Automating Involutive MCMC using Probabilistic and Differentiable Programming

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Abstract

Involutive MCMC is a unifying mathematical construction for MCMC kernels that generalizes many classic and state-of-the-art MCMC algorithms, from reversible jump MCMC to kernels based on deep neural networks. But as with MCMC samplers more generally, implementing involutive MCMC kernels is often tedious and error-prone, especially when sampling on complex state spaces. This paper describes a technique for automating the implementation of involutive MCMC kernels given (i) a pair of probabilistic programs defining the target distribution and an auxiliary distribution respectively and (ii) a differentiable program that transforms the execution traces of these probabilistic programs. The technique, which is implemented as part of the Gen probabilistic programming system, also automatically detects user errors in the specification of involutive MCMC kernels and exploits sparsity in the kernels for improved efficiency. The paper shows example Gen code for a split-merge reversible jump move in an infinite Gaussian mixture model and a state-dependent mixture of proposals on a combinatorial space of covariance functions for a Gaussian process.

1 INTRODUCTION

Markov chain Monte Carlo (MCMC) algorithms are powerful tools for approximate sampling from probability distributions and are central to modern Bayesian statistics, probabilistic machine learning, statistical physics, and numerous application areas where probabilistic modeling and inference are used. But designing and deriving efficient MCMC algorithms is mathematically involved, and implementing MCMC kernels is tedious and notoriously error-prone. These challenges are especially pronounced when sampling from probability distributions on complex state spaces that combine symbolic, numeric, and structural uncertainty, such as those arising in computational biology [Huelsenbeck et al., 2004], robotics and scene understanding [Geiger et al., 2011], and models of human cognition [Tenenbaum et al., 2011].

Involutive MCMC is a mathematical construction for MCMC kernels that gives a simplifying and unifying perspective on a number of previously disparate classes of kernels, including reversible jump MCMC [Green, 1995], which is the dominant mathematical framework for MCMC on complex state spaces. Involutive MCMC constructs an MCMC kernel from three components: (i) the unnormalized target density, (ii) a sampler and density for an auxiliary probability distribution, and (iii) an involution on an extended state space. While this construction is mathematically clarifying, correctly implementing involutive MCMC kernels on complex state spaces remains challenging due to tedious density and Jacobian computations and the need for careful reasoning about the state space.

This paper formulates involutive MCMC on general state spaces and shows how to automate the implementation of an involutive MCMC kernel from three declarative programs that define the target probability distribution, auxiliary probability distribution, and the involution, respectively. The probability distributions are defined as probabilistic programs, and the involution is defined as a differentiable program that transforms the execution traces of the probabilistic programs. We use probabilistic programming techniques and automatic differentiation to automatically compute the acceptance probability. We also show how to automatically detect mathematical errors in the specification of an involutive MCMC kernel, and how to improve the efficiency by automatically exploiting the sparsity structure in the involution. We implemented the approach within the Gen probabilistic pro-

1 An involution is a bijection that is its own inverse (that is, $f$ where $f(f(z)) = z$).
The involutive MCMC construction encompasses many existing classes of MCMC kernels, some of which explicitly make use of bijective or involutive deterministic maps. In particular, the reversible jump framework [Green, 1995; Hastie and Green, 2012] employs a family of continuously differentiable bijections between the parameter spaces of different models. Tierney (1998) described a family of deterministic proposals based on a deterministic involution that is equivalent to involutive MCMC but without the auxiliary probability distribution. More recently, Spanbauer et al. (2020) defined a class of deep generative models based on differentiable involutions and trained these models to serve as efficient proposal distributions on continuous state spaces; the resulting algorithm is an instance of the construction presented in this paper.

In recent decades, a number of probabilistic programming systems have automated the implementations of probabilistic inference algorithms (Gilks et al., 1994; Milch et al., 2005; Pfeffer, 2007; Goodman et al., 2008; Gehr et al., 2016; Carpenter et al., 2017). Most of these systems support generic built-in inference algorithms, with user-customization limited to tweaking algorithm parameters. Some systems allow for user-defined variational families or proposal distributions (Ritchie et al., 2016; Bingham et al., 2019). Programmable inference (Mansinghka et al., 2018) proposes that inference algorithms be programmed by users using new high-level inference abstractions. The Gen probabilistic programming system (Cusumano-Towner et al., 2019) exposes an API that supports high-level user implementations of an open-ended set of inference algorithms, and abstracts away low-level implementation details of inference algorithms.

One other probabilistic programming system besides Gen supports custom reversible jump samplers: Roberts et al. (2019) present a system embedded in Haskell that automatically generates the implementation of some reversible jump MCMC kernels from a high-level specification. Narayanan and Shan (2020) give a technique that automatically computes Metropolis-Hastings acceptance probabilities in some settings; however, these approaches do not handle many kernels that can be handled by our technique, including the example in Figure 2.
(a) A pair of split-merge transitions in a Gaussian mixture model. The split transition splits the orange component into purple and blue components.

\begin{align*}
\text{k} & \sim \text{poisson} + 1(1) \\
\text{means} & \sim \text{normal}(0, 10) \\
\text{weights} & \sim \text{dirichlet}(1.0 \text{ for k in 1:k}) \\
\end{align*}

(b) An infinite Gaussian mixture model expressed in a Gen probabilistic modeling language.

\begin{align*}
@gen function p(n::Int)
   k ~ poisson_plus_one(1)
   means = [((\text{mu}, j)) ~ normal(0, 10) for j in 1:k]
   vars = [((\text{var}, j)) ~ inv\_gamma(1, 10) for j in 1:k]
   for i in 1:n
      (x, i) ~ mixture_of_normals(weights, means, vars)
   end
   weights ~ dirichlet([2.0 for j in 1:k])
   \text{means} = [((\text{mu}, j)) ~ normal(0, 10) for j in 1:k]
   \text{vars} = [((\text{var}, j)) ~ inv\_gamma(1, 10) for j in 1:k]
end

(c) Auxiliary proposal distribution \(q\) for the split-merge reversible jump MCMC move, expressed in a Gen probabilistic modeling language.

\begin{align*}
@gen function q(n::Int)
   k = \text{trace}[k] \# current number of clusters
   \text{split} = (k = 1) \? \text{true} : ((\text{split}) \sim \text{bernoulli}(0.5))
   \text{if split}
      \text{cluster\_to\_split} \sim \text{uniform\_discrete}(1, k)
      u1 ~ \text{beta}(2, 2); u2 ~ \text{beta}(2, 2); u3 ~ \text{beta}(1, 1)
      \text{else}
      \text{cluster\_to\_merge} \sim \text{uniform\_discrete}(1, k-1)
   \text{end}
end

(d) Involution \(f\) for the split-merge reversible jump MCMC move, expressed in a Gen differentiable programming language.

@transform \# (model\_in, aux\_in) to (model\_out, aux\_out) begin
   k \sim \text{read}(model\_in[:k], :discrete)
   \text{split} = (k = 1) \? \text{true} : \text{read}(aux\_in[:split], :discrete)
   \text{if split}
      \text{cluster\_to\_split} \sim \text{read}(aux\_in[:cluster\_to\_split], :discrete)
      \text{write}(model\_out[:k], k+1, :discrete)
      \text{copy}(aux\_in[:cluster\_to\_split], aux\_out[:cluster\_merge])
      \text{write}(aux\_out[:split], false, :discrete)
   \text{else}
      \text{cluster\_to\_merge} \sim \text{read}(aux\_in[:cluster\_to\_merge], :discrete)
      \text{write}(p\_out, k, k+1, :discrete)
      \text{copy}(aux\_in[:cluster\_merge], aux\_out[:cluster\_to\_split])
      \text{if (k > 2) write}(aux\_in[:split], true, :discrete)
   \text{end}
end

\[=\] model traces (traces of \(p\))
\[=\] auxiliary proposal traces (traces of \(q\))

Figure 1: Example of reversible jump MCMC (Green, 1995) implemented using involutive MCMC in Gen. The example implements a ‘split-merge move’ in an infinite Gaussian mixture model (Richardson and Green, 1997) using three Gen programs: (1) a probabilistic program \(p\) encoding the generative model (shown in b), (2) a probabilistic program \(q\) encoding an auxiliary probability distribution (shown in c), and (3) a differentiable program \(f\) that encodes an involution on the space of pairs of traces of \(p\) and \(q\) (shown in d). Gen’s involutive MCMC operator (shown in e) automatically computes the acceptance probability.
@gen function p(x_values::Vector)
    cov_function = cov_function_prior()
    cov_matrix = compute_cov_matrix(cov_function, x_values)
    n = length(xs)
    y_values = mvnormal(zeros(n), cov_matrix .+ 0.01*I(n))
end

@gen function cov_function_prior()
    node_type = categorical(production_rule_probs))
    if node_type == CONSTANT
        param ~ uniform(0, 1)
    return ConstantNode(param)
    elseif node_type == PLUS
        left_node ~ cov_function_prior()
        right_node ~ cov_function_prior()
        return PlusNode(left_node, right_node)
    elseif node_type == TIMES
        left_node ~ cov_function_prior()
        right_node ~ cov_function_prior()
        return TimesNode(left_node, right_node)
    elseif node_type == TIMES
        left_node ~ cov_function_prior()
        right_node ~ cov_function_prior()
        return TimesNode(left_node, right_node)
    elseif node_type == SQUARED_EXP
        length_scale ~ uniform(0, 1)
        return SquaredExponentialNode(length_scale)
    elseif node_type == LINEAR
        param ~ uniform(0, 1)
        return LinearNode(param)
    elseif node_type == PERIODIC
        return PeriodicNode(length_scale)
    end
end

@gen function q(trace)
    prev_cov_function = trace[:cov_function]
    path ~ walk_tree(prev_cov_function, [:cov_function])
    new_subtree ~ cov_function_prior()
    return path
end

@gen function walk_tree(node::Node, path)
    if isa(node, LeafNode)
        done = bernoulli(1)
        return path
    elseif (::done) ~ bernoulli(0.5)
        return path
    elseif (::recurse_left) ~ bernoulli(0.5)
        path = (path..., :left_node)
        return (::left) ~ walk_tree(node.left, path)
    else
        path = (path..., :right_node)
        return (::right) ~ walk_tree(node.right, path)
    end
end

@transform f (model_in, aux_in) to (model_out, aux_out) begin
  model_subtree_address = foldr(=>, path)
  new_subtree ~ cov_function_prior()
  prev_cov_function = trace[:cov_function]
  path ~ walk_tree(prev_cov_function, [:cov_function])
  new_subtree ~ cov_function_prior()
  return path
end

Figure 2: A mixture kernel implemented using involutive MCMC in Gen, applied to infer the covariance function of a Gaussian process. The prior on covariance functions is based on a probabilistic context-free grammar. Each component kernel in the mixture replaces a subtree of the covariance function parse tree with a new subtree. The mixture kernel chooses a random subtree to replace via a random walk on the parse tree. The mixture kernel is composed from three Gen programs: (1) a probabilistic program p encoding the generative model (shown in a), (2) a probabilistic program q encoding an auxiliary probability distribution (shown in b), and (3) a differentiable program f that encodes an involution (shown in d).
3 INVOLUTIVE MCMC ON GENERAL STATE SPACES

Involutive MCMC is a general framework for constructing MCMC kernels that are stationary for a target probability distribution $p$. Informally, the algorithm works as follows: starting at some state $x$, we first sample an auxiliary variable $y \sim q_x$ from a state-dependent auxiliary distribution. We then apply an involution $f$ to the pair $(x, y)$ to obtain $(x', y')$. Finally, we compute an acceptance probability $\alpha$ and either accept $x'$ as the new state, or reject it and repeat the previous state $x$. Different choices of $q$ and $f$ recover many algorithms from the literature (Neklyudov et al., 2020).

In this section, we present involutive MCMC for models $p$ and auxiliary kernels $q$ defined over general state spaces. By emphasizing general state spaces, we intend to clarify a potential point of confusion regarding the involutive MCMC algorithm: as presented by Neklyudov et al. (2020), the acceptance probability $\alpha$ depends on the Jacobian of the involution $f$, but it is not immediately clear how to define this Jacobian when $f$ may operate on samples from arbitrary measurable spaces, rather than on vectors in $\mathbb{R}^n$. Our reformulation of the algorithm below is general enough to handle arbitrary model and auxiliary distributions, and precise enough to enable automation via probabilistic and differentiable programming: the rest of this paper uses it to develop a technique for deriving efficient implementations of involutive MCMC algorithms automatically, given only declarative specifications of $p$, $q$, and $f$.

3.1 General Involutive MCMC

Let $(X, \Sigma_P, \mu_P)$ and $(Y, \Sigma_Q, \mu_Q)$ denote two general measure spaces with $\sigma$-finite $\mu_P$ and $\mu_Q$. Involutive MCMC (Algorithm 1) implements a transition kernel that is invariant for a model distribution given by $p : X \rightarrow [0, \infty)$, a probability density over $X$ with respect to $\mu_P$. Each iteration, the algorithm first samples auxiliary variables $y \in Y$ from an auxiliary distribution $q_x$ based on the model’s current state $x$: for each $x \in X$ such that $p(x) > 0$, $q_x : Y \rightarrow [0, \infty)$ is a probability density with respect to $\mu_Q$.

The resulting pair $(x, y)$ of the current model state and the newly sampled auxiliary state will be an element of the joint space $Z := \{ (x, y) \in X \times Y \mid p(x)q_x(y) > 0 \}$. We can equip $Z$ with the $\sigma$-algebra $\Sigma := \{ A \cap Z \mid A \in \Sigma_P \otimes \Sigma_Q \}$ (assuming $Z$ is a $\mu_P \times \mu_Q$-measurable set), and a reference measure $\mu(A) := (\mu_P \times \mu_Q)(A)$.

Let $f : Z \rightarrow Z$ denote an involution ($f^{-1} = f$) such that the pushforward of $\mu$ under $f$, denoted $\mu \circ f^{-1}$, is absolutely continuous with respect to $\mu$, with Radon-Nikodym derivative $d(\mu \circ f^{-1})/d\mu : Z \rightarrow [0, \infty)$. Involutive MCMC runs $f$ on $(x, y)$ to obtain $(x', y')$, then computes an acceptance probability $\alpha$. With probability $\alpha$, the new state $x'$ is returned; otherwise, the previous state $x$ is repeated.

Algorithm 1 Involutive MCMC

```
procedure involutive-mcmc(p, q, f, x)
    y \sim q_x(\cdot) \triangleright \text{Sample auxiliary state}
    (x', y') \leftarrow f(x, y) \triangleright \text{Apply involution}
    \alpha \leftarrow \frac{p(x')q_y(y')}{p(x)q_y(y)} \cdot \left( \frac{d(\mu \circ f^{-1})}{d\mu}(x, y) \right)
    r \sim \text{Uniform}(0, 1)
    \text{if } r \leq \alpha \text{ then return } x' \text{ else return } x
end procedure
```

Theorem 3.1 (Involutive MCMC is stationary). Involutive MCMC defines a probability kernel $k$ on $X$ that is stationary with respect to the model probability distribution. That is, $\int_B k_x(B)p(x)d\mu_X(dx) = \int_B p(x)d\mu_X(dx)$ for all $B \in \Sigma_X$.

Proof. The proof is presented in stages in the appendix (see Section A.2, Section A.3, and Section A.4). □

3.2 Probability Distributions on Dictionaries

While maximally general, the measure-theoretic formulation of involutive MCMC in Algorithm 1 is not amenable to an automated implementation, because it does not indicate how to compute the Radon-Nikodym derivative that is required for the acceptance probability, and it is unclear how to specify the probability measures involved.

While restricting the state space to vectors of real numbers would address these issues, we seek a representation that remains flexible enough to represent complex hybrid state spaces with numeric, symbolic, and structure uncertainty. Therefore, we use state spaces consisting of finite dictionaries that map (possibly random) keys to (possibly random) values. Dictionaries include vectors as a special case (a vector $x \in \mathbb{R}^n$ can be represented as a dictionary mapping the keys $1, \ldots, n$ to the values $x_1, \ldots, x_n$), but are more flexible: different keys can hold values of different types (e.g. integers, strings), and we can also consider distributions in which the set of keys is itself random, which is useful for model selection problems and structure uncertainty more generally.

This section describes probability distributions on dictionaries, and gives a constructive definition of the involutive MCMC acceptance probability in this setting in terms of a Jacobian. Section 3 will then show how probability distributions on dictionaries can be specified with probabilistic programs, and how probabilistic
programming techniques can automatically compute probability densities on spaces of dictionaries.

The space of finite dictionaries. We fix a countably infinite set $\mathcal{K}$ of possible keys, such that each key $k$ is either called discrete ($k \in \mathcal{I}$) or continuous ($k \in \mathcal{J}$), where $\mathcal{K} = \mathcal{I} \cup \mathcal{J}$. Let $V_k$ denote the set of possible values for key $k$, where $V_k$ is a countable set for each discrete key, and where $V_k = \mathbb{R}^{d_k}$ for each continuous key for some $d_k$. Given a set of keys $K$, let $V_K = \times_{k \in K} V_k$ denote the set of assignments of values to each key. Then the set of all finite dictionaries is $\mathcal{D} := \bigcup_{K \subset \mathcal{K}, |K| < \infty} \{(K, x) \mid x \in V_K\}$. That is, a dictionary specifies a finite set of keys $K \subset \mathcal{K}$ at which it has values, and an assignment of values $x_k$ for each key.

Relationship to representation of Green (1995). Green (1995) uses a state space that is the countable union of ‘models’, where each model is typically a vector of real-valued parameters. Dictionaries have substantially more structure: Instead of monolithic ‘models’, dictionaries use a more elaborate discrete state that includes the set of keys and the assignment to the discrete keys. Also, because continuous keys play the role of real-valued parameters, it is possible to express that a given real-valued parameter is shared between models. The additional structure of dictionaries enables the automation techniques in Section 4.

A measure space of finite dictionaries. We associate a measure $\mu_k$ on $V_k$ for each key $k$—the counting measure for each discrete key and the Lebesgue-measure on $\mathbb{R}^{d_k}$ for each continuous key. For each finite set of keys $K$, we make $V_K$ a measure space using the standard product $\sigma$-algebra $\Sigma_K = \otimes_{k \in K} \Sigma_k$ and the product measure $\mu_K = \times_{k \in K} \mu_k$. We equip $\mathcal{D}$ with the $\sigma$-algebra $\Sigma_{\mathcal{D}} := \bigcup_{K \subset \mathcal{K}, |K| < \infty} \{(K, x) \mid x \in B_K\} \cap B_K \in \Sigma_K$ for each finite $K \subset \mathcal{K}$ to obtain a measurable space of dictionaries. A reference measure $\mu_{\mathcal{D}}$ on this space can be constructed using the product measures $\mu_K$: we set $\mu(B) := \sum_{K \in \mathcal{K}, |K| < \infty} \mu_K(\{x \mid (K, x) \in B\})$.

Notation for dictionaries. Given a dictionary $m = (K, x)$, we write $K_m$ for $K$ and $m[k]$ for the value $x_k$ associated with a key $k \in K$. We also denote specific dictionaries using notation $\{k_1 \mapsto v_1, k_2 \mapsto v_2, \ldots\}$. For example, the dictionary $(K, x)$ with $K = \{1, "foo"\}$ and $x_1 = 0.123$ and $x_{\text{foo}^\ast} = 5$ is denoted $\{1 \mapsto 0.123, "foo" \mapsto 5\}$.

Probability distributions on finite dictionaries. When $V_k$ is discrete for all keys $k$, a probability distribution on dictionaries is defined by a probability mass function $p : \mathcal{D} \to [0, 1]$ that assigns a probability $p(m)$ to each dictionary $m \in \mathcal{D}$ such that $\sum_{m \in \mathcal{D}} p(m) = 1$. More generally a probability distribution on dictionaries is defined by a probability density $p : \mathcal{D} \to (0, \infty)$ such that $\int p(m) \mu_{\mathcal{D}}(dm) = 1$. The probability mass is distributed among the finite sets of keys $K \subset \mathcal{K}$:

$$1 = \sum_{K \subset \mathcal{K}, |K| < \infty} \left( \sum_{x_1} \left( \int_{\mathbb{R}^{d_K}} p((K, (x_1, x_2))) \, dx_2 \right) \right)$$

where $d_K := \sum_{k \in K \cup J} d_k$ is the total continuous dimension for keys $K$, and where $x_1$ is an assignment to the discrete choices in $K$ and $x_2$ is an assignment to the continuous choices.

We now give an example to build intuition. Consider a generative model of univariate data points $y_1, \ldots, y_n$ from a Gaussian mixture with an unknown number of components $k$, each with unknown mean $m_i$ and variance $s_i$. If we place a Gaussian prior on $m_i$, an inverse Gamma prior on $s_i$, and a Poisson prior on $k$, the resulting density on dictionaries $d$ is:

$$p(d) = \frac{p_{\text{poisson}}(3)(d[k])}{\prod_{i=1}^n \text{normal}(0,1)(d[m_i]) \cdot \text{inversedgamma}(1,10)(d[s_i]) \cdot \prod_{i=1}^n \frac{1}{\pi s_i} \sum_{j=1}^k p_{\text{normal}}(d[n_i], d[s_i])(d[y_i])}$$

when $K_d = \{k, y_1, \ldots, y_n\} \cup \{m_i \mid 1 \leq i \leq d[k]\} \cup \{s_i \mid 1 \leq i \leq d[k]\}$, and 0 otherwise. In this case, we have $V_k = \mathbb{N}$ with the counting measure for $\mu_k$, and for all other keys $k \in \mathcal{K}$, $V_k = \mathbb{R}$ with the Lebesgue measure for $\mu_k$. For each $j \in \{0,1,\ldots\}$, the probability mass assigned to key set $\{k, y_1, \ldots, y_n\} \cup \{m_i \mid 1 \leq i < j\} \cup \{s_i \mid 1 \leq i \leq j\}$ is $p_{\text{poisson}}(s)(j)$ (via Equation (1)).

Conditional distributions via disintegration. Consider a probability density $p$ on the space $\mathcal{D}$ of dictionaries. We say a key $k \in \mathcal{K}$ almost always appears if $\int 1[k \in K_m] p(m) \mu_{\mathcal{D}}(dm) = 1$. Suppose $B$ is a set of keys that almost always appear for $p$, and that both $(B, b)$ is a dictionary with keys $B$. Furthermore, let $(K_m, m) \oplus (K_n, n) := (K_m \cup K_n, (m, n))$ be the merge of two dictionaries $m$ and $n$ defined on disjoint key sets $K_m$ and $K_n$. Then we can define the conditional density $p(d \mid b) := \int_{[K_d \cap B = \emptyset]} \frac{p(d \oplus b)}{p(d \oplus b)} \mu_{\mathcal{D}}(dm)$ when the denominator is finite. If each key $k \in B$ is discrete (e.g. $\mu_k$ is the counting measure), then this definition corresponds to the ordinary notion of conditioning on an event (namely, the event that a sample from $p$ agrees with the dictionary $b$ on all keys in $B$). When this is not the case, it corresponds to a more general measure-theoretic notion called disintegration (Chang and Pollard, 1997).

Consider the infinite univariate mixture model, and the conditional density given observed data $(B, b) := \ldots$
\{y_1 \mapsto y_1, \ldots, y_n \mapsto y_n\}. \) The conditional density \( p(d|b) \) is nonzero only if \( K_d = \{k\} \cup \{m_i \mid 1 \leq i \leq k\} \cup \{s_i \mid 1 \leq i \leq k\} \) for some \( k \) (\( d \) does not contain \( y \)-values), and the denominator in the definition of \( p(d|b) \) simplifies to the familiar sum of marginal likelihoods over all \( k \), where each marginal likelihood is a Riemann integral over \( \mathbb{R}^{2k} \).

### 3.3 Involutional MCMC with Dictionaries

Suppose that the model distribution and auxiliary distributions are probability distributions on dictionaries, with densities \( p \) and \( q_e \). Then, \( X \) and \( Y \) are both sets of dictionaries, and the joint space \( Z \) is a set of pairs \((x, y)\) of dictionaries with keys \( K_P \) and \( K_Q \) respectively, so that \( Z = X \times Y \subseteq D_P \times D_Q \) where \( D_P \) is the set of dictionaries on keys taken from \( K_P \) and similarly for \( D_Q \). To simplify the notation, and without loss of generality, we will assume that \( K_P \) and \( K_Q \) are disjoint\(^4\) and we define \( Z := \{x \oplus y : p(x)q_e(y) > 0\} \subseteq D \), where \( D \) is the set of dictionaries on keys from \( K_P \cup K_Q \) (recall \( x \oplus y \) denotes the dictionary resulting from merging dictionaries \( x \) and \( y \) with disjoint keys).

Suppose there is a countable partition of \( Z \) into \( \{Z_e : e \in E\} \) such that if \((K_1, x_1)\) and \((K_2, x_2)\) are two dictionaries in the same component \( Z_e \), then \( K_1 = K_2 \) and they agree on all discrete values: \( x_{1k} = x_{2k} \) for all \( k \in K_1 \cap I \). Then each set \( Z_e \) is isomorphic to a Euclidean space of assignments to the continuous keys in the two dictionaries. Suppose there is an involution \( g : E \rightarrow E \) between elements of the partition, and a family of continuously differentiable bijections \( h_e : Z_e \rightarrow Z_{g(e)} \) indexed by \( e \in E \), with \( h_e = h_{g(e)}^{-1} \).

Let \( e(z) \in E \) denote which element of the partition a dictionary \( z \in Z \) belongs to. Then \( f : Z \rightarrow Z \) given by \( f(z) := h_{e(z)}(z) \) is an involution:

\[
f(f(z)) = h_{e(f(z))}(h_{e(z)}(z)) = h_{g(e(z))}(h_{e(z)}(z)) = z.
\]

Let \( \|Jh_e\| (z) \) denote the absolute value of the determinant of the Jacobian of \( h_e \), evaluated at \( z \). Then, the acceptance probability in Algorithm 1 simplifies to:

\[
\frac{p(x')q_e(y')}{p(x)q_e(y)} \cdot \|Jh_e\| (z).
\]

One example of a valid partition of \( Z \) is given by equivalence classes of the following equivalence relation:

\[ z_1 \sim z_2 \iff (K_{z_1} = K_{z_2}) \land (z_1[k] = z_2[k] \forall k \in K_{z_1} \cap I) \]

(dictionaries are equivalent if they contain the same keys and they agree on the value of all discrete keys). See Section A.1 of the appendix for details.

### 4 Automating Involutional MCMC with Traces

Involutional MCMC is a general framework that can be used to develop diverse MCMC algorithms for models over arbitrary state spaces. We wish to automate the implementation details for involutional MCMC algorithms, given only a specification of the model \( p \), the auxiliary distribution \( q \), and the involution \( f \). To do so, we require a representation for the distributions \( p \) and \( q \) that is flexible enough to represent the full variety of models and auxiliary distributions of interest to practitioners. The representation must support density evaluation and sampling. It is also desirable that the representation be structured: the more information available to us (e.g., about the decomposition of a distribution’s state space into individual univariate and multivariate random variables, or about conditional independence relationships in a model), the easier it will be for the implementation to exploit this structure automatically by using more efficient data structures and low-level manipulations.

#### 4.1 Trace-Based Probabilistic Programming

Probabilistic programs are flexible and structured representations for probability distributions. Unlike densities (but like Bayesian networks), probabilistic programs can be efficiently sampled and contain explicitly represented information about some conditional independence relationships in a model. But unlike Bayesian networks, they do not assume a fixed number of random variables, state space dimension, or dependency structure.

At the most basic level, a probabilistic program is a program that makes random choices. Any such program induces a probability distribution over its possible execution traces, records of each random choice it makes. If each random choice is associated with a unique address from the set of dictionary keys \( K \), then these traces can be viewed as finite dictionaries, mapping the address of each random choice to its value. The distribution induced by a probabilistic program over its execution traces can thus be understood as a measure on the space \( (D, \Sigma_D, \mu_D) \) introduced in the previous section. Furthermore, densities of trace distributions with respect to \( \mu_D \) are typically easy to compute.

In this section, we introduce a probabilistic programming language from the Gen probabilistic programming system (Cusumano-Towner et al., 2019), and present a technique for automating the implementation of involutional MCMC algorithms when the model \( p \) and auxiliary distribution \( q_e \) are both represented...
as probabilistic programs in this language. But the technique is not limited to the Gen system—we also provide the implementation of a minimal probabilistic programming language in PyTorch that supports the automation technique.

4.1.1 A Probabilistic Programming Language

Our probabilistic programming language augments the syntax of Julia [Bezanson et al., 2017] with a single new construct, the `\{address\} \sim \text{distribution}` expression, for making a named random choice. An
execution trace of a Gen probabilistic program is a dictionary that can be sampled by running the program according to Julia’s usual semantics, and upon encountering an expression of the form `{address} ~ distribution`, (i) evaluating the address expression (`address`) to obtain an address \( k \in K \); (ii) evaluating the distribution expression (`distribution`) to obtain a probability distribution over the measurable space \( V_k \); (iii) sampling a value \( x_k \) from this distribution and adding the mapping \( \{ k \mapsto x_k \} \) to the execution trace; and (iv) returning the sampled value \( x_k \) to the program, to continue execution. When execution terminates, the execution trace has accumulated a mapping for each random choice encountered during the program’s execution.

For example, consider the probabilistic program below, which defines a Gaussian mixture model with an unknown number of components:

```julia
@gen function p(n::Int)
    k ~ poisson_plus_one(1)
    means = [{(:mu, j) ~ normal(0, 10) for j in 1:k}]
    vars = [{(:var, j) ~ inv_gamma(1, 10) for j in 1:k}]
    weights ~ dirichlet([2.0 for j in 1:k])
    for i in 1:n
        {(:x, i)} ~ mixture_of_normals(weights, means, vars)
    end
end
```

The program \( p \) accepts as input an integer \( n \), a number of data points. Each \( n \) defines a distinct distribution over dictionaries. The first line of the program samples a number of mixture components from a Poisson prior using the address `:k`. (This line could also be written \( k \in \{ :k \} \sim \text{poisson\_plus\_one}(1) \): the address is the symbol `:k`, and the result of the choice is assigned to a Julia variable called `k`. Because this is a common pattern, Gen provides the syntactic sugar \( x \sim d \) as shorthand for \( x \sim \{ :x \} \sim d \).) The program then samples \( k \) means and \( k \) variances from Gaussian and inverse Gamma priors, respectively. Each of these \( 2k \) random choices has its own address, determined by the address expression preceding it. For example, the mean for the fourth mixture component (if \( k \geq 4 \) has address `:mu`, 4). The mixture weights are then sampled at the address `:weights` from a Dirichlet distribution, and \( n \) data points are sampled at addresses `(:x, 1), \ldots, (:x, n)`.

The density of an arbitrary dictionary \((K, x)\) under any probabilistic program’s distribution on traces can be computed using \( \text{SCORE} \). The idea is to run the probabilistic program, and whenever a random choice `{address} ~ distribution` is encountered, to look up the value \( x_k \) in the dictionary, compute its density under the primitive distribution \( d \), multiply this density into a running total, and return control to the probabilistic program as if the sampling instruction had executed and returned \( x_k \). At the end, the running total can be returned as the trace’s density. If at any point an address \( k \notin K \) is encountered, or if not all addresses in \( K \) have been visited at the end of execution, the algorithm returns 0 as the density.

### 4.1.2 Automatically Computing Density Ratios in Involutive MCMC

We can use two probabilistic programs \( P \) and \( Q \) to specify the model density \( p \) and auxiliary densities \( q_x \) that appear in involutive MCMC (Algorithm 1). In this case, the program \( Q \) accepts a trace \( x \) of \( P \) as

\[ p(n)(|K, x|) = \frac{p(\text{poisson}(1)(x_k - 1)) \prod_{i=1}^{n} p(\text{normal}(0, 10)(x_{(\mu, i)})) \prod_{i=1}^{n} p(\text{inversegamma}(1, 10)(x_{(\var, i)})) \prod_{i=1}^{n} \sum_{j=1}^{k} x_{(\text{weights}, i)} \cdot p(\text{normal}(x_{(\mu, j)}, x_{(\var, j)})(x_{(x, i)}))}{\text{dirichlet}(2.0, \ldots, 2.0)(x_{(\text{weights})})} \]

when \( K \) contains exactly the addresses \(:k, \text{weights}, (:x, i)\) for \( i = 1, \ldots, n \), and \((:\mu, j)\) and \((:\var, j)\) for \( j = 1, \ldots, x_k \); otherwise, the density is 0.
input, we denote a probabilistic program \( Q \) applied to input \( x \) by \( Q_x \).

Typically, we cannot use a probabilistic program \( P \) to represent the target distribution directly: probabilistic programs implement simulators for a distribution, but target densities are typically not tractable to simulate (hence the need for MCMC). Instead, we may wish to sample from a target \( p \) that arises from conditioning a probabilistic program \( P \)'s distribution over traces on observations of the values at some addresses. Let \( \tilde{p} \) denote \( P \)'s distribution over traces, and let \( b = (B, b) \) be a dictionary of observations, as described in Section 3.2. Then, as shown in that section, the target distribution \( p(x) = \tilde{p}(x | b) = \frac{\tilde{p}(x \oplus b)}{\tilde{L}(b)} \), where

\[
\tilde{L}(b) = \int_{\{m|m \cap B = b\}} \tilde{p}(m \oplus b) \mu_P(dm) \quad \text{is the marginal likelihood of} \ b \quad \text{and does not depend on} \ x.
\]

If we use \( \tilde{p}(x \oplus b) = \tilde{L}(b)p(x) \). We use the \( \tilde{p}(x \oplus b) \) in place of \( p(x) \) to compute the ratio of densities in Algorithm 1, we will wind up with the same output, because \( \tilde{L}(b) \) will cancel in the numerator and denominator:

\[
\frac{p(x')q_x(y')}{p(x)q_x(y)} = \frac{\tilde{p}(x' \oplus b)q_x(y')}{\tilde{p}(x \oplus b)q_x(y)} = \frac{\tilde{p}(x'|b)q_x(y')}{\tilde{p}(x|b)q_x(y)} \quad (3)
\]

Thus, this ratio can be computed term-by-term using \textsc{score} on the probabilistic programs \( P \) and \( Q \) (Algorithm 2): to compute \( q_x(y') \), we run the algorithm directly on the program \( Q_x \), and to compute \( p(x) \) and \( p(x') \), we actually merge the dictionary \( x \) with the observations \( b \) and compute \( \tilde{L}(b)p(x) = \tilde{p}(x \oplus b) \) instead, by running the algorithm on \( P \) with trace \( x \oplus b \). The density \( q_x(y) \) can be computed while \( y \) is being sampled, using \textsc{trace-and-score}.

Section 5 describes a more efficient approach that exploits sparsity in the involution and cancellations in the acceptance ratio for improved efficiency, but requires a more sophisticated probabilistic programming runtime system.

Figure 1 and Figure 2 show examples of probabilistic programs \( P \) and \( Q \) respectively, for a split-merge reversible jump move.

### 4.2 Differentiable Programming with Traces

Section 4.1 showed that if the densities \( p \) and \( q \) are specified using probabilistic programs \( P \) and \( Q \), then the density ratio in the acceptance probability for involutive MCMC on dictionaries (Equation 2) can be automated using probabilistic programming techniques. This section shows that if the involution \( f \) is specified using a differentiable program \( F \) that transforms the execution traces of probabilistic programs, then the Jacobian factor in Equation 2 can also be automated, using automatic differentiation. The procedure AUTO-INVLUTIVE-MCMC in Algorithm 2 combines these two ideas and automates involutive MCMC given the programs \( P \), \( Q \) and \( F \).

#### 4.2.1 A Differentiable Programming Language for Manipulating Traces

Recall that for involutive MCMC on a state space of dictionaries, we define \( Z := \{x \oplus y : p(x)q_x(y) > 0\} \subseteq D \), where \( x \oplus y \) is the dictionary resulting from merging dictionaries \( x \) and \( y \) with disjoint keys. The involution is a function \( f : Z \to Z \).

We now introduce a simple differentiable programming language for specifying involutions \( f \). The language needs to have syntax for reading the value from an address in \( x \oplus y \in Z \) and writing to an address in \( x' \oplus y' \in Z \). To read a value \( (x \oplus y)[a] \) at address \( a \), we use the \texttt{@read} keyword:

\[
\text{value} = \texttt{@read}(\langle\text{address}\rangle, \langle\text{type}\rangle)
\]

The first argument is the address \( a \) and the second argument is either \texttt{discrete} or \texttt{continuous}, and informs the interpreter whether the random choice at that address is drawn from a discrete or continuous distribution (this information will be used to support automatic differentiation). Recall that \( x \) is the trace of the model probabilistic program, and \( y \) is the trace of the auxiliary probabilistic program. Each address \( a \) therefore needs to specify which of these traces to read from, and the address within that trace. The traces are given names in the function signature:

\[
\texttt{@transform} f (\texttt{model}_i, \texttt{aux}_i) \text{ to } (\texttt{model}_o, \texttt{aux}_o)
\]

\[
\texttt{begin}
\texttt{. . .}
\texttt{end}
\]

Here, the traces \( x, y, x' \) and \( y' \) are given names \texttt{model}_i, \texttt{aux}_i, \texttt{model}_o, and \texttt{aux}_o, respectively. The syntax for address \( a \) within trace \texttt{trace} is \texttt{trace}[a]. For example, to read the value of a continuous address \( :a \) from the input model trace \( x \):

\[
\text{val} = \texttt{@read}(\texttt{model}_i[\langle a \rangle], \texttt{:continuous})
\]

The syntax for writing to an address in \( x' \oplus y' \in Z \) is

\[
\texttt{@write}(\texttt{model}_o[\langle a \rangle], \texttt{val}, \texttt{:continuous})
\]

Note that the input traces \( x, y \) are distinct from the output traces \( x', y' \); input traces can only be read from, and output traces can only be written to. For example, it is not possible to write an output trace and then read the written value from it later.
Often, we want to simply copy the value from some address in the input traces to some address in the output trace. While this is possible via a @read followed by a @write, the language provides a special syntax:

```
@copy(<source-address>, <destination-address>)
```

For example, to copy the value from address `x` in `x` to address `v` in `x'`, we use:

```
@copy(model_in[:u], model_out[:v])
```

Of course, it is also possible to copy from `x` to `y'` from `y` to `x'` and from `y` to `y'`. As we will see in Section 5, it is preferable to use @copy when possible instead of reading and then writing, as this can make the acceptance probability calculation more efficient.

### Constructing an Involution

Consider the following generative model, which posits that a vector of univariate data is either generated from a single normal distribution or a mixture of two normal distributions. The model is expressed as a probabilistic program:

```plaintext
@gen function p()
    k ~ uniform_discrete(1, 2)
    means = [1:] for j in 1:k
    weights = ones(k)
    vars = ones(k)
    for i in 1:100
        {1:2} ~ mixture_of_normals(weights, means, vars)
    end
end
```

This is a simplified version of the infinite Gaussian mixture model in Figure 1. Each key of the form `(x, i)` will be observed (in the dictionary `x`) contains the other keys `k` and `(mu, j)` and `(mu, 1)` and `(mu, 2)`.

We will now walk through how to express a simple ‘split-merge’ move [Richardson and Green, 1997] using our differentiable programming language. Suppose we want to construct an involutive MCMC kernel that changes `k` from 2 to 1 or vice versa. The discrete part of the involution is straightforward:

```plaintext
@gen function q(model_trace)
    if model_trace"k" == 1
        # we are doing a split, sample extra DoF
        u ~ beta(2, 2)
    end
end
```

Our involution is on the space of combined dictionaries `x ⊕ y` where `y` are traces of `q`. Note that for each `(x ⊕ y)` where `x[k] = 1`, `y` has a key `u`, and for each `(x ⊕ y)` where `x[k] = 2`, `y` is empty. We extend the involution using a pair of bijections between `(mu1, mu2)` and `(mu, u)` that show how two cluster means should be transformed into one cluster mean (merge), and vice versa (split):

\[
\begin{align*}
\mu_1, \mu_2 &\mapsto ((\mu_1 + \mu_2)/2, \mu_2 - (1 + \mu_2)/2) \quad [\text{Merge}] \\
\mu_1, u &\mapsto (\mu_1 - u, \mu_1 + u) \quad [\text{Split}]
\end{align*}
\]

The value of `x[k]` determines which of these functions is executed. The full involution program \(\mathcal{F}\) is then:

```plaintext
@transform f (model_in, aux_in) to (model_out, aux_out)
begin
    k = @read(model_in["k"], discrete)
    if k == 1
        @write(model_out["k"], 2, discrete)
        # split bijection
        mu = @read(model_in["mu", 1], continuous)
        u = @read(aux_in["u"], continuous)
        mu1 = mu - u; mu2 = mu + u
        @write(model_out["mu", 1], mu1, continuous)
        @write(model_out["mu", 2], mu2, continuous)
    else
        @write(model_out["k"], 1, discrete)
        # merge bijection
        mu1 = @read(model_in["mu", 1], continuous)
        mu2 = @read(model_in["mu", 2], continuous)
        mu = (mu1 + mu2) / 2
        u = mu2 - mu
        @write(model_out["mu", 1], mu, continuous)
        @write(aux_out["u"], u, continuous)
    end
end
```

The two continuous bijections (implemented in blocks of code in the two branches) are inverses of one another. This is a common pattern in involution programs—an involution on the discrete parts of the traces (in this case, just `x[k]`) determines via control flow which continuous code blocks get executed, such that the end-to-end program defines an involution.

Note that the observations `b` (in this case, the x-coordinates) are included in traces of \(p\), which take the form `x ⊕ b` where `x` is the latent part and `b` is the observed part. The involution program \(\mathcal{F}\) is allowed to read from the the observations in the model trace using the same syntax as used to read from the latent part of the trace `x`. (The example given here does not
utilize this feature).

4.2.2 Computing the Jacobian with Automatic Differentiation

Recall that the involution \( f \) must decompose into (i) an involution \( g \) on elements \( e \in E \) of a partition of the state space, and (ii) a pair of continuous differentiable bijections \( h_e \) and \( h_{g(e)} = h_e^{-1} \) between each pair of corresponding elements of the partition. Each function \( h_e \) is a function from the values at continuous addresses in the input trace \( (z[k] \mid k \in K_z \cap J) \) to the values at continuous addresses in the output trace \( (z'[k] \mid k \in K_{z'} \cap J) \). In the example above, the partition \( E \) is given by the equivalence classes of the relation \( (x_1, y_1) \sim (x_2, y_2) \iff x_1[k] = x_2[k] \) (there are two equivalence classes), \( g \) maps the \( k \) = 1 class to the \( k \) = 2 class and vice versa, and the continuous bijections \( h_e \) and \( h_{g(e)} \) are the functions in Equation (4).

We compute the Jacobian using automatic differentiation. (The Gen implementation uses forward-mode AD whereas our PyTorch implementation uses reverse-mode AD.) The procedure \textsc{run-involution} in Algorithm 2 shows the implementation of the interpreter for the language that uses reverse-mode AD. The interpreter executes \( F \) using regular Julia or Python semantics, but intercepts calls to \texttt{@write}, \texttt{@read}, and \texttt{@copy} statements, and in addition to performing the desired operation, records the set of continuous addresses that are read, written, and copied. After \( F \) is finished executing, AD uses the recorded addresses to compute the Jacobian \( Jh_e(z) \); in the case of reverse-mode AD, this is accomplished by iterating over output continuous addresses and backpropagating from each one to all of the input continuous addresses, computing the Jacobian column-by-column. Keys with an \( n \)-dimensional Lebesgue measure as their reference measure, corresponding to vector-valued random choices, are unpacked into \( n \) separate columns in the Jacobian; this detail is elided in Algorithm 2. The discrete and continuous labels are also omitted from the syntax in \textsc{run-involution} to simplify notation (\( a \in \mathbb{I} \) indicates a discrete choice and otherwise a choice is continuous).

5 EXPLOITING SPARSITY FOR IMPROVED PERFORMANCE

Suppose \( N \) and \( N' \) are the total number of random choices in the input traces \( x, y \) and output traces \( x', y' \) respectively (note that the observations \( b \) are excluded—\( x \) and \( x' \) are the latent part of the model’s traces only). Let \( M \) be the number of continuous random choices among these (which must be the same in the input traces and output traces). Then, the number of operations used in Algorithm 2 grows as \( O(N + N') + O(M^3) \). The linear term is due to sampling \( y' \) and computing the four log-densities required for the acceptance probability. The cubic term is due to computing the Jacobian determinant, which is also required for the acceptance probability (Equation 3).

It is possible to reduce the number of operations performed in an automated involutive MCMC kernel by exploiting special structure in the involution \( f \). In some cases, this structure can lead to \( O(1) \) operations per kernel application (i.e. constant in \( N, N', \) and \( M \)). This section describes techniques for exploiting involution structure within an automated involutive MCMC implementation. These techniques are used in the Gen implementation, and one of the techniques is used in our minimal PyTorch implementation.

5.1 Sparsity-Aware Automatic Jacobian Computation

The naïve implementation of Algorithm 2 computes the Jacobian by first computing the \( M \)-by-\( M \) Jacobian matrix \( Jh_e(z) \) via automatic differentiation, and then computing the absolute value of its determinant. However, we observe that in many applications of involutive MCMC, the values at continuous choices in the input traces are directly copied into the output traces (either at the same key or a different key). These copy operations result in columns in the Jacobian matrix that have a single 1 entry with remaining entries equal to 0. For example, for the function \( (u, v, x, y) \mapsto (u, 2u - v, y, x) = (u', v', x', y') \), the Jacobian is (with columns corresponding to \( u', v', x', \) and \( y' \) and rows corresponding to \( u, v, x, \) and \( y \)):

\[
\begin{bmatrix}
1 & 2 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{bmatrix}
\]

Using the cofactor expansion of the determinant, we note that for any ‘copy’ column in an \( M \)-by-\( M \) Jacobian matrix (a column with a single 1 and all other entries 0), the absolute value of the determinant is equivalent to that of the \((M-1)\)-by-\((M-1)\) sub-matrix with the corresponding column and row omitted (even if that would remove other nonzero entries from the matrix). By applying this rule recursively, we can instead compute the determinant of a much smaller matrix; for the example above with \( M = 4 \), the absolute value of the determinant simplifies to the absolute value of a single entry (\((-1)^{3}\)). Indeed, if some input key is copied to some output key, then we can entirely avoid computing its row (and corresponding column) of the Jacobian. Therefore, the number of operations (which is dominated by the determinant) reduces from \( M^3 \) to \((M - |C|)^3\) where \(|C|\) is the number of input
writing the value for each element of \((x', y')\) for involutive MCMC move only updates a portion of the model trace and not the observed part \(b\). Suppose that \(N_1 := |K_x|, N_2 := |K_y|, N'_1 := |K_{x'}|\) and \(N'_2 := |K_{y'}|\), and \(N := N_1 + N_2\) and \(N' := N'_1 + N'_2\). Suppose that \(N_1 + N'_1 \gg N_2 + N'_2\), which often occurs when the the number of latent variables is large, but the involutive MCMC move only updates a portion of the latent variables. Algorithm \(\mathcal{F}\) runs \(\mathcal{F}\), which explicitly writes the value for each element of \((x', y')\), requiring \(N' = N'_1 + N'_2 \approx N'_1\) ‘write’ or ‘copy’ operations. The algorithm also uses approximately \(N_1 + N'_1\) operations to evaluate the log-densities, because it accumulates the log-density of each random choice in \(x\), and \(x'\).

We now show how to modify the program \(\mathcal{F}\) and its interpreter, so that both computing \(z' = (x', y')\) from \(z = (x, y)\), and computing the log density ratio \(\log(\tilde{p}(x' \oplus b)/\tilde{p}(x \oplus b))\), can take \(O(1)\) operations (that is, constant in \(N_1 + N'_1\)) when the involuntion \(f\) has sparse structure and the model density \(p\) has conditional independencies.

Note that \(x\) and \(x'\) may both have values for certain keys, and \(x\) may contains keys not present in \(x'\), and vice versa. Often, an involuntion does not modify the values of many keys in the trace—this is the case in the split-merge reversible jump move described earlier. Suppose that \(A \subseteq K_x \cap K_{x'}\) is the set of keys \(k\) in both \(x\) and \(x'\) for which \(x'[k] = x[k]\). Let \(\Delta := K_x \setminus A\) be the set of keys in \(x'\) that are either (i) not in \(x\), or (ii) in \(x\) but have their value changed. Then, the previous trace \(x\) and a dictionary \(\delta\) with \(K_\delta = \Delta\) and \(\delta[k] = x'[k]\) and the density function \(p\) suffice to uniquely define the trace \(x'\), provided the density satisfies the following condition, which is satisfied by densities defined by probabilistic programs\(^4\): \(p(x) > 0\) and \(p(x') > 0\) and \(x \neq x'\) implies there exists \(k \in K_x \cap K_{x'}\) with \(x[k] \neq x'[k]\). Let \(|x|_A\) denote the restriction of a dictionary \(x\) to only keys in \(A\). Then, naive-trace-update (Algorithm \(\mathcal{F}\)) computes the new trace \(x'\) and log-densities ratio \(\log(p(x')/p(x))\) of a probabilistic program from a previous trace \(x\) and a dictionary \(\delta\) (and observations \(b\)), provided there exists \(x' = \delta \oplus x|_A\) for some \(A\) where \(p(x') > 0\).

Naive-trace-update is a naive implementation of a general trace-update operation that is part of Gen’s API (Cusumano-Towner et al. 2019). While the naive implementation requires \(O(N_1 + N'_1)\) operations, it is possible for more sophisticated implementations of trace-update to run in approximately \(O(\|K_\delta\|)\) operations for certain probabilistic programs \(\mathcal{P}\) by exploiting conditional independence structure program that leads to cancellations in the density ratio \(\tilde{p}(x' \oplus b)/\tilde{p}(x \oplus b)\). The details of these more efficient implementations are outside the scope of this paper, but are implemented as part of the Gen system.

Given an implementation of trace-update (that has the same input and output signature of naive-trace-update) we can optimize Algorithm \(\mathcal{F}\) by modifying the requirement for the involution program \(\mathcal{F}\): Instead of explicitly specifying a value for all keys in

\(^{4}\)Intuitively, two traces of a probabilistic program cannot have different sets of addresses unless they share an address and disagree on its value.
\textbf{Algorithm 3} Naive Trace Update
\begin{algorithmic}
\Require probabilistic program $\mathcal{P}$; previous trace $x$; observations $b$; dictionary $\delta$ such that there exists $x' = (\delta \oplus x | A)$ for some $A$ where $p(x') > 0$.
\Procedure{naive-trace-update}{\mathcal{P}, x, b, \delta}
\State $x' \leftarrow \{\}$
\State $s' \leftarrow 0$
\State Execute $\mathcal{P}$, but with "$k \sim \text{distribution}$" $\equiv \{$
\State \hspace{1cm} 1. if $k \in K_b$ then $v \leftarrow \delta[k]$ else $v \leftarrow (x \oplus b)[k]$
\State \hspace{1cm} 2. if $k \notin K_b$ then set $x'[k] \leftarrow v$
\State \hspace{1cm} 3. set $s' \leftarrow s' + \logpdf(distribution, v)$
\State \hspace{1cm} 4. evaluate to $v$
\State $s \leftarrow \text{score}(\mathcal{P}, x \oplus b)$
\State \Return $(x', s' - s)$
\EndProcedure
\end{algorithmic}

$x'$, it need only explicitly specify values in $\delta$. (We call the other values in $x'$ implicit copies—they could be explicitly copied within $\mathcal{F}$, but this would result in unecessary code and possibly unnecessary computation.) Therefore, the involution program can run in $O(|K_3| + N_2 + N_1')$ operations. We remove the separate calls to score for the log-densities $\log(\tilde{p}(x \oplus b))$ and $\log(\tilde{p}(x' \oplus b))$ and replace them with a single call to \texttt{trace-update} on $\mathcal{P}$ that takes in $x$ and $\delta$ and returns $x'$ and $\log(\tilde{p}(x' \oplus b)/\tilde{p}(x \oplus b))$. When $|K_3|$ and $N_2$ and $N_1'$ are all constant in the size $N_1$ of the latent part of model trace $x$, the resulting algorithm uses a number of operations that does not grow with $N_1 + N_1'$.

6 DYNAMICALLY DETECTING BUGS IN INVOLUTIONS

The automated technique described in the previous sections allows users to implement involutive MCMC algorithms by writing probabilistic programs for $p$ and $q$ and a differentiable program for the involution $f$, avoiding the need to derive and implement the accept/reject formula by hand. This eliminates certain classes of errors that could otherwise be difficult to root out in hand-coded implementations of MCMC algorithms. However, it is still of course possible to implement $p$, $q$, or $f$ incorrectly, introducing bugs that may invalidate the correctness proofs for the involutive MCMC algorithm.

Fortunately, the factorization of diverse algorithms into a common template, involving an explicitly represented model, auxiliary distribution, and involution, enables simple and automated debugging checks that can catch a wide variety of such errors dynamically.

\begin{algorithm}
\caption{Dynamic Check for Bugs}
\Procedure{involutive-mcmc-check}{\mathcal{P}, \mathcal{Q}, \mathcal{F}}
\State Generate a randomized test case $((x \oplus b), .) \sim \text{trace-and-score}(\mathcal{P})$
\State $(y, .) \sim \text{trace-and-score}(\mathcal{Q}_x)$
\State Run involution and perform dimension check $x' \oplus y' \leftarrow \text{run-involution}(\mathcal{F}, x \oplus y, b)$
\State Support check $\log p(x') \leftarrow \text{score}(\mathcal{P}, x')$
\State $\log q_x'(y') \leftarrow \text{score}(\mathcal{Q}_x', y')$
\State \Return $(\log p(x') > -\infty) \land (\log q_x'(y') > -\infty)$
\State Involution check $\tilde{x} \oplus \tilde{y} \leftarrow \text{run-involution}(\mathcal{F}, x' \oplus y', b)$
\State \Return $(\tilde{x} = x) \land (\tilde{y} = y)$
\EndProcedure
\end{algorithm}

The check first randomly samples a model trace $x$ and simulated observations $b$ from the model prior $p$, and auxiliary trace $y$ from the $q_x$. It then runs three tests on this simulated test case:

1. \textbf{Support check}. The \textit{support check} runs the involution $\mathcal{F}$ on $(x, y)$ and checks that the resulting pair of traces, $(x', y')$, are within the set $Z$ of positive-density elements for $\pi$.

2. \textbf{Dimension check}. The \textit{dimension check} runs the involution $\mathcal{F}$ on $(x, y)$ and checks that the sizes of these sets match. (This check is part of computing the determinant of the Jacobian in \texttt{run-involution}).

3. \textbf{Involution check}. The \textit{involution check} runs $\mathcal{F}$ twice to compute $f(f(x, y))$ and checks that the result is equal to $(x, y)$. If $f$ is an involution on $Z$, then this check will always succeed; if there is a set $\tilde{Z}$ of positive $\pi$-measure on which $f(f(z)) \neq z$ (i.e., $f$ is not an involution), then this check has positive probability of failing.

These checks each catch qualitatively different bugs in user programs. We now give several examples.

\textit{Incorrectly transformed continuous variables}. Many bugs in the design or implementation of deterministic transformations of continuous variables are naturally detected by the involution check. Consider, for example, the Hamiltonian Monte Carlo algorithm \cite{Duane1987}.
Marco Cusumano-Towner, Alexander K. Lew, Vikash K. Mansinghka

et al., 1987], which, as [Neklyudov et al., 2020] observe, is an instance of the involutive MCMC framework. When applied to HMC, the dynamic bug check involves: (a) sampling a model state \( x \) from the prior; (b) sampling a momentum \( y \); (c) running the leapfrog integrator forward to get a new state \( x' \) and new momentum \( -y' \); (d) running the leapfrog integrator backward from state \( x' \) with momentum \( y' \), and (e) checking that this results in the state-momentum pair \( x, -y \). If the momentum is not properly negated, or if the leapfrog integrator is incorrectly implemented, this check can fail.

As another, simpler example of this type of error, consider the `split_params` and `merge_params` functions invoked in Figure 1 as part of a reversible-jump MCMC kernel for inferring a mixture of Gaussians with an unknown number of components. Considering only the \( \mu \) parameter, suppose the `split` move samples an auxiliary variable \( u_1 \) and computes \( \mu_1 = \mu + u_1, \mu_2 = \mu - u_1 \) as the means of the two new clusters. If the `merge` move joins two clusters and assigns \( \mu = \sqrt{\mu_1 \mu_2} \), there is a mismatch: a split move cannot be reversed by a corresponding merge, because in general, \( (\mu + u_1)(\mu - u_1) \neq \mu \). This error could be fixed either by changing the split to compute \( \mu_1 = \mu u_1, \mu_2 = \frac{\mu}{u_1} \), or by changing the merge to compute \( \mu = \frac{\mu_1 + \mu_2}{2} \).

Discrete logic errors. Another common class of errors is for the discrete logic of an involution to be flawed. Consider the following incorrect implementation of a `birth-death` move for the mixture model in Figure 1 which either adds a new mixture component or selects an existing one at random to delete (we name the traces \( \text{tr1}, \text{tr2}, \text{tr3}, \text{ad tr4} \) for reasons of space):

```plaintext
@gen function q(trace)
    current_k = trace[:k]
    is_birth ~ bernoulli(current_k == 1 ? 1.0 : 0.5)
    if is_birth
        new_mu = normal(0, 10)
        new_var ~ inv_gamma(1, 10)
    else
        deletion_idx ~ uniform_discrete(1, current_k)
    end
end
```

```plaintext
@transform h (tr1, tr2) to (tr3, tr4) begin
    is_birth = @read(tr2, :is_birth, :discrete)
    @write(tr4[:is_birth], !is_birth, :discrete)
    k = @read(tr1[:k], :discrete)
    weights = @read(tr1[:weights], :continuous)
    if is_birth
        @write(tr3[:k], k+1, :discrete)
        new_mu = @read(tr2[:new_mu], :continuous)
        new_var = @read(tr2[:new_var], :continuous)
        @write(tr3[:,:mu], new_mu, :continuous)
        @write(tr3[:,:var], new_var, :continuous)
        new_weights = add_weight(weights)
        @write(tr4[:deletion_idx], k+1, :discrete)
    else
        idx = @read(tr2[:deletion_idx], :discrete)
        @copy(tr1[(:mu, i)], tr4[(:new_mu)])
        @copy(tr1[(:var, i)], tr4[(:new_var)])
        for i in (idx+1):k
            @copy(tr1[(:mu, i)], tr3[(:mu, i-1)])
            @copy(tr1[(:var, i)], tr3[(:var, i-1)])
        end
        @write(tr3[:k], k-1, :discrete)
        new_weights = delete_weight(weights, idx)
        @write(tr3[:weights], new_weights, :continuous)
    end
end
```

The flaw in this implementation is that although the death move can delete any of the \( k \) mixture components, the birth move can only add a new component to the \( \text{end} \) (index \( k+1 \)), so the move is not reversible. The involution check will discover that the deletion of a component with index \( i < k \) is not reversed by a corresponding birth move, and will thus raise an error.

Other miscellaneous errors. When implementing distributions as probabilistic programs, it is also possible for users to make more mundane errors, such as spelling the name of a random choice inconsistently, or characterizing random choices using the wrong `type` tags (`:continuous` and `:discrete`). Such errors can be difficult to detect statically, because the addresses at which a probabilistic program makes random choices, and the distributions of those choices, may change from sample to sample. (Previous work has explored static analyses based on types [Lew et al., 2019] and abstract interpretation [Lee et al., 2019], but these each work on limited subsets of the programs that Gen’s full modeling language permits, and it is often precisely these more complex programs that require the flexibility of the involutive MCMC framework in the first place). Our dynamic support and dimension checks can help to detect bugs like these. For example, if the involution \( f \) writes to a misspelled address, the support check will determine that the resulting trace’s density is 0.

Dynamic checks during inference. These dynamic assertions can also be run during inference, at each application of the transition kernel. This can be useful to catch bugs that only occur in regions of the state
space with low prior mass (but perhaps high posterior mass). When enabled, we can run dynamic checks after each application of the kernel, and when they fail, write to a debugging log and reject the proposed new state. As it turns out, the kernel induced by this procedure is still stationary for $p$

**Lemma 6.1.** Let $p$ and $q_h$ be model and auxiliary densities as above, but suppose $f : D \times D \rightarrow D \times D$ may not be an involution on $Z$. Trace-based involutive MCMC with dynamic checks enabled, rejecting whenever such a check fails, still yields a kernel that is stationary for $p$.

**Proof.** Let $R = \{ x \in Z \mid f(f(x)) = x \wedge \pi(f(x)) > 0 \}$, and let $h(x) := 1[x \in R]f(x) + 1[x \notin R]x$. Then $h$ is an involution on $Z$, and trace-based involutive MCMC with $p$, $q_x$, and $h$ yields a stationary kernel. But this kernel is the same one induced by using $f$ with dynamic checks. For $x$ on which dynamic checks succeed, $h$ is equivalent to $f$. For $x$ on which dynamic checks fail, $h$ is equivalent to the identity; thus, accepting a move produced by $h$ is equivalent to rejecting. 

7 EXAMPLES

7.1 Reversible Jump MCMC

Reversible jump MCMC (Green 1995 Hastie and Green 2012) is a special case of involutive MCMC, and the implementation of reversible jump MCMC kernels can be automated using the probabilistic and differentiable programming languages presented in this paper. We now review reversible jump MCMC, then show how it can be automated using the techniques presented earlier, and give an example.

Review of reversible jump MCMC. The reversible jump MCMC framework involves a set of ‘models’ $h \in \mathcal{H}$, and a prior distribution on models $p(h)$. For each model, there is a latent continuous parameter vector $\theta_h \in \mathbb{R}^{n(h)}$ where $n(h)$ is the dimension of model $h$, and a likelihood function $L_{D,h}(\theta_h)$ for each $h$ given data $D$. The latent state $x$ is a pair $(h, \theta_h)$ of model and continuous parameter. There is a set of move types $\mathcal{M}$. Each move type $m \in \mathcal{M}$ is associated with an unordered pair of models $(h_1, h_2)$ and a dimensionality $d(m)$ such that $d(m) \geq n(h_1)$ and $d(m) \geq n(h_2)$ (zero, one, or more than one move types may be associated with a given pair of models). For each latent state $x = (h, \theta_h)$, there is a probability distribution $q_x(m)$ on move types such that $\int q_x(m) > 0$ implies that $x$ is one of the models for move type $m$. For each move type $m \in \mathcal{M}$ between $h_1$ and $h_2$ there is a pair of continuously differentiable bijections $g_{m,h_1 \rightarrow h_2} : \mathbb{R}^{d(m)} \rightarrow \mathbb{R}^{d(m)}$ and $g_{m,h_2 \rightarrow h_1} := g_{m,h_1 \rightarrow h_2}^{-1}$, and a pair of proposal densities $q_{m,h_1 \rightarrow h_2}(u_{h_1 \rightarrow h_2})$ and $q_{m,h_2 \rightarrow h_1}(u_{h_2 \rightarrow h_1})$ where $u_{h_1 \rightarrow h_2} \in \mathbb{R}^{d(m) - n(h_1)}$ and $u_{h_2 \rightarrow h_1} \in \mathbb{R}^{d(m) - n(h_2)}$. A proposal is made from state $x = (h, \theta_h)$ by (i) sampling a move type $m \sim q_x(\cdot)$, and (ii) sampling continuous variable $u \sim q_{m,h \rightarrow h'}(\cdot)$ for $(h, h')$ associated with $m$, and (iii) computing $(\theta', u') := g_{m,h \rightarrow h'}(\theta_h, u)$, and proposing new state $x' = (h', \theta'_h)$.

Encoding reversible jump in involutive MCMC.

To encode reversible jump MCMC in our framework, we write a probabilistic program $P$ that encodes the space of models $\mathcal{H}$, the prior distribution on models $p(h)$, the per-model priors $p_\theta(\theta_h)$ and the per-model likelihoods $L_{D,h}(\theta_h)$. The set of all models $h$ is encoded in the set of all pairs $(K_P, \mathbf{d}_P)$ where $K_P$ represent possible trace structures (i.e. control-flow paths through $P$) and $\mathbf{d}_P$ are the set of assignments to discrete random choices made by $P$. The per-model continuous parameters $\theta$ are encoded via continuous random choices $\mathbf{c}_P$. The auxiliary probabilistic program $Q$ encodes both the probability distribution on moves types using discrete random choices and possibly stochastic control flow (where $P$ and $Q$), and the per-move-type probability densities on $u$ using continuous random choices $\mathbf{c}_Q$. The involution $f$ factors into an (i) involution $f_1$ on pairs $i = (K_P, \mathbf{d}_P), (H_P, \mathbf{d}_Q))$ that defines the association between move types $M$ and the model pairs $(h_1, h_2)$; and (ii) a family of bijections $f_{1,i}$ on the space of pairs $(\mathbf{c}_P, \mathbf{c}_Q)$ of continuous random choices for both programs for fixed values of the discrete random choices and fixed trace structure.

Example: Split-merge reversible jump. Figure 1 shows a split-merge reversible jump kernel for an infinite Gaussian mixture model (Richardson and Green 1997) implemented using the probabilistic and differentiable programming languages described in this paper. Figure 1 shows the infinite Gaussian mixture model, specified as a probabilistic program $p$. The program takes the number of data points as input, then samples the number of clusters from a Poisson distribution, then samples cluster parameters and mixture proportions, and finally samples the data points from the resulting finite mixture. Figure 1 shows the auxiliary probabilistic program $q$ for the split-merge kernel. This program takes a trace of the model program as input, and randomly decides whether to split a cluster and increase the number of clusters by one or merge two clusters and decrease the number of clusters by one. Then, the program randomly picks which cluster to split, or which clusters to merge. This kernel always merges the last cluster with a random other cluster; for ergodicity the move can be composed with a simple move (that has acceptance probability 1) that swaps a
random cluster with the last cluster. If a split is chosen, then the program also samples the three degrees of freedom necessary to generate the new parameters for the clusters in an invertible manner. Figure 1 shows a differentiable program specifying the involution for the split-merge kernel, and Figure 1 shows graphically how this involution acts on pairs of traces. The yellow section (1) defines an involution \( f \) on the discrete random choices that specifies that (i) the split choice should be flipped (so that split moves are always mapped to merge moves and vice versa) and that (ii) the number of clusters should be increased by one for a split move and decreased by one for a merge move, and (iii) which merged cluster corresponds to which split clusters. The green section (2) specifies the continuous bijections that govern the transformation of continuous random choices during split moves and the purple section (3) specifies the inverses of these bijections, which govern the transformation of continuous choices during merge moves.

7.2 State-Dependent Mixture Proposals

Example: Bayesian structure learning for Gaussian processes. Figure 2 shows automated involutive MCMC being applied to fully Bayesian inference over the covariance function of a Gaussian process, where the prior on covariance functions (Figure 2) is based on a probabilistic context-free grammar. The inference algorithm is based on an involutive MCMC kernel that uses a state-dependent mixture of proposals. A variant of this inference algorithm was previously studied in [Schaechtle et al., 2016; Saad et al., 2019] based on a model of Grosse et al. (2012).

Hierarchical address spaces. This example uses probabilistic programs that invoke other probabilistic programs, sometimes recursively. For example, the model probabilistic program \( p \) invokes the probabilistic program \( \text{cov_function_prior} \), which is itself recursive. Similarly, the auxiliary probabilistic program \( q \) invokes \( \text{walk_tree} \) (which is recursive) as well as \( \text{cov_function_prior} \). Consider the syntax used to recursively invoke \( \text{walk_tree} \) within \( \text{walk_tree} \):

\[
(\{\text{:left}\} \sim \text{walk_tree}(\text{node}.\text{left}, \text{path}))
\]

This expression resembles a random choice expression. However, instead of associating the return value of the function \( \text{walk_tree} \) with the address \( \text{:left} \), the address \( \text{:left} \) is associated with the entire trace of random choices made within \( \text{walk_tree} \). That is, \( \text{:left} \) is the namespace for the addresses of all random choice made within the invocation. Further invocations by the callee themselves result in nested namespaces. This process results in a hierarchical address space for random choices, as shown in Figure 2. This does not modify the mathematical formalism—each random choice made during the execution of a probabilistic program still has a unique address, but the address has multiple components that localize it within the hierarchy. For example, the choice \( \text{done} \) a recursive call to \( \text{walk_tree} \) might have address:

\[
k = (\text{:left} => \text{right} => \text{done})
\]

(‘=>’ is the Gen syntax for constructing hierarchical addresses).

A complex state-dependent distribution. At each iteration of the MCMC algorithm, the auxiliary probabilistic program \( q \) (Figure 2) first picks a random node in the parse tree of the covariance function, by doing a stochastic walk of the existing parse tree that terminates at the chosen node.

\[
\text{prev_cov_function} = \text{trace}[\text{cov_function}]
\text{path} \sim \text{walk_tree}(\text{prev_cov_function}, \ldots)
\]

The code that walks the tree uses the following recursion, which results in a probability distribution that assigns exponentially lower probability to nodes that are deeper in the tree.

\[
\text{if } (\{\text{done}\} \sim \text{bernoulli}(0.5))
\text{return } \text{path}
\text{elseif } (\{\text{recurse_left}\} \sim \text{bernoulli}(0.5))
\text{path} = (\text{path}..., \text{:left_node})
\text{return } (\{\text{left}\} \sim \text{walk_tree}(\text{node}.\text{left}, \text{path}))
\text{else}
\text{path} = (\text{path}..., \text{:right_node})
\text{return } (\{\text{right}\} \sim \text{walk_tree}(\text{node}.\text{right}, \text{path}))
\text{end}
\]

The resulting distributions on selected nodes for two possible input trees are shown below:

![Distributions on selected nodes for two possible input trees](image)

The first part of the involution (Figure 2) copies the random choices made during this walk from the input auxiliary trace to the output auxiliary trace.

\[
@\text{copy}(\text{aux_in}[\text{path}], \text{aux_out}[\text{path}])
\]

Note that here, \( @\text{copy} \) is being used to copy the entire set of random choices from the namespace \( \text{path} \) in \( \text{aux_in} \) to the namespace \( \text{path} \) in \( \text{aux_out} \).

Because the mixture distribution is specified using a probabilistic program, it is straightforward to modify
the program \( p \) to define a different mixture distribution. The code below specifies a mixture distribution that is uniform over all nodes in the tree.

\[
\begin{align*}
n_1 &= \text{size}(\text{node.left}); n_2 = \text{size}(\text{node.right}) \\
\text{if} \ (\{\text{:done}\} \sim \text{bernoulli}(1 / (1 + n_1 + n_2))) & \text{ return path} \\
\text{elseif} \ (\{\text{:recurse_left}\} \sim \text{bernoulli}(n_1 / (n_1+n_2)) & \text{ path = (path..., :left_node)} \\
& \text{ return } (\{\text{:left}\} \sim \text{walk_tree(node.left, path)}) \\
\text{else} & \text{ path = (path..., :right_node)} \\
& \text{ return } (\{\text{:right}\} \sim \text{walk_tree(node.right, path)}) \\
\end{align*}
\]

The resulting distributions, for two possible input trees, are:

Note that the probability of choosing a given subtree to propose to is itself changed when the subtree changes. Therefore, the mixture probabilities do not in general cancel in the acceptance probability calculation, and must be accounted for. For the original mixture distribution, the ratio of mixture probabilities is either 1, 0, or 2 depending on whether the previous and new subtrees are leaf or internal nodes. For this alternative mixture distribution, the ratio of mixture probabilities is the ratio of sizes of the two trees (e.g. 9/5 or 5/9 for the trees above). In both cases, our automated involutive MCMC algorithm automatically computes the acceptance probability.

A general pattern for state-dependent mixtures of proposals in Metropolis-Hastings. The other parts of the auxiliary probabilistic program and the involution program specifies a proposal distribution for the subtree of the parse tree that is rooted at the chosen node. In particular, the rest of the auxiliary probabilistic program \( q \) proposes a new subtree by sampling from the same process used to recursively define the prior distribution:

\[
\text{new_subtree} \sim \text{cov_function_prior()}
\]

The involution program swaps the old subtree with the newly proposed subtree:

```plaintext
@copy(model_in[subtree_address], aux_out[:new_subtree])
@copy(aux_in[:new_subtree], model_out[subtree_address])
```

This is an instance of a more general pattern for implementing state-dependent mixture proposals:

1. The auxiliary probabilistic program \( Q \) samples from a distribution over different sets of random choices that will be proposed to (in this case, each set is a different subtree of the parse tree).
2. The auxiliary probabilistic program \( Q \) then samples new values for those random choices (in this case, a new subtree).
3. The involution program \( F \) swaps the previous values of those random choices with their new values, by swapping data between the model trace and the auxiliary trace.
4. The involution program \( F \) copies the random choices that determined what subset of random choices to propose to from the input auxiliary trace to the output auxiliary trace.

8 DISCUSSION

Involutive MCMC is a unifying construction (Neklyudov et al., 2020) for MCMC algorithms that encompasses both classic approaches to constructing kernels like reversible jump MCMC (Green, 1995), but also recently introduced classes of MCMC kernels based on neural networks (Spanbauer et al., 2020). Therefore, the approach to automating involutive MCMC kernels presented in this paper makes a number of classic MCMC techniques easier to use and broadens their accessibility, and may potentially aid in development of novel MCMC techniques as well. The implementation of our approach in the Gen probabilistic programming system has already been used by researchers in computational biology (Merrell and Gitter, 2020) and artificial intelligence (Zhi-Xuan et al., 2020) to prototype and develop new reversible-jump MCMC algorithms.

The technique for automating involutive MCMC presented in this paper can be generalized to the setting of sequential Monte Carlo samplers (Del Moral et al., 2006). Instead of one model probabilistic program, one auxiliary probabilistic program and one involution program, there are two model probabilistic programs, two auxiliary probabilistic programs, and a pair of bijective differentiable programs that transform traces of one model into traces of the other. This more general construct, which builds on earlier work on sequential Monte Carlo and probabilistic programs (Cusumano-Towner et al., 2018), has already been implemented as part of the Gen probabilistic programming system.

Improving the performance of automated involutive MCMC and of flexible probabilistic programming systems like Gen more generally is an important area
The approach described in this paper is largely dynamic and is not performance-competitive with optimized hand-coded implementations in performance-oriented languages like C. While our approach is already valuable for use cases where the best performance is not necessary or the expertise or time needed for an optimized hand-coded implementation is not available, more research into compilers and automatic code generation of custom inference algorithms from high-level user specifications would broaden the applicability of systems like Gen.

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References

Bezanson, J., Edelman, A., Karpinski, S., and Shah, V. B. (2017). Julia: A fresh approach to numerical computing. *SIAM Review*, 59(1):65–98.

Bingham, E., Chen, J. P., Jankowiak, M., Obermeyer, F., Pradhan, N., Karaletsos, T., Singh, R., Szerlip, P., Horsfall, P., and Goodman, N. D. (2019). Pyro: Deep universal probabilistic programming. *The Journal of Machine Learning Research*, 20(1):973–978.

Carpenter, B., Gelman, A., Hoffman, M. D., Lee, D., Goodrich, B., Betancourt, M., Brubaker, M., Guo, J., Li, P., and Riddell, A. (2017). Stan: A probabilistic programming language. *Journal of statistical software*, 76(1).

Chang, J. T. and Pollard, D. (1997). Conditioning as disintegration. *Statistica Neerlandica*, 51(3):287–317.

Cusumano-Towner, M. (2018). Inference library of the Gen probabilistic programming system. [https://github.com/probcomp/Gen.jl/blob/b9d72b/src/inference/mh.jl#L73-L108](https://github.com/probcomp/Gen.jl/blob/b9d72b/src/inference/mh.jl#L73-L108) Accessed: 2018-12-27.

Cusumano-Towner, M., Bichsel, B., Gehr, T., Vechev, M., and Mansinghka, V. K. (2018). Incremental inference for probabilistic programs. In *Proceedings of the 39th ACM SIGPLAN Conference on Programming Language Design and Implementation*, PLDI 2018, pages 571–585. ACM.

Cusumano-Towner, M. F., Saad, F. A., Lew, A. K., and Mansinghka, V. K. (2019). 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. ACM.

Del Moral, P., Doucet, A., and Jasra, A. (2006). Sequential Monte Carlo samplers. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 68(3):411–436.

Duane, S., Kennedy, A. D., Pendleton, B. J., and Roweth, D. (1987). Hybrid Monte Carlo. *Physics letters B*, 195(2):216–222.

Gehr, T., Misailovic, S., and Vechev, M. (2016). Psi: Exact symbolic inference for probabilistic programs. In *International Conference on Computer Aided Verification*, pages 62–83. Springer.

Geiger, A., Lauer, M., and Urtasun, R. (2011). A generative model for 3D urban scene understanding from movable platforms. In *CVPR 2011*, pages 1945–1952. IEEE.

Gilks, W. R., Thomas, A., and Spiegelhalter, D. J. (1994). A language and program for complex Bayesian modelling. *Journal of the Royal Statistical Society: Series D (The Statistician)*, 43(1):169–177.

Goodman, N., Mansinghka, V., Roy, D. M., Bonawitz, K., and Tenenbaum, J. B. (2008). Church: a language for generative models. In *Proceedings of the 24th Annual Conference on Uncertainty in Artificial Intelligence*, UAI 2008, pages 220–229. AUAI Press.

Green, P. J. (1995). Reversible jump Markov chain Monte Carlo computation and Bayesian model determination. *Biometrika*, 82(4):711–732.

Grosse, R. B., Salakhutdinov, R., Freeman, W. T., and Tenenbaum, J. B. (2012). Exploiting compositionality to explore a large space of model structures. In *Proceedings of the 28th Conference on Uncertainty in Artificial Intelligence*, UAI 2012, pages 306–315. AUAI Press.

Hastie, D. I. and Green, P. J. (2012). Model choice using reversible jump Markov chain Monte Carlo. *Statistica Neerlandica*, 66(3):309–338.

Huelsenbeck, J. P., Larget, B., and Alfaro, M. E. (2004). Bayesian phylogenetic model selection using reversible jump Markov chain Monte Carlo. *Molecular biology and evolution*, 21(6):1123–1133.

Lee, W., Yu, H., Rival, X., and Yang, H. (2019). Towards verified stochastic variational inference for probabilistic programs. *Proceedings of the ACM on Programming Languages*, 4(POPL):1–33.
Lew, A. K., Cusumano-Towner, M. F., Sherman, B., Carbin, M., and Mansinghka, V. K. (2019). Trace types and denotational semantics for sound programmable inference in probabilistic languages. *Proceedings of the ACM on Programming Languages*, 4(POPL):1–32.

Mansinghka, V. K., Schaechtle, U., Handa, S., Radul, A., Chen, Y., and Rinard, M. (2018). Probabilistic programming with programmable inference. In *Proceedings of the 39th ACM SIGPLAN Conference on Programming Language Design and Implementation*, pages 603–616.

Merrell, D. and Gitter, A. (2020). Inferring signaling pathways with probabilistic programming. *Proceedings of the Nineteenth European Conference of Computational Biology*.

Milch, B., Marthi, B., Russell, S., Sontag, D., Ong, D. L., and Kolobov, A. (2005). BLOG: Probabilistic models with unknown objects. In *Proceedings of the Nineteenth International Joint Conference on Artificial Intelligence*, IJCAI 2005, pages 1352–1359. Morgan Kaufmann Publishers Inc.

Narayanan, P. and Shan, C.-c. (2020). Symbolic disintegration with a variety of base measures. *ACM Transactions on Programming Languages and Systems (TOPLAS)*, 42(2):1–60.

Neklyudov, K., Welling, M., Egorov, E., and Vetrov, D. (2020). Involutive MCMC: A Unifying Framework. *arXiv preprint arXiv:2006.16653*.

Pfeffer, A. (2007). The design and implementation of IBAL: A general-purpose probabilistic language. *Introduction to statistical relational learning*, page 399.

Richardson, S. and Green, P. J. (1997). On Bayesian analysis of mixtures with an unknown number of components (with discussion). *Journal of the Royal Statistical Society: series B (statistical methodology)*, 59(4):731–792.

Ritchie, D., Horsfall, P., and Goodman, N. D. (2016). Deep amortized inference for probabilistic programs. *arXiv preprint arXiv:1610.05735*.

Roberts, D. A., Gallagher, M., and Taimre, T. (2019). Reversible jump probabilistic programming. In Chaudhuri, K. and Sugiyama, M., editors, *Proceedings of Machine Learning Research*, volume 89 of *Proceedings of Machine Learning Research*, pages 634–643. PMLR.

Saad, F. A., Cusumano-Towner, M. F., Schaechtle, U., Rinard, M. C., and Mansinghka, V. K. (2019). Bayesian synthesis of probabilistic programs for automatic data modeling. *Proceedings of the ACM on Programming Languages*, 3(POPL):1–32.
A APPENDIX

A.1 Derivation of the pushforward Radon-Nikodym derivative for a special case

Implementing Algorithm \[\text{APPENDIX}\] requires computing the Radon-Nikodym derivative \(d(\mu \circ f^{-1})/d\mu\). This section derives that function for the special case in which the involution \(f\) can be factored into an involution on a countable set \(I\) and a family of bijections on \(\mathbb{R}^{n_i}\) for some \(n_i\) for each \(i \in I\). Suppose \(Z = \{(i,x) : i \in I, x \in \mathbb{R}^{n_i}\}\). Suppose \(f_1\) is an involution on \(I\) and \(n_i = n_{f_1(i)}\) and \(f_2\) is a family of continuously differentiable bijections indexed by \(i \in I\), such that \(f_{2,i} : \mathbb{R}^{n_i} \to \mathbb{R}^{n_i}\). Also suppose that \(f_{2,i} = f_{2,i}^{-1}\) for all \(i \in I\). That is,

\[
f_{2,i}(f_{2,i}(x)) = x \text{ for all } x \in \mathbb{R}^{n_i} \text{ and all } i \in I
\]

Then, \(f : Z \to Z : (i,x) \mapsto (f_1(i), f_{2,i}(x))\) is an involution because:

\[
f(f(i,x)) = f(f_1(i), f_{2,i}(x)) = (f_1(f_1(i)), f_{2,i}(f_2,i)(f_{2,i}(x))) = (i,x)
\]

Let \(\Sigma_n\) and \(\mu_n\) denote the Lebesgue \(\sigma\)-algebra and Lebesgue measure on \(\mathbb{R}^{n_i}\), respectively. Let \(\Sigma \subset \mathcal{P}(Z)\) be the \(\sigma\)-algebra of sets of the form \(\cup_{i \in I} \{(i,x) : x \in K_i\}\) for some \(K_i \in \Sigma_n\) for each \(i \in I\). Let \(\mu\) denote the measure on measurable space \((Z, \Sigma)\) given by:

\[
\mu(\cup_{i \in I} \{(i,x) : x \in K_i\}) := \sum_{i \in I} \mu_n(K_i)
\]

We wish to show that the Radon-Nikodym derivative of the pushforward of \(\mu\) by \(f\) with respect to \(\mu_i\), evaluated at \((i,x)\), is the absolute value of the Jacobian (determinant) of the function \(f_{2,i}\) evaluated at \(x\), which is denoted \((Jf_{2,i})(x)\):

\[
d(\mu \circ f^{-1})/d\mu(i,x) = |(Jf_{2,i})(x)|
\]

Consider \((\mu \circ f^{-1})(A)\) for \(K \in \Sigma\):

\[
(\mu \circ f^{-1})(\cup_{i \in I} \{(i,x) : x \in K_i\}) = \mu(f^{-1}(\cup_{i \in I} \{(i,x) : x \in K_i\}))
\]

\[
= \mu(\cup_{i \in I} f^{-1}(\{(i,x) : x \in K_i\}))
\]

\[
= \mu(\cup_{i \in I} \{(f_1(i), x) : x \in f_{2,i}(K_i)\})
\]

\[
= \sum_{i \in I} \mu_n(f_{2,i}(K_i))
\]

It suffices to show that for all \(K \in \Sigma\):

\[
\int_K |(Jf_{2,i})(x)| \mu(dx) = \sum_{i \in I} \mu_n(f_{2,i}(K_i))
\]

Expanding the left-hand side:

\[
\int_K |(Jf_{2,i})(x)| \mu(dx) = \sum_{i \in I} \int_{K_i} |(Jf_{2,i})(x)| \mu_n(dx) = \sum_{i \in I} \mu_n(f_{2,i}(K_i))
\]

where the final step uses Bogachev Theorem 3.7.1 with \(g := 1\), and \(F := f_{2,i}\).

A.2 Proof of detailed balance for involution

The involutive MCMC kernel is composed of two parts: An extension of the state space, and an involution on the extended state space. First, we show detailed balance for the deterministic involution move applied to the extended state space.

Tierney [1998] gives a class of MCMC kernels based on involutions that satisfy detailed balance. We now reproduce the result in our notation:
Lemma A.1 (Detailed balance for involution move (Tierney 1998)). Let \((Z, \Sigma, \pi)\) denote a measure space. Suppose \(f\) is a one-to-one function from \(Z\) onto \(Z\) such that \(f^{-1} = f\). Consider the probability kernel \(k\) defined by \(k_z(A) := [f(z) \in A | \alpha(z, f(z)) + |z| \in A (1 - \alpha(z, f(z)))\) (where \(\alpha(z, f(z))\) gives the probability of accepting a proposed transition from \(z\) to \(f(z)\)). Let \(v(dz) := \pi(dz) + (\pi \circ f^{-1})(dz)\). Let \(h(z)\) be a density for \(\pi\) with respect to \(\nu\). Let \(K := \{z \in Z : h(z) > 0 \text{ and } h(f(z)) > 0\}\). \(k\) satisfies detailed balance with respect to \(\pi\) if and only if:

1. \(\alpha(z, f(z)) = 0\) for \(\pi\)-almost all \(z \not\in K\)
2. \(\alpha(z, f(z)) h(f(z))^{-1} = \alpha(f(z), z)\)

Now we apply Lemma A.1 to our setting where \(\pi\) is \(\sigma\)-finite, there exists a \(\sigma\)-finite reference measure \(\mu\) for measurable space \((Z, \Sigma)\) such that \(\pi\) is mutually absolutely continuous with respect to \(\mu\), and where the pushforward of \(\mu\) by \(f\), denoted \(\mu \circ f^{-1}\), is absolutely continuous with respect to \(\mu\).

In our setting, \(\alpha\) is defined as:

\[
\alpha(z, f(z)) := \min \left\{ 1, \frac{d\pi}{d\mu}(f(z)) \cdot \frac{d(\mu \circ f^{-1})}{d\mu}(z) \right\}
\]  

(15)

This definition of \(\alpha\) satisfies:

\[
\alpha(z, f(z)) \frac{d\pi}{d\mu}(z) \cdot \left( \frac{d(\mu \circ f^{-1})}{d\mu}(z) \right)^{-1} = \alpha(f(z), z)
\]

(16)

Therefore, to apply Lemma A.1 it suffices to show \(\pi\) has density with respect to \(\nu\) (denoted \(h(z)\)) such that:

\[
\frac{h(z)}{h(f(z))} = \frac{d\pi}{d\nu}(z) \left( \frac{d(\mu \circ f^{-1})}{d\mu}(z) \right)^{-1}
\]

(17)

Since \(\pi\) and \(\pi \circ f^{-1}\) are both absolutely continuous with respect to \(\mu\), \(\pi\) is also absolutely continuous with respect to \(\mu\), and has density:

\[
\frac{d\pi}{d\mu}(z) = \frac{d\pi}{d\nu}(z) + \frac{d(\pi \circ f^{-1})}{d\mu}(z)
\]

(18)

\(\pi\) is absolutely continuous with respect to \(\nu\), and therefore:

\[
\frac{d\pi}{d\mu}(z) = \frac{d\pi}{d\nu}(z) \cdot \frac{d\nu}{d\mu}(z)
\]

(19)

Because \((d\pi/d\mu)(z) > 0\) for all \(z \in Z\), \((d\nu/d\mu)(z) > 0\) for all \(z \in Z\). Therefore,

\[
\frac{h(z)}{h(f(z))} = \frac{d\pi}{d\nu}(z) = \frac{d\pi}{d\mu}(z)
\]

(20)

Therefore:

\[
\frac{h(z)}{h(f(z))} = \frac{d\pi}{d\mu}(z) \cdot \frac{d\nu}{d\mu}(f(z))
\]

(21)

It suffices to show that:

\[
\frac{d\nu}{d\mu}(f(z)) = \left( \frac{d(\mu \circ f^{-1})}{d\mu}(z) \right)^{-1}
\]

(22)

First, we prove a Lemma:

Lemma A.2. If \((Z, \Sigma)\) is a measurable space and \(f : Z \to Z\) is a measurable function that is an involution, \(\nu\) and \(\mu\) are \(\sigma\)-finite measures such that \(\nu\) is absolutely continuous with respect to \(\mu\), and such that the pushforward measures \(\nu \circ f^{-1}\) and \(\mu \circ f^{-1}\) are both \(\sigma\)-finite, then \(\nu \circ f^{-1}\) is absolutely continuous with respect to \(\mu \circ f^{-1}\) and

\[
\frac{d(\nu \circ f^{-1})}{d(\mu \circ f^{-1})}(z) = \frac{d\nu}{d\mu}(f(z))
\]
Proof. First, $\nu \circ f^{-1}$ is absolutely continuous with respect to $\mu \circ f^{-1}$ because $(\mu \circ f^{-1})(A) = 0$ implies $\mu(f^{-1}(A)) = 0$ implies $\nu(f^{-1}(A)) = 0$ implies $(\nu \circ f^{-1})(A) = 0$. To show that $z \mapsto (d\nu/d\mu)(f(z))$ is the Radon-Nikodym derivative $d(\nu \circ f^{-1})/d(\mu \circ f^{-1})$, it suffices to show that for all $K \in \Sigma$:

$$\int_K \left( \frac{d\nu}{d\mu}(f(z)) \right) (\mu \circ f^{-1})(dz) = (\nu \circ f^{-1})(A) := \nu(f^{-1}(A))$$

(23)

Applying Theorem 3.6.1 in Bogachev with $\nu$ and $\mu$ implies $\nu(f^{-1}(A)) = 0$ implies $(\nu \circ f^{-1})(A) = 0$. To show that $z \mapsto (d\nu/d\mu)(f(z))$ is the Radon-Nikodym derivative $d(\nu \circ f^{-1})/d(\mu \circ f^{-1})$, it suffices to show that for all $K \in \Sigma$:

$$\int_K \left( \frac{d\nu}{d\mu}(f(z)) \right) (\mu \circ f^{-1})(dz) = (\nu \circ f^{-1})(A) := \nu(f^{-1}(A))$$

(23)

First, $\nu \circ f^{-1}$ is absolutely continuous with respect to $\mu \circ f^{-1}$ because $(\mu \circ f^{-1})(A) = 0$ implies $\mu(f^{-1}(A)) = 0$ implies $\nu(f^{-1}(A)) = 0$ implies $(\nu \circ f^{-1})(A) = 0$. To show that $z \mapsto (d\nu/d\mu)(f(z))$ is the Radon-Nikodym derivative $d(\nu \circ f^{-1})/d(\mu \circ f^{-1})$, it suffices to show that for all $K \in \Sigma$:

$$\int_K \left( \frac{d\nu}{d\mu}(f(z)) \right) (\mu \circ f^{-1})(dz) = (\nu \circ f^{-1})(A) := \nu(f^{-1}(A))$$

(23)

Now, note that $\nu$ and $\nu \circ f^{-1}$ are the same measure:

$$\nu(A) = \pi(A) + \pi'(A) = \pi(A) + \pi(f^{-1}(A))$$

(29)

$$\nu(f^{-1}(A)) = \pi(f^{-1}(A)) + \pi(f^{-1}(f^{-1}(A))) = \pi(f^{-1}(A)) + \pi(A)$$

(30)

Therefore,

$$\frac{d(\nu \circ f^{-1})}{d\nu}(z) = 1 \text{ for all } z$$

Expanding $d(\nu \circ f^{-1})/d\nu$ using the chain rule:

$$1 = \frac{d(\nu \circ f^{-1})}{d\nu}(z)$$

(31)

$$= \frac{d(\nu \circ f^{-1})}{d(\mu \circ f^{-1})}(z) \cdot \frac{d(\mu \circ f^{-1})}{d\mu}(z) \cdot \frac{d\mu}{d\nu}(z)$$

(32)

$$= \frac{d\nu}{d\mu}(f(z)) \cdot \frac{d(\mu \circ f^{-1})}{d\mu}(z) \cdot \frac{d\mu}{d\nu}(z) \text{ [Lemma A.2]}$$

(33)

$$= \frac{d\nu}{d\mu}(f(z)) \cdot \frac{d(\mu \circ f^{-1})}{d\mu}(z) \cdot \frac{1}{\frac{d\nu}{d\mu}(z)}$$

(34)

$$\left( \frac{d(\mu \circ f^{-1})}{d\mu}(z) \right)^{-1} = \frac{d\nu}{d\mu}(f(z)) \frac{d\mu}{d\nu}(z)$$

(35)

### A.3 Proof of stationarity for involution

Detailed balance of the the involution kernel with respect to the measure induced by $\pi$ implies:

$$\int_B \pi(z)k_z^x(A)\mu(dz) = \int_K \pi(z)k_z^x(B)\mu(dz) \quad \text{for all } K, B \in \Sigma$$

(36)

Stationarity with respect to $\pi$ follows by substituting $Z$ for $B$:

$$\int_Z \pi(z)k_z^x(A)\mu(dz) = \int_K \pi(z)k_z^x(Z)\mu(dz) = \int_K \pi(z)\mu(dz) \quad \text{for all } A \in \Sigma$$

(37)
A.4 Proof of stationarity for end-to-end kernel

We are given that the involution is stationary with respect to (the measure induced by) $\pi(x, u) := p(x)q_x(u)$:

$$
\int_Z k'_x(A) \pi(z) \mu(dz) = \int_K \pi(z) \mu(dz) \text{ for all } A \in \Sigma
$$

(39)

The end-to-end kernel is defined for all $x \in \mathcal{X}$ such that $p(x) > 0$ as:

$$
k_x(A) := \int_U k'_{x,u}(A \times U)q_x(u)\mu_U(du) \text{ for all } A \in \Sigma, x \in \mathcal{X}
$$

(40)

Stationarity of the end-to-end kernel with respect to the measure induced by $p$ is:

$$
\int_X k_x(A) p(x) \mu_P(dx) = \int_K p(x) \mu_P(dx) \text{ for all } A \in \Sigma
$$

(41)

Expanding:

$$
\int_X k_x(A) p(x) \mu_P(dx) = \int_X \left( \int_U k'_{x,u}(A \times U)q_x(u)\mu_Q(du) \right) p(x) \mu_P(dx)
$$

$$
= \int_{X \times U} k'_{x,u}(A \times U)q_x(u)p(x)\mu_P(dz)
$$

$$
= \int_Z k'_{x,u}((x', u') \in Z : x' \in A)\pi(z)\mu(dz)
$$

$$
= \int \{ (x, u) \in Z : x \in A \} q_x(u)p(x)\mu(dz)
$$

$$
= \int_X \{ (x, u) \in Z : x \in A \} q_x(u)\mu_Q(du) p(x)\mu_P(dx)
$$

$$
= \int_X p(x) \mu_P(dx)
$$



A.5 A Sufficient Condition for Involutive MCMC with Dictionaries

Our formulation of involutive MCMC requires the following technical condition to hold: $Z := \{(x, y) \in X \times Y : \pi(x, y) > 0\}$ is $\mu_P \times \mu_Q$-measurable. We now give a sufficient condition for this to hold, when $X$ and $Y$ are spaces of dictionaries. Let $D \subseteq K$ denote the subset of addresses that are discrete (i.e. where $V_k$ is a countable set and $\mu_k$ is the counting measure). For $x \in \times_{k \in Q} V_k$ let $x = (d, c)$ where $d \in \times_{k \in A \cap D} V_k$ and $c = \times_{k \in A \setminus D} V_k$, so that $d$ is the discrete part of $x$ and $c$ is the non-discrete part.

Lemma A.3. Suppose that $p$ and $q$ are such that $p(K,(d,c)) > 0$ implies $p(K,(d,c')) > 0$ for all $c' \in \prod_{k \in A \setminus D} V_k$, and that $q_x(K,(d,c)) > 0$ where $x = (A, d, c)$ implies that $q_{x'}(K,(d,c')) > 0$ for all $c' \in \prod_{k \in A \setminus D} V_k$ and all $x' = (A, d, c')$ where $c' \in \prod_{k \in A \setminus D} V_k$. Then, $Z := \{(x, y) \in X \times Y : \pi(x, y) > 0\}$ is $\mu \times \mu$-measurable where $\mu$ is the reference measure on traces.

Proof. For $p$ and $q$ satisfying these conditions, $Z = \cup_{(K_1,K_2,d_1,d_2) \in E} \{(K_1,(d_1,c_1)),(K_2,(d_2,c_2))) : c_1 \in \times_{k \in K_1 \setminus D} V_k, c_2 \in \times_{k \in K_2 \setminus D} V_k\}$ for some countable set $E \subseteq \{(K_1,K_2,d_1,d_2) : K_1, K_2 \subseteq K, |K_1| < \infty, |K_2| < \infty, d_1 \in \times_{k \in K_1 \setminus D} V_k, d_2 \in \times_{k \in K_2 \setminus D} V_k\}$ of address sets and discrete choice values for both programs. The measure of $Z$ is $\mu \times \mu(Z) = \sum_{(K_1,K_2,d_1,d_2) \in E} \prod_{k \in (K_1 \cup K_2) \setminus (K_1 \cup K_2)} \mu_k(V_k)$. □

When $p$ and $q$ are defined via probabilistic programs $P$ and $Q$ respectively, this requirement means that for both the model probabilistic program $P$ and the auxiliary probabilistic program $Q$, the support of a random choice that is not discrete cannot depend on the value of another non-discrete random choice. Additionally, the support of non-discrete random choices in $Q$ cannot depend on the value of non-discrete random choices in the input $x$, which is a trace of $P$. This requirement defines a notion well-behavedness for a probabilistic program $(P)$ and an additional notion of well-behavedness for a pair of probabilistic programs that are sequenced one after the other $(P$ and $Q)$. 
