Autoconj (Hoffman et al., 2018) proposes a term-graph rewriting system that can be used for marginalizing a log joint density with conjugacy. Our approach is distinct in that we operate on the graphical model and computation graph for the generative process, as opposed to the log-density. Gorinova et al. (2021) propose an information flow type system that could be applied to automatic marginalization of discrete random variables. Following the exploration of more expressive PPLs, streaming models have attracted much attention. Murray et al. (2018) proposed delayed sampling, which uses automatic marginalization to improve inference via the Rao-Blackwellized particle filter (RBPF) (Doucet et al., 2000). Delayed sampling has been developed in Birch (Murray & Schön, 2018), Pyro (Bingham et al., 2018) with functors (Obermeyer et al., 2019a;b), Anglican (Lundén, 2017) and ProbZelus (Baudart et al., 2020). Atkinson et al. (2022) propose semi-symbolic inference, which further expands the applicability of delayed sampling to models with arbitrary structure. Our work is distinct in that we statically analyze a model prior to performing inference for the purpose of improving MCMC: this makes our approach “fully symbolic” (no concrete values are available) and leads to different algorithmic considerations, though our Algorithm 1 shares technical underpinnings with the hoisting algorithm in Atkinson et al. (2022); see Appendix E for more details.

There are many works that improve HMC inference in PPLs from different perspectives. Stan (Carpenter et al., 2017) has had tremendous impact using HMC inference for PPLs.

Because Stan programs specify a log-density and not a sampling procedure, our idea does not directly apply to Stan programs. However, many Stan programs are generative in spirit, and Baudart et al. (2021) characterize a subset of Stan programs on which the methods of this paper can be applied directly. Papaspiliopoulos et al. (2007) propose a general framework for non-centered (re)parameterization in MCMC. Gorinova et al. (2020) automate the procedure of choosing parameterizations of models using variational inference. In Parno & Marzouk (2018) and Hoffman et al. (2019), the parameterizations of all latent variables are learned as normalizing flows (Papamakarios et al., 2021; Rezende & Mohamed, 2015). In models where some variables are marginalizable, our method works better than reparameterization: see Section 5.2 for an example. Mak et al. (2022) use the framework of involutive MCMC (Neklyudov et al., 2020; Cusumano-Towner et al., 2020) to extend the applicability of MCMC to non-parametric models in PPLs.

## 5. Experiments

We evaluate the performance of our method on two classes of hierarchical models where conjugacy plays an important role. We use NumPyro’s no-U-turn sampler (NUTS) (Hoffman & Gelman, 2014) in all experiments, denoted HMC hereafter. Our approach is “HMC with marginalization” (HMC-M). For all experiments, we use 10,000 warm up samples to tune the sampler, 100,000 samples for evaluation, and evaluate performance via effective sample size (ESS) and time (inclusive of JAX compilation time).

### 5.1. Hierarchical partial pooling models

A hierarchical partial pooling (HPP) model (Gelman et al., 1995) has the form  $p(\theta, z_{1:n}, y_{1:n}) = p(\theta) \prod_{i=1}^n p(z_i | \theta) p(y_i | \theta, z_i, x_i)$ , where  $(x_i, y_i)$  are observed covariate and response values for the  $i$ th data point,  $z_i$  is a local latent variable, and  $\theta$  is a global latent variable to model shared dependence. In some HPPs, the distribution of  $z_i$  is chosen to be a conjugate to  $y_i$ . The eight schools model is one such example. Figure 5 shows samples of  $\theta = [\mu, \tau]$  for the eight schools model obtained by both HMC and HMC-M. Without marginalization, HMC struggles to sample small values of  $\tau$  and the chain gets stuck due to the “funnel” relationship between  $\tau$  and  $x_i$  (Papaspiliopoulos et al., 2007). With marginalization, both  $x_i$  and the funnel are eliminated (from HMC), and the quality of the final samples significantly improves.

Another application of HPPs is repeated binary trials, where we observe the number of successes  $y_i$  out of  $K_i$  trials for each unit  $i$ , and assume a partially shared structure for the

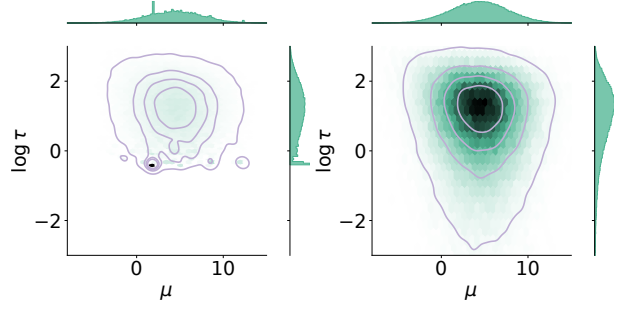


Figure 5. Histogram and contour of samples from  $\mu$  and  $\log \tau$  from the eight schools model with different algorithms. In both cases, 100k samples were taken. Left: using HMC, with very low ESS, the chain fails to mix getting stuck in a particular region with almost no exploration of low values of  $\tau$ . Right: using HMC-M, the posterior is evenly explored.

success probabilities, such as (Carpenter et al., 2017):

$$m \sim \text{Uniform}(0, 1), \quad \kappa \sim \text{Pareto}(1, 1.5), \\ \theta_i \sim \text{Beta}(m\kappa, (1 - m)\kappa), \quad y_i \sim \text{Binomial}(K_i, \theta_i).$$

Applications include the rat tumors dataset (Tarone, 1982), the baseball hits 1970 dataset (Efron & Morris, 1975) and the baseball hit 1996 AL dataset (Carpenter et al., 2017). This model is again difficult for HMC due to a funnel relationship between  $\kappa$  and  $\theta_i$  (Carpenter et al., 2017). Suggested remedies are to model  $\kappa$  with an exponential distribution (Patil et al., 2010) or rewrite the model to one where reparameterization is applicable (Carpenter et al., 2017).

We observe that, since  $\theta_i$  (Beta) is locally conjugate to  $y_i$  (Bernoulli), marginalization is a better strategy. In the marginalized model,  $y_i$  is a beta-binomial random variable, HMC samples only  $m$  and  $\kappa$ , and each  $\theta_i$  is sampled afterward from  $p(\theta_i | m, \kappa, y_i)$ , a beta distribution. The funnel problem is eliminated and the HMC dimension is reduced from  $n + 2$  to 2. Our methods achieve this automatically.

Table 2 shows the results. Sampling  $\kappa$  is known to be difficult in this model, but HMC-M achieves an ESS with similar magnitude to the number of samples. The HMC problem dimension is also reduced, which leads to faster running time. These factors combined lead to more than 100x ESS/s improvement on the baseball hit 1996 AL data set.

### 5.2. Hierarchical linear regression

Similar to partial pooling, hierarchy can be introduced in linear regression models. We demonstrate with two examples how our methods can improve inference in such models.

**Electric company:** The electric company model (Gelman & Hill, 2006) studies the effect of an educational TV program on children’s reading abilities. There are  $C = 192$  classes in  $G = 4$  grades divided into  $P = 96$  treatment-control pairs.

Table 2. Min ESS across all dimensions, time (s) and min ESS/s for HMC and HMC-M on the repeated binary trials model. Mean and std over 5 independent runs are reported.

DATASET	ALGORITHM	MIN ESS	TIME (s)	MIN ESS/s
BASEBALL HITS 1970 ( $n = 18$ )	HMC	1384.1 (1156.7)	<b>94.5</b> (5.7)	14.8 (12.7)
	HMC-M	<b>39001.8</b> (20030.4)	110.5 (89.2)	<b>592.3</b> (304.2)
RAT TUMORS ( $n = 71$ )	HMC	24632.3 (1494.5)	654.8 (43.9)	37.7 (2.1)
	HMC-M	<b>77644.5</b> (9570.8)	<b>72.4</b> (0.3)	<b>1072.7</b> (134.0)
BASEBALL HITS 1996 AL ( $n = 308$ )	HMC	9592.3 (260.1)	2746.1 (107.6)	3.5 (0.2)
	HMC-M	<b>61109.0</b> (3344.9)	<b>130.9</b> (1.4)	<b>467.0</b> (29.5)

Class  $k$  is represented by  $(g_k, p_k, t_k, y_k)$  where  $g_k$  is the grade,  $p_k$  is the index of pair,  $t_k \in \{0, 1\}$  is the treatment variable and  $y_k$  is the average score. The classes in pair  $j$  belong to grade  $gp[j]$ . The full model is

$$\begin{aligned}\mu_i &\sim \mathcal{N}(0, 1), \quad a_j \sim \mathcal{N}(100\mu_{gp[j]}, 1), \\ b_i &\sim \mathcal{N}(0, 100^2), \quad \log \sigma_i \sim \mathcal{N}(0, 1), \\ y_k &\sim \mathcal{N}(a_{p_k} + t_k b_{g_k}, \sigma_{g_k}^2).\end{aligned}$$

where  $i \in \{1, \dots, G\}$ ,  $j \in \{1, \dots, P\}$  and  $k \in \{1, \dots, C\}$ . Observe that  $\mu_i$ ,  $a_j$ ,  $b_i$  and  $y_k$  are all normally distributed with affine dependencies. Therefore, it is possible to marginalize  $\mu_i$ ,  $a_j$  and  $b_i$  from the HMC process. As Section 2 points out, it is very difficult to manually do so, but our methods do so automatically.

We observed that marginalization of  $\mu_i$  led to very high JAX compilation times even though the computation graph for the log-density was not much larger than the one before marginalization (14606 primitive operations vs. 9186). We attribute this to a current JAX limitation. See Appendix F for experimental evidence. As a workaround, we manually prevented  $\mu_i$  from being marginalized.

Figure 6 shows the results. In this model, HMC on the original model performs poorly, but reparameterizing the  $a_j$  variables is very helpful: this alternative is shown as HMC-R, and achieves excellent ESS (comparable to the number of samples). However, HMC-R does not reduce the dimension and solves a  $3G + P = 108$  dimension problem, while automatic marginalization reduces the problem dimension to 8 and results in an additional 4x speed up.

**Pulmonary fibrosis:** The Pulmonary fibrosis dataset (Shahin et al., 2020) has patient observation records over time of forced vital capacity (FVC), a disease indicator. The FVC of each patient is assumed to be linear with respect to time and regression slopes and intercepts are generated by a hierarchical model; see Appendix G. We again prevent two top-level variables from being marginalized and remove  $\frac{2}{3}$  of the data points due to slow JAX compilation. Under these settings, HMC-M again outperforms HMC and HMC-R by producing more effective samples in less time (Table 3).

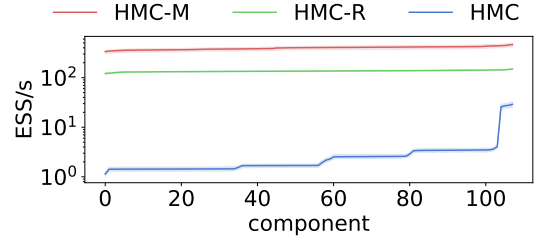


Figure 6. Component-wise ESS/s on the electric company model. Our method (HMC-M) is compared against HMC and HMC with reparameterization (HMC-R). Components ordered by ESS/s.

Table 3. Min ESS across all dimensions, time (min) and min ESS/s for HMC, HMC-R and HMC-M on the pulmonary fibrosis model. Mean and std over 5 independent runs are reported.

ALGORITHM	MIN ESS	TIME (MIN)	MIN ESS/s
HMC	19817 (1207)	51.8 (0.1)	0.1 (0.0)
HMC-R	11362 (1567)	51.5 (1.3)	0.1 (0.0)
HMC-M	<b>96135</b> (557)	<b>14.9</b> (1.3)	<b>1.8</b> (0.1)

## 6. Discussion

We proposed a framework to automatically marginalize variables in a graphical model obtained from a PPL for the purpose of accelerating MCMC. Our results show significant performance improvements in models with conjugacy. The process can be fully automated to free users from cumbersome derivations and implementations. The method is limited to graphical models, which excludes some PPL features but covers a huge range of applied statistical models. Our current implementation is limited to scalar and element-wise array operations. An important direction for future work is to support a wider range of array operations, including matrix operations, indexing, slicing, and broadcasting. Another interesting direction is to introduce automatic marginalization to MCMC applicable to higher order PPLs. We believe this work is an important step towards an automatic MCMC system that performs well on a wide range of models with minimal input from users.

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## A. Proof of the correctness of Definition 1

Definition 1 in the main text is

**Definition 1** (Edge reversal). Assume  $G$  is a graphical model where node  $v$  is a parent of  $c$  and there is no other path from  $v$  to  $c$ . Reversing the  $v \rightarrow c$  edge replaces factors  $p(x_v | \mathbf{x}_{\text{pa}(v)})p(x_c | x_v, \mathbf{x}_{\text{pa}(c) \setminus \{v\}})$  by  $p(x_c | \mathbf{x}_U)p(x_v | x_c, \mathbf{x}_U)$  and updates the parent sets as  $\text{pa}'(c) = U$ ,  $\text{pa}'(v) = U \cup \{c\}$ , where  $U = \text{pa}(v) \cup \text{pa}(c) \setminus \{v\}$ .

It was claimed that the operation yields a graphical model with the same joint distribution as the original. Now we prove it.

*Proof.* It is enough to show that (1) the graphical model after reversal is still valid; (2) the joint distribution does not change, which requires

$$p(x_v | \mathbf{x}_{\text{pa}(v)})p(x_c | x_v, \mathbf{x}_{\text{pa}(c) \setminus \{v\}}) = p(x_c | \mathbf{x}_U)p(x_v | x_c, \mathbf{x}_U).$$

For (1), we need to show that no cycles could be formed during the process. For any  $p_v \in \text{pa}(v)$ , an edge  $p_v \rightarrow c$  is added. Because there does not exist a path from  $c$  to  $p_v$  (otherwise there will be a loop in the original model), this edge will not cause a loop. For any  $p_c \in \text{pa}(c) \setminus \{v\}$ , an edge  $p_c \rightarrow v$  is introduced. This edge will also not cause a loop; otherwise another path from  $v$  to  $c$  will be found. Finally, the edge  $v \rightarrow c$  is replaced with  $c \rightarrow v$ , this edge will also not introduce a loop because there are no other paths from  $v$  to  $c$ .

Now we show (2). Since there is no other paths from  $v$  to  $c$ , there is no path from  $v$  to any nodes in  $\mathbf{x}_{\text{pa}(c) \setminus \{v\}}$ . Conditioned on  $\mathbf{x}_{\text{pa}(v)}$ , by conditional independence, we have that  $p(x_v | \mathbf{x}_{\text{pa}(v)}) = p(x_v | \mathbf{x}_U)$ . Also, all paths from nodes in  $\text{pa}(v)$  to  $c$  are blocked either by  $v$ , or by a parent of  $c$ , so conditioned on  $\mathbf{x}_{\text{pa}(c) \setminus \{v\}}$ , by independence,  $p(x_c | x_v, \mathbf{x}_{\text{pa}(c) \setminus \{v\}}) = p(x_c | x_v, \mathbf{x}_U)$ . By the properties of conjugacy, we have that

$$\begin{aligned} p(x_v | \mathbf{x}_{\text{pa}(v)})p(x_c | x_v, \mathbf{x}_{\text{pa}(c) \setminus \{v\}}) &= p(x_v | \mathbf{x}_U)p(x_c | x_v, \mathbf{x}_U) \\ &= p(x_c | \mathbf{x}_U)p(x_v | x_c, \mathbf{x}_U). \end{aligned}$$

□

## B. Proof of the Theorem 1

We first restate Theorem 1.

**Theorem 1.** Let  $G$  be a graphical model where node  $v$  has children  $c_1, \dots, c_H$ . If  $x_v$  is locally conjugate to each of  $x_{c_1}, \dots, x_{c_H}$ , then node  $v$  can be turned into a leaf by sorting  $c_1, \dots, c_H$  by any topological ordering and reversing the edges from  $v$  to each child following this ordering.

*Proof.* Without loss of generality, assume  $c_1, \dots, c_H$  are sorted according to topological ordering. We prove by induction. Assume for  $k \in \{0, \dots, H\}$ , we have reversed the edges  $v \rightarrow c_1, \dots, v \rightarrow c_k$ , and have the following properties:

- (1) The children of  $v$  are  $c_{k+1}, \dots, c_H$ .
- (2)  $c_{k+1}, \dots, c_H$  are ordered topologically;
- (3)  $x_v$  is a local conjugate prior for each of  $x_{c_{k+1}}, \dots, x_{c_H}$ .

We show that the edge  $v \rightarrow c_{k+1}$  is reversible and the properties still hold for  $k+1$  after the reversal. By (1) and (2),  $c_{k+1}$  is minimal among the children of  $v$  in topological order, so there does not exist a path from  $v$  to  $c_{k+1}$  other than  $v \rightarrow c_{k+1}$ . By (3),  $x_v$  is a local conjugate prior to  $x_{c_{k+1}}$ . Then we can apply edge reversal to  $v \rightarrow c_{k+1}$ . Now we check all the conditions after the replacement. For property (1), the children of  $v$  now become  $c_{k+2}, \dots, c_H$ . For property (2), the nodes with edges that changed (either incoming or outgoing) were  $v$ ,  $c_{k+1}$ , and their parents; these nodes all preceded  $c_{k+2}, \dots, c_H$  in topological order prior to the reversal and continue to do so afterward, so the relative ordering of  $c_{k+2}, \dots, c_H$  does not change. For (3), the distribution family of  $x_v$  does not change, and the conditional distribution of each of  $x_{c_{k+2}}, \dots, x_{c_H}$  does not change. So all conditions of local conjugacy in Table 1 will not change for them, which means the distribution of  $x_v$  is still a local conjugate prior for the distributions of each of  $x_{c_{k+2}}, \dots, x_{c_H}$ .

In summary, the three conditions holds for  $k = H$  by induction, which means  $v$  can be converted to a leaf following the said procedure. □

**Algorithm 3** Determining dependency of a variable on an input.  $\mathbf{x}_{1:M}$  is the set of all random variables.

```

1: function DEPENDENT ( $w_j, x$ )
2:   if  $w_j = x$  then
3:     return True
4:   if  $w_j \in \mathbf{x}_{1:M}$  then
5:     return False
6:   for  $p \in \text{pred}(j)$  do
7:     if DEPENDENT( $w_p, x$ ) then
8:       return True
9:   return False
    
```

### C. Details of conjugacy detection

Conjugacy detection requires looking into the computation graph of functions. In this section, we introduce how conjugacy detection is performed on a computation graph. During the tracing of a program, the procedure of computation is compiled into intermediate representations consisting of basic operations. For example, the function

```

def f(x, y):
    p = (x - y) ** 2
    q = (x + y) ** 2
    return p + q
    
```

could be represented as

```

INPUTS: a, b
c = SUB a b
d = SQUARE c
e = ADD a b
f = SQUARE e
g = ADD d f
OUTPUTS: g
    
```

By looking at the intermediate representations, it is possible to reason about the relationship between outputs and inputs. For a function  $f(x_{i_1}, x_{i_2}, \dots, x_{i_k})$ , we defined its computation graph to be a sequence of  $N_f$  *primitive operations* in Section 3.2. The sequence  $w_1, w_2, \dots, w_{k+N_f}$  is computed, where: (1) the first  $k$  are the inputs to the function, i.e.,  $w_j = x_{i_j}$  for  $j = 1$  to  $k$ , and (2) each subsequent value is computed from the preceding values as

$$w_j = \phi_j(\mathbf{w}_{\text{pred}(j)}), \quad (2)$$

where  $\phi_j$  is a primitive operation on the set of values  $\mathbf{w}_{\text{pred}(j)}$ , where  $\text{pred}(j) \subseteq \{1, \dots, j-1\}$  is the set of predecessors of  $j$ . In Section 3.5, we have reduced conjugacy detection to affinity, linearity and dependency detections. We first introduce the details of dependency detection with the above definition.

Given a function with a computation graph, we may want to determine whether a variable  $w_j$  depends on an input  $x_a$ . We define the result to be  $\text{DEPENDENT}(w_j, x_a)$ , which could be obtained recursively through the equations shown in Algorithm 3. Note that in this paper, the inputs of functions are always random variables in  $\mathbf{x}_{1:M}$ . For  $\text{DEPENDENT}(w_j, x_a)$ , if  $w_j$  is a random variable in  $\mathbf{x}_{1:M}$ , then it must be an input of the function. Then  $\text{DEPENDENT}$  would return whether  $w_j$  is  $x_a$ . If  $w_j$  is the result of a basic operator, it would enumerate the inputs of that operator. If any of those inputs are dependent on  $x_a$ , then the result is true. The recursive algorithm could be of exponential complexity in some special cases. We store intermediate results in a dictionary and refer to it before recursion to avoid redundant computation. Then the complexity is linear with respect to the number of variables involved.

Affinity and linearity can be included in the same framework. In addition to determining whether  $w_j$  is affine to  $x_a$ , we further return whether the slope and intercept are non-zero. If affinity is detected with zero intercept, the relationship is then linear. We define  $\text{AFFINE\_ALL}(w_j, x_a)$  to be a tuple of three bool variables - whether  $w_j$  is affine on  $x_a$ ,

---

**Algorithm 4** Determining affinity and linearity of a variable on an input.  $\mathbf{x}_{1:M}$  is the set of all random variables.

---

```

1: function AFFINE_ALL ( $w_j, x$ )
2:   if  $w_j = x$  then
3:     return True, True, False
4:   if  $w_j \in \mathbf{x}_{1:M}$  then
5:     return True, False, True
6:   if  $\phi_j \in \{\text{ADD}, \text{SUB}\}$  and  $\text{pred}(j) = \{p_1, p_2\}$  then
7:      $r_1, s_2, t_1 = \text{AFFINE\_ALL}(w_{p_1}, x)$ 
8:      $r_2, s_2, t_2 = \text{AFFINE\_ALL}(w_{p_2}, x)$ 
9:     return  $r_1$  and  $r_2, s_1$  or  $s_2, t_1$  or  $t_2$ 
10:  if  $\phi_j = \text{MUL}$  and  $\text{pred}(j) = \{p_1, p_2\}$  then
11:     $r_1, s_2, t_1 = \text{AFFINE\_ALL}(w_{p_1}, x)$ 
12:     $r_2, s_2, t_2 = \text{AFFINE\_ALL}(w_{p_2}, x)$ 
13:    if not  $s_1$  then
14:      return  $r_1$  and  $r_2, t_1$  and  $s_2, t_1$  and  $t_2$ 
15:    if not  $s_2$  then
16:      return  $r_1$  and  $r_2, s_1$  and  $t_2, t_1$  and  $t_2$ 
17:    return False, False, False
18:  if  $\phi_j = \text{DIV}$  and  $\text{pred}(j) = \{p_1, p_2\}$  then
19:     $r_1, s_2, t_1 = \text{AFFINE\_ALL}(w_{p_1}, x)$ 
20:     $r_2, s_2, t_2 = \text{AFFINE\_ALL}(w_{p_2}, x)$ 
21:    if not  $s_2$  then
22:      return  $r_1$  and  $r_2, s_1, t_1$ 
23:    return False, False, False
24:  for  $p \in \text{pred}(j)$  do
25:     $r, s, t = \text{AFFINE\_ALL}(w_p, x)$ 
26:    if not  $r$  or  $s$  then
27:      return False, False, False
28:  return True, False, True
29:
30: function AFFINE ( $w_j, x$ )
31:   $r, s, t = \text{AFFINE\_ALL}(w_j, x)$ 
32:  return  $r$ 
33:
34: function LINEAR ( $w_j, x$ )
35:   $r, s, t = \text{AFFINE\_ALL}(w_j, x)$ 
36:  return  $r$  and not  $t$ 

```

---

whether the slope is non-zero and whether the intercept is non-zero. Then LINEAR and AFFINE could be obtained from  $\text{AFFINE\_ALL}(w_j, x_a)$ . Our algorithm of affinity detection is adapted from [Atkinson et al. \(2022\)](#) with slight modification to setting that has no concrete values. The pseudocodes are in Algorithm 4. The result of  $\text{AFFINE\_ALL}(w_j, x_a)$  could be obtained by enumeration of cases of  $\phi_j$  and induction in the structure of the computation graph. For example, if we know  $w_j = \text{ADD}(w_{p_1}, w_{p_2})$ , and  $r_1, s_1, t_1 = \text{AFFINE\_ALL}(w_{p_1}, x_a)$  and  $r_2, s_2, t_2 = \text{AFFINE\_ALL}(w_{p_2}, x_a)$ , then  $w_j$  is affine to  $x_a$  if both of  $w_{p_1}$  and  $w_{p_2}$  are affine to  $x_1$ , which means ( $r_1$  **and**  $r_2$ ). The slope is non-zero if any of the slope of  $p_1$  or  $p_2$  is non-zero, so the second return value is ( $s_1$  **or**  $s_2$ ). The same applies to whether the intercept is non-zero, which is ( $t_1$  **or**  $t_2$ ).

## D. Details of reversing an edge

We have constructed the parts of conjugacy detection. In this section we discuss the details of reversing an edge in the marginalized MCMC. In Algorithm 2 a function AFFINE\_COEFF is defined to get the coefficients when affinity is detected. The pseudocode of it is in Algorithm 5, which is similar to AFFINE. We emphasize that the computations in Algorithm 5 are fully symbolic. Each variable corresponds to a sequence of operations which could be regarded as a computation graph.

---

**Algorithm 5** Getting the coefficients of affine relationship between a variable  $w_j$  on an input  $x$ .  $\mathbf{x}_{1:M}$  is the set of all random variables.

---

```

1: function AFFINE_COEFF( $w_j, x$ )
2:   if  $w_j = x$  then
3:     return 1, 0
4:   if  $w_j \in \mathbf{x}_{1:M}$  then
5:     return 0, 1
6:   if  $\phi_j = \text{ADD}$  and  $\text{pred}(j) = \{p_1, p_2\}$  then
7:      $s_1, t_1 = \text{AFFINE\_COEFF}(w_{p_1}, x)$ 
8:      $s_2, t_2 = \text{AFFINE\_COEFF}(w_{p_2}, x)$ 
9:     return  $s_1 + s_2, t_1 + t_2$ 
10:  if  $\phi_j = \text{SUB}$  and  $\text{pred}(j) = \{p_1, p_2\}$  then
11:     $s_1, t_1 = \text{AFFINE\_COEFF}(w_{p_1}, x)$ 
12:     $s_2, t_2 = \text{AFFINE\_COEFF}(w_{p_2}, x)$ 
13:    return  $s_1 - s_2, t_1 - t_2$ 
14:  if  $\phi_j = \text{MUL}$  and  $\text{pred}(j) = \{p_1, p_2\}$  then
15:     $s_1, t_1 = \text{AFFINE\_COEFF}(w_{p_1}, x)$ 
16:     $s_2, t_2 = \text{AFFINE\_COEFF}(w_{p_2}, x)$ 
17:    if  $s_1$  is zero then
18:      return  $t_1 * s_2, t_1 * t_2$ 
19:    if  $s_2$  is zero then
20:      return  $s_1 * t_2, t_1 * t_2$ 
21:    raise Error
22:  if  $\phi_j = \text{DIV}$  and  $\text{pred}(j) = \{p_1, p_2\}$  then
23:     $s_1, t_1 = \text{AFFINE\_COEFF}(w_{p_1}, x)$ 
24:     $s_2, t_2 = \text{AFFINE\_COEFF}(w_{p_2}, x)$ 
25:    if  $s_2$  is zero then
26:      return  $s_1/t_2, t_1/t_2$ 
27:    raise Error
28:  return 0,  $w_j$ 

```

---

So each  $+$ ,  $-$ ,  $*$  and  $/$  is applied as merging two (potentially overlapping) computation graphs. One issue is we need to define whether some variables are zero (lines 17,19,25). So operations of zeros should be specially dealt with. For example, if we find a  $0 + 0$ , instead of declaring an operation that adds two zeros, we should instead use the result 0.

Now we are only left with the full version of Algorithm 2, which could be found in Algorithm 6.

## E. Relations to the hoisting algorithm

The hoisting algorithm in [Atkinson et al. \(2022\)](#) is an online algorithm that can be used for automatically running Rao-Blackwellized particle filters (RBPF) ([Doucet et al., 2000](#)). Our Algorithm 1 is highly related to the hoisting algorithm. Both algorithms can perform conjugacy detection and marginalize all possible random variables. One apparent difference is that Algorithm 1 is written as loops while the hoisting algorithm uses recursions. However, the main difference between the two algorithms comes from the application. In RBPF, all non-marginalizable random variables are sampled from the model, allowing the representations to be semi-symbolic, where non-marginalizable random variables are replaced with sampled values during the execution of the hoisting algorithm. In HMC, no random variables are directly sampled, and the same computation graph will be executed many times, so marginalization should be performed before running with fully symbolic representations. In the mean time, Theorem 1 allows us to separate the conjugacy detections and the reversals in two different loops, which reduces the running time in large scale models. This improvement is not possible with the hoisting algorithm as an online algorithm, so some unnecessary reversals are performed. Furthermore, from the perspective of implementation, the parent node is fixed inside the loop of  $v$  in Algorithm 1. So in one iteration, all the calls to CONJUGATE and REVERSE are with respect to the same  $v$ . It is therefore possible to save the intermediate results of these functions to avoid redundant computation on the computation graph. So the time complexity of Algorithm 1 is  $O(M|C|)$ , where  $|C|$  is the size of the

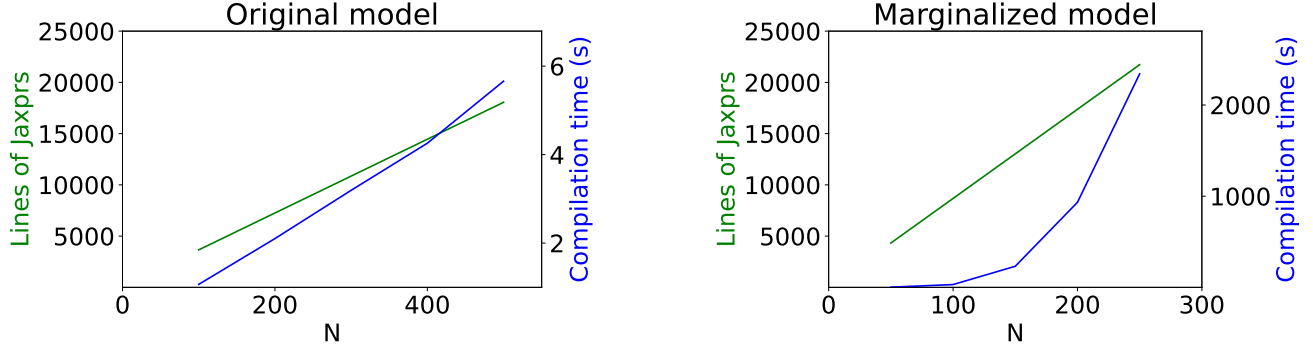


Figure 7. Lines of Jaxprs of the gradient of the log density function and JIT compilation time with respect to  $N$  for the simple hierarchical model. With similar lines of Jaxprs, the compilation time can be hundreds of times slower on the marginalized model than on the original model.

computation graph. With the above considerations, we think that Algorithm 1 is an important contribution in the area.

## F. Slow compilation of JAX

In the experiments, we discover that the compilation time of JAX can be slow for some models. We identify the problem specifically at the structure of marginalized hierarchical models. To demonstrate, we consider the simple model

$$x \sim \mathcal{N}(0, 1), \log \sigma \sim \mathcal{N}(0, 1), y_i \sim \mathcal{N}(x, 1),$$

where  $i = 1, \dots, N$  and  $y_i = 0$  for all  $i$  are provided as pseudo observations. It is possible to marginalize  $x$  by reversing edges to each of  $y_i$ . However, we found that the JIT compilation time scales super-linear with respect to  $N$  for the marginalized model. See Figure 7. Regardless of the performance, the JIT compilation time for the gradient function of the marginalized model can be hundreds larger than that of the original model when  $N$  is large enough, with similar lines of Jaxprs. This is probably because marginalization creates a chain shaped computation graph for all the observations, and it is difficult for JAX to work in this case. We do not regard it as a core limitation of our idea.

## G. Pulmonary fibrosis model

Records from the pulmonary fibrosis dataset (Shahin et al., 2020) have the form  $(\text{ID}_i, t_i, y_i)$ , where  $\text{ID}_i$  is the patient id,  $t_i$  is the observation time, and  $y_i$  is forced vital capacity (FVC), a measure of disease progression. The FVC of each patient is assumed to be linear with respect to time and regression slopes and intercepts are generated by the following hierarchical model:

$$\begin{aligned} \mu_\alpha &\sim \mathcal{N}(0, 500^2), \sigma_\alpha \sim \text{HalfCauchy}(100), \\ \mu_\beta &\sim \mathcal{N}(0, 3^2), \sigma_\beta \sim \text{HalfCauchy}(3), \\ \alpha_j &\sim \mathcal{N}(\mu_\alpha, \sigma_\alpha^2), \beta_j \sim \mathcal{N}(\mu_\beta, \sigma_\beta^2), \\ \sigma &\sim \text{HalfCauchy}(100), y_i \sim \mathcal{N}(\alpha_{\text{ID}_i} + t_i \beta_{\text{ID}_i}, \sigma^2), \end{aligned}$$

where  $i \in \{1, \dots, 549\}$  and  $j \in \{1, \dots, 173\}$ . We prevented the variables  $\mu_\alpha$  and  $\mu_\beta$  from being marginalized to avoid slow JAX compilation.

---

**Algorithm 6** The full version of Algorithm 2: reversing an edge
 

---

```

1: function REVERSE ( $G = (D_i, \text{pa}(i), f_i)_{i=1}^M, v, c$ )
2:   //  $\text{pa}(v), \text{pa}(c), f_v, f_c, D_c$  updated in place
3:   // all variables represent symbolic expressions
4:   if  $D_c$  is normal and  $D_v$  is normal then
5:     Let  $\mu_v$  and  $\sigma_v^2$  be the two output expressions  $f_v$ , and  $\mu_c$  and  $\sigma_c^2$  be the output expressions of  $f_c$ .
6:      $p, q = \text{AFFINE\_COEFF}(\mu_c, x_v)$ 
7:      $k = \sigma_v^2 p / (p^2 \sigma_v^2 + \sigma_c^2)$ 
8:      $\mu'_c = p \mu_v + q$ 
9:      $\sigma'^2_c = p^2 \sigma_v^2 + \sigma_c^2$ 
10:     $\mu'_v = \mu_v + k(x_c - \mu'_c)$ 
11:     $\sigma'^2_v = (1 - kp) \sigma_v^2$ 
12:     $f_c = (\mu'_c, \sigma'^2_c), f_v = (\mu'_v, \sigma'^2_v)$ 
13:  if  $D_v$  is Beta and  $D_c \in \{\text{Bernoulli}, \text{Binomial}\}$  then
14:    Let  $\alpha_v$  and  $\beta_v$  be the two output expressions of  $f_v$ 
15:    if  $D_c = \text{Bernoulli}$  then
16:       $n_c = 1$ 
17:       $p_c = \lambda_c$ 
18:    else
19:      Let  $n_c$  and  $p_c$  be the two output expressions of  $f_c$ 
20:       $\alpha'_v = \alpha_v + x_c$ 
21:       $\beta'_v = \beta_v + n_c - x_c$ 
22:       $D_c = \text{BetaBinomial}$ 
23:       $f_c = (n_c, \alpha_v, \beta_v), f_v = (\alpha'_v, \beta'_v)$ 
24:  if  $D_v$  is Gamma and  $D_c \in \{\text{Exponential}, \text{Gamma}\}$  then
25:    Let  $\alpha_v$  and  $\beta_v$  be the two output expressions of  $f_v$ 
26:    if  $D_c = \text{Exponential}$  then
27:       $\alpha_c = 1$ 
28:       $\beta_c = \lambda_c$ 
29:    else
30:      Let  $\alpha_c$  and  $\beta_c$  be the two output expressions of  $f_c$ 
31:       $p, q = \text{AFFINE\_COEFF}(\beta_c, x_v)$ 
32:       $\alpha'_v = \alpha_v + \alpha_c$ 
33:       $\beta'_v = \beta_v + p * x_c$ 
34:       $D_c = \text{CompoundGamma}$ 
35:       $f_c = (\alpha_c, \alpha_v, \beta_v/p), f_v = (\alpha'_v, \beta'_v)$ 
36:   $\text{pa}(c) = (\text{pa}(c) \setminus \{v\}) \cup \text{pa}(v)$ 
37:   $\text{pa}(v) = \text{pa}(v) \cup \{c\} \cup \text{pa}(c)$ 
38:  return  $G$ 

```

---