

# Address-Based Semantics and Static Factorisation Analysis For Probabilistic Programs

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While probabilistic programming has been studied from a mathematical perspective for over 40 years, its formalisations often differ from the systems used in practice. In this work, we introduce address-based operational semantics for a formal probabilistic programming language (PPL). Our semantics more closely model the inner workings of PPLs which make use of user-defined sample addresses like Gen, Pyro, or PyMC. Furthermore, by translating a program to its control-flow-graph, we define a sound static analysis that approximates the dependency structure of random variables in the program. As a result, we obtain a factorization of the implicitly defined program density, which allows us to show the equivalence of programs to either Bayesian or Markov networks. Lastly, we demonstrate how this statically obtained dependency structure can be used to speed up posterior inference for probabilistic programs in a case study.

CCS Concepts: • **Theory of computation** → **Operational semantics; Program analysis**; • **Mathematics of computing** → *Bayesian computation; Bayesian networks; Markov networks*.

Additional Key Words and Phrases: Probabilistic programming, operational semantics, static program analysis, factorisation, Bayesian networks, Markov networks

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## 1 INTRODUCTION

Probabilistic programming provides an intuitive means to specify probabilistic models as programs. Typically, probabilistic programming systems enable automatic posterior inference for these programs. Besides these practical aspects, probabilistic programming has been examined from a mathematical perspective for over 40 years [Barthe et al. 2020; Kozen 1979]. However, there often is a gap between the formalisation of probabilistic programs and their practical implementation. Stan [Carpenter et al. 2017] is one of the few probabilistic programming languages (PPLs) that is formalised and widely used in real-world applications [Gorinova et al. 2019].

In this work, we present novel operational semantics for PPLs that make use of user-defined addresses in sample statements, like Gen [Cusumano-Towner et al. 2019], Turing [Ge et al. 2018], Pyro [Bingham et al. 2019], PyMC [Salvatier et al. 2016], or BeanMachine [Tehrani et al. 2020]. Below are examples of such address-based sample statements in several PPLs, where the address expressions are highlighted with red:

```
x = { :x => i } ~ Normal(0.,1)           # Gen
x = pyro.sample(f"x_{i}", Normal(0.,1.)) # Pyro
x = pymc.Normal(f"x_{i}", mu=0., sigma=1.) # PyMC
x = sample("x_"+str(i), Normal(0.,1.))   # our formal syntax
```

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Addresses are dynamically computed identifiers for random variables, which can be different from the name of the program variable they are assigned to.

We will interpret a probabilistic program as a function  $p$ , called program density, that maps a trace  $\text{tr}$  to its (unnormalised) density  $\in \mathbb{R}_{\geq 0}$ . In this context, a trace is simply a map from addresses to values, where we need not further specify how these values are set. In practice, the values are set depending on the used inference algorithm. For instance, for a Metropolis Hastings algorithm, one could sample these values from a proposal distribution [Wingate et al. 2011], whereas for the Hamiltonian Monte Carlo algorithm one would set these values by simulating a Hamiltonian physics system [Hoffman et al. 2014]. In variational inference methods, these values are perturbed by gradient ascent [Kucukelbir et al. 2017].

Having described the syntax and semantics of our formal PPL in Section 2, we will prove a factorisation of the program density. Namely, if a program contains  $K$  sample statements, then the program density can be written as a product of  $K$  terms:

$$p(\text{tr}) = \prod_{k=1}^K p_k(\text{tr}).$$

For each factor  $p_k$ , we can *statically* determine the set of addresses that contribute to it. If the program contains no loops and uses unique constant addresses for each sample statement, then the factorisation theorem implies that the program is equivalent to a Bayesian network. If the program contains loops, has dynamically computed addresses, or has non-unique addresses, then the program density still factorises into  $K$  terms. However, only an equivalence to the more general Markov networks can be shown. The reason is that we have to consider a potentially unbounded number of random variables and cyclic dependencies.

## 1.1 Overview

**Section 2. Address-Based Semantics For Probabilistic Programs** introduces our novel semantics for a formal probabilistic programming language. It is a generalisation of the operational semantics of Core Stan [Gorinova et al. 2019]. Instead of interpreting a program as a function over only a fixed set of finite variables, we extended this approach to interpret programs as functions over traces. Gorinova et al. injected the values of the random variables directly into the initial program state, whereas in our semantics the elements of the trace are used depending on dynamically evaluated addresses. Furthermore, our formal PPL and semantics support while loops.

**Section 3. Static Factorisation for Programs Without Loops** examines the factorisation of the program density for the simplified case where programs do not contain while loops.

In Section 3.2, we present a static provenance analysis that finds the dependencies of a program variable  $x$  at any program state  $\sigma$ . The dependencies are described by specifying at which addresses a trace needs to be known to also know the value of  $x$  in  $\sigma$ . This analysis forms the basis for finding the factorisation over addresses and operates on the control-flow-graph (CFG) of a program.

We formally describe the well-known correspondence between a program and its CFG. Mapping the operational semantics onto the CFG allows us to prove soundness of the provenance analysis in Section 3.2. This is achieved by constructing evaluation functions that map traces directly to the values of variables at program states. These functions require the traces to be only evaluated at the addresses the variable statically depends on. This constitutes the mathematical heavy lifting of this paper.

In Section 3.3, we prove the factorisation theorem for programs without loops by explicitly constructing the factors from the evaluation functions. In this section, we also discuss the equivalence of programs to either Bayesian or Markov networks.

**Section 4. Static Factorisation for Programs With Loops** presents a clever trick to generalise the factorisation result of Section 3 to programs that may contain while loops. The idea is to mathematically unroll while loops to obtain a directed acyclic graph with a countably infinite number of nodes that essentially represent all possible program paths. This *unrolled CFG* preserves the program semantics and allows us to effectively reuse the proofs of Section 3. Again, with the resulting factorisation, equivalence of programs to Markov networks can be shown.

**Section 5. Case Study: Speeding-Up Posterior Inference** demonstrates how the statically obtained factorisation of the program density can be used to decrease the runtime of a Metropolis Hastings inference algorithm for the probabilistic model at hand by a factor of 10.

## 2 ADDRESS-BASED SEMANTICS FOR PROBABILISTIC PROGRAMS

First, we introduce the syntax of our formal probabilistic programming language in terms of expressions and statements similar to [Gorinova et al. 2019] and [Hur et al. 2014].

### Syntax of Expressions:

$E ::=$	expression
$c$	constant
$x$	variable
$g(E_1, \dots, E_n)$	function call

### Syntax of Statements:

$S ::=$	statement
$x = E$	assignment
$S_1; S_2$	sequence
if $E$ then $S_1$ else $S_2$	if statement
skip	skip
while $E$ do $S$	while loop

$x = \text{sample}(E_0, f(E_1, \dots, E_n))$     sample

We assume that the constants of this language range over a set of values including booleans, integers, real numbers, and strings. However, for our purposes it is not necessary to characterise this set in detail and we define  $\mathcal{V}$  to be the set of all values. A program contains a finite set of program variables denoted by  $x$  or  $x_i$ . We further assume a set of built-in functions  $g$ . The only non-standard construct in the language are sample statements. For sample statements, the expression  $E_0$  corresponds to the user-defined sample address, which is assumed to evaluate to a string. The symbol  $f$  ranges over a set of built-in distributions which are parameterised by arguments  $E_1, \dots, E_n$ .

### 2.1 Operational Semantics

The meaning of a program is the density implicitly defined by its sample statements. This density is evaluated for *program trace* and returns a real number. A program trace is a (partial) mapping from addresses to values,  $\text{tr}: \text{Strings} \rightarrow \mathcal{V}$ . How the value at an address is determined is not important for this work and in practice it typically depends on the algorithm that is used to perform posterior inference for the program. We denote the set of all traces with  $\mathcal{T}$ .

For each trace  $\text{tr}$ , the operational semantics of our language are defined by the big-step relation  $(\sigma, S) \Downarrow^{\text{tr}} \sigma'$ , where  $S$  is a statement and  $\sigma \in \Sigma$  is a program state – a finite map from program variables to values

$$\sigma ::= x_1 \mapsto V_1, \dots, x_n \mapsto V_n, \quad x_i \text{ distinct, } V_i \in \mathcal{V}.$$

A state can be naturally lifted to a map from expressions to values  $\sigma: \text{Exprs} \rightarrow \mathcal{V}$ :

$$\sigma(x_i) = V_i, \quad \sigma(c) = c, \quad \sigma(g(E_1, \dots, E_n)) = g(\sigma(E_1), \dots, \sigma(E_n)).$$

The operational semantics for the non-probabilistic part of our language are standard:

$$\begin{array}{c}
\frac{}{(\sigma, x = E) \Downarrow^{\text{tr}} \sigma[x \mapsto \sigma(E)]} \quad \frac{(\sigma, S_1) \Downarrow^{\text{tr}} \sigma' \quad (\sigma', S_2) \Downarrow^{\text{tr}} \sigma''}{(\sigma, S_1; S_2) \Downarrow^{\text{tr}} \sigma''} \\
\\
\frac{\sigma(E) = \text{true} \quad (\sigma, S_1) \Downarrow^{\text{tr}} \sigma'}{(\sigma, \text{if } E \text{ then } S_1 \text{ else } S_2) \Downarrow^{\text{tr}} \sigma'} \quad \frac{\sigma(E) = \text{false} \quad (\sigma, S_2) \Downarrow^{\text{tr}} \sigma'}{(\sigma, \text{if } E \text{ then } S_1 \text{ else } S_2) \Downarrow^{\text{tr}} \sigma'} \\
\\
\frac{\sigma(E) = \text{false}}{(\sigma, \text{while } E \text{ do } S) \Downarrow^{\text{tr}} \sigma} \quad \frac{\sigma(E) = \text{true} \quad (\sigma, (S; \text{while } E \text{ do } S)) \Downarrow^{\text{tr}} \sigma'}{(\sigma, \text{while } E \text{ do } S) \Downarrow^{\text{tr}} \sigma'}
\end{array}$$

Above,  $\sigma[x \mapsto V]$  denotes the updated program state  $\sigma'$ , where  $\sigma'(x) = V$  and  $\sigma'(y) = \sigma(y)$  for all other variables  $y \neq x$ .

At sample statements, we inject the value of the trace at address  $V_0$ . We multiply the density, represented by the reserved variable  $\mathbf{p}$ , with the value of function  $\text{pdf}_f$  evaluated at  $\text{tr}(V_0)$ . Note that the function  $\text{pdf}_f$  may be an arbitrary function to real values. However, in the context of probabilistic programming it can be interpreted as the density function of distribution  $f$ . Lastly, the value  $\text{tr}(V_0)$  is stored in the program state at variable  $x$ . The semantics of sample statements are summarised in the following rule:

$$\frac{\forall i: \sigma(E_i) = V_i \quad V_0 \in \mathbf{Strings} \quad V = \text{tr}(V_0)}{(\sigma, x = \text{sample}(E_0, f(E_1, \dots, E_n))) \Downarrow^{\text{tr}} \sigma[x \mapsto V, \mathbf{p} \mapsto \sigma(\mathbf{p}) \times \text{pdf}_f(V; V_1, \dots, V_n)]}$$

Finally, the meaning of a program  $S$  is defined as the mapping of trace to density. This definition is well-defined, because the semantics are deterministic for each trace.

DEFINITION 1. *The meaning of a program  $S$  is a function  $p_S: \mathcal{T} \rightarrow \mathbb{R}_{\geq 0}$  given by*

$$p_S(\text{tr}) := \begin{cases} \sigma(\mathbf{p}) & \text{if } \exists \sigma: ((x_i \mapsto \text{null}, \mathbf{p} \mapsto 1), S) \Downarrow^{\text{tr}} \sigma \\ \text{undefined} & \text{otherwise} \end{cases}$$

Listing 1. Simple probabilistic program with stochastic branching.

```

p = sample("p", Uniform(0,1))
x = sample("x", Bernoulli(p))
if x == 1 then
  y = sample("y", Bernoulli(0.25))
else
  z = sample("z", Bernoulli(0.75))

```

Consider the simple probabilistic program in Listing 1. The density defined by our operational semantics is given below, where  $\delta_v$  denotes the delta function whose value is 1 if  $v$  equals true and 0 otherwise.

$$\begin{aligned}
p(\text{tr}) = & \text{pdf}_{\text{Uniform}}(\text{tr}(\text{"p"}); 0, 1) \\
& \times \text{pdf}_{\text{Bernoulli}}(\text{tr}(\text{"x"}); \text{tr}(\text{"p"})) \\
& \times (\delta_{\text{tr}(\text{"x"})} \text{pdf}_{\text{Bernoulli}}(\text{tr}(\text{"y"}); 0.25) + (1 - \delta_{\text{tr}(\text{"x"})})) \\
& \times (\delta_{\text{tr}(\text{"x"})} + (1 - \delta_{\text{tr}(\text{"x"})}) \text{pdf}_{\text{Bernoulli}}(\text{tr}(\text{"z"}); 0.75)).
\end{aligned}$$

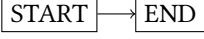
### 3 STATIC FACTORISATION FOR PROGRAMS WITHOUT LOOPS

#### 3.1 Control-Flow-Graph

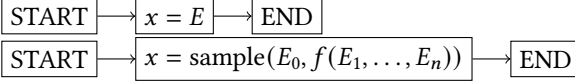
The goal of this work is to statically find a factorisation of the density implicitly defined by a probabilistic program in terms of addresses. This static analysis will operate on the control-flow-graph (CFG) of a program. We begin by considering programs without loops first and describe how we can formally translate such a program to its corresponding CFG. We will equip this CFG with semantics equivalent to the operational semantics of the original program.

A CFG has five types of nodes: start, end, assign, branch, and join nodes. Branch nodes have two successor nodes, end nodes have no successor, all other nodes have one. The CFG contains exactly one start node from which every other node is reachable. Further, it contains exactly one end node that is reachable from any other node. We describe the recursive translation rules for program  $S$  both mathematically and as diagrams. Sub-graphs are drawn by circular nodes, branch and join nodes are drawn as diamond nodes, and assign, start, and end nodes have rectangular shape.

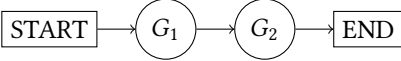
- The CFG of a skip-statement,  $S = \text{skip}$ , consists of only start and end node.



- The CFG of an assignment,  $x = E$ , or sample statement  $x = \text{sample}(E_0, f(E_1, \dots, E_n))$ , is a sequence of start, assign, and end node:



- The CFG for a sequence of statements,  $S = S_1; S_2$ , is recursively defined by the CFGs  $G_1$  and  $G_2$  of  $S_1$  and  $S_2$  respectively.

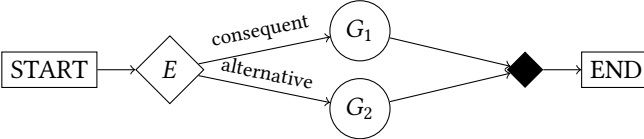


The resulting CFG can be written as  $G = (G_1 \cup G_2) \setminus \{N_{\text{end}}^1, N_{\text{start}}^2\}$ , with

$$N_{\text{start}} = N_{\text{start}}^1, \quad N_{\text{end}} = N_{\text{end}}^2, \quad \text{predecessor}(N_{\text{end}}^1) \rightarrow \text{successor}(N_{\text{start}}^2),$$

where  $N_{\text{start}}^i$  is the start node of  $G_i$  and  $N_{\text{end}}^i$  is the end node of  $G_i$ .

- The CFG of an if statement,  $S = (\text{if } E \text{ then } S_1 \text{ else } S_2)$ , is also defined in terms of the CFGs of  $S_1$  and  $S_2$



The resulting CFG can be written as

$$G = G_1 \setminus \{N_{\text{start}}^1, N_{\text{end}}^1\} \cup G_2 \setminus \{N_{\text{start}}^2, N_{\text{end}}^2\} \cup \{N_{\text{start}}, N_{\text{end}}, N_{\text{branch}}, N_{\text{join}}\}, \text{ where}$$

$$N_{\text{branch}} = \text{Branch}(E), \quad N_{\text{start}} \rightarrow N_{\text{branch}}, \quad N_{\text{join}} \rightarrow N_{\text{end}},$$

$$N_{\text{branch}} \rightarrow \text{successor}(N_{\text{start}}^1) =: \text{consequent}(N_{\text{branch}}),$$

$$N_{\text{branch}} \rightarrow \text{successor}(N_{\text{start}}^2) =: \text{alternative}(N_{\text{branch}}),$$

$$\text{predcons}(N_{\text{join}}) := \text{predecessor}(N_{\text{end}}^1) \rightarrow N_{\text{join}},$$

$$\text{predalt}(N_{\text{join}}) := \text{predecessor}(N_{\text{end}}^2) \rightarrow N_{\text{join}}.$$

We say the tuple  $(N_{\text{branch}}, N_{\text{join}}) \in \text{BranchJoin}(G)$  is a branch-join pair.

**3.1.1 CFG Semantics.** For a control-flow-graph  $G$  we define the small-step semantics for a trace  $\text{tr}$  as a relation that models the transition from node to node depending on the current program state:

$$(\sigma, N) \xrightarrow{\text{tr}} (\sigma', N')$$

The semantics for the CFG of program  $S$  are set-up precisely such that they are equivalent to the operational semantics of program  $S$ . The transition rules depending on node type and program state are given below:

$$\begin{array}{c} \frac{N = \text{START} \quad N' = \text{successor}(N)}{(\sigma, N) \xrightarrow{\text{tr}} (\sigma, N')} \quad \frac{N = \text{Assign}(x = E) \quad N' = \text{successor}(N)}{(\sigma, N) \xrightarrow{\text{tr}} (\sigma[x \mapsto \sigma(E)], N')} \\[10pt] \frac{N = \text{Join} \quad N' = \text{successor}(N)}{(\sigma, N) \xrightarrow{\text{tr}} (\sigma, N')} \quad \frac{N = \text{Branch}(E) \quad \sigma(E) = \text{true}}{(\sigma, N) \xrightarrow{\text{tr}} (\sigma, \text{consequent}(N))} \quad \frac{N = \text{Branch}(E) \quad \sigma(E) = \text{false}}{(\sigma, N) \xrightarrow{\text{tr}} (\sigma, \text{alternative}(N))} \\[10pt] \frac{N = \text{Assign}(x = \text{sample}(E_0, f(E_1, \dots, E_n))) \quad \sigma(E_i) = V_i \quad V_0 \in \mathbf{Strings} \quad N' = \text{successor}(N)}{(\sigma, N) \xrightarrow{\text{tr}} (\sigma[x \mapsto V, \mathbf{p} \mapsto \sigma(\mathbf{p}) \times \text{pdf}_f(V; V_1, \dots, V_n)], N')} \end{array}$$

Finally, the meaning of a CFG is a mapping from trace to density. It is defined for traces  $\text{tr}$  if there exists a path of node transitions from start to end node.

**DEFINITION 2.** Let  $\sigma_0 = (x_i \mapsto \text{null}, \mathbf{p} \mapsto 1)$  be the initial program state. The semantics of a CFG  $G$  is the function  $p_G: \mathcal{T} \rightarrow \mathbb{R}_{\geq 0}$  given by

$$p_G(\text{tr}) := \begin{cases} \sigma(\mathbf{p}) & \text{if } \exists \sigma, \sigma_i, N_i: \\ & (\sigma_0, \text{START}) \xrightarrow{\text{tr}} \dots \xrightarrow{\text{tr}} (\sigma_i, N_i) \xrightarrow{\text{tr}} \dots \xrightarrow{\text{tr}} (\sigma, \text{END}) \\ \text{undefined} & \text{otherwise} \end{cases}$$

**PROPOSITION 1.** For all programs  $S$  without while loops and corresponding control-flow-graph  $G$ , it holds that for all traces  $\text{tr}$

$$p_S(\text{tr}) = p_G(\text{tr}).$$

**PROOF.** See Appendix A.1. □

## 3.2 Static Provenance Analysis

The provenance of variable  $x$  in CFG node  $N$  are all the addresses  $\subseteq \mathbf{Strings}$  that contribute to the computation of its value in node  $N$ . In this section, we define an algorithm that operates on the CFG, which statically determines the provenance for any variable  $x$  at any node  $N$ . As this is a static algorithm it is an over-approximation of the true provenance. In Section 3.2.1, we will prove soundness of the presented algorithm, i.e., we show that indeed the value of variable  $x$  at node  $N$  can be computed from the values in the trace  $\text{tr}$  at the addresses which make up the provenance. But first, we introduce some useful concepts which are similar to definitions found in data-flow analysis [Cooper and Torczon 2011; Hennessy and Patterson 2011].

**DEFINITION 3.** For a CFG  $G$ , let  $\text{AssignNodes}(G, x)$  be all nodes  $N'$  in  $G$  that assign variable  $x$ ,  $N' = \text{Assign}(x = \dots)$ . The set of reaching definitions for variable  $x$  in node  $N$  are defined as

$$\text{RD}(N, x) = \{N' \in \text{AssignNodes}(G, x) : \exists \text{path}(N', \dots, N_i, \dots, N), N_i \notin \text{AssignNodes}(G, x)\}.$$

Intuitively, the set of reaching definitions are all nodes that could have written the value of  $x$  in the program state before executing node  $N$ .

DEFINITION 4. For CFG  $G$  and node  $N$  the set of branch parents is defined as

$$BP(N) = \{B : (B, J) \in \text{BranchJoin}(G) \wedge \exists \text{ path } (B, \dots, N, \dots, J)\}.$$

A branch node  $B$  and join node  $J$  are a branch-join pair  $(B, J) \in \text{BranchJoin}(G)$  if they belong to the same if-statement (see the translation rule for if-statements to CFGs).

The set of branch parents are all parent branch nodes of  $N$  that determine if the program branch of  $N$  is executed. Lastly, we need the set of all strings that the address expression of a sample statement may evaluate to.

DEFINITION 5. For a sample CFG node  $N = \text{Assign}(x = \text{sample}(E_0, f(E_1, \dots, E_n)))$ , we define the set of all possible addresses as

$$\text{addresses}(N) = \{\sigma(E_0) : \sigma \in \Sigma\} \subseteq \text{Strings}.$$

Now we are able to define the algorithm to statically approximate the provenance of any variable  $x$  at any node  $N$  denoted by  $\text{prov}(N, x)$  in Algorithm 1. In the algorithm we use  $\text{vars}(E)$ , which is defined as the set of all program variables in expression  $E$ . It is often useful to determine the provenance of an entire expression instead of only a single variable. For expressions  $E$ , we lift the definition of  $\text{prov}$

$$\text{prov}(N, E) = \bigcup_{y \in \text{vars}(E)} \text{prov}(N, y).$$

---

**Algorithm 1** Computing the provenance set  $\text{prov}(N, x)$  statically from the CFG.

---

**Input** CFG node  $N$ , variable  $x$

$\text{prov} \leftarrow \text{EmptySet}()$

$\text{queue} \leftarrow [(N, x)]$

**while**  $\text{queue.is\_not\_empty}()$  **do**

$(N, x) \leftarrow \text{queue.pop}()$

**for**  $N' \in \text{RD}(N, x)$  **do**

**if**  $N' = \text{Assign}(x = \text{sample}(E_0, f(E_1, \dots, E_n)))$  **then**

$\text{prov} \leftarrow \text{prov} \cup \text{addresses}(N')$

$E' \leftarrow E$

**else if**  $N' = \text{Assign}(x = E)$  **then**

$E' \leftarrow E_0$

**for**  $y \in \text{vars}(E')$  **do**

**if**  $\text{is\_unmarked}((N', y))$  **then**

$\text{mark}((N', y))$

$\text{queue.push}((N', y))$

**for**  $N_{bp} \in \text{BP}(N')$  **do**

**for**  $y \in \text{vars}(E_{N_{bp}})$  **do**

**if**  $\text{is\_unmarked}((N_{bp}, y))$  **then**

$\text{mark}((N_{bp}, y))$

$\text{queue.push}((N_{bp}, y))$

$\triangleright N_{bp} = \text{Branch}(E_{N_{bp}})$

**return**  $\text{prov}$

---

The algorithm works as follows. If we want to find  $\text{prov}(N, x)$ , we first have to find all reaching definitions for  $x$ . If the reaching definition  $N'$  is a sample node,  $x = \text{sample}(E_0, \dots)$ , then the value of  $x$  can only depend on the addresses generated by  $E_0$ ,  $\text{addresses}(N')$ , and the provenance of  $E_0$ . If  $N'$  is an assignment node  $x = E$ , we have to recursively find the provenance of the expression  $E$ . Lastly, there can be multiple reaching definitions for  $x$  in different branches and the value of  $x$  also depends on the branching condition. Thus, we also find all branch parents and recursively determine their provenance and add it to the final result.

In practice the potentially infinite set  $\text{addresses}(N)$  can be represented by the CFG node  $N$  itself. An implementation of Algorithm 1 would return a set of CFG sample nodes rather than a potentially infinite set of strings.

```

b = sample("b", Bernoulli(0.5))
s = sample("s", InverseGamma(1., 1.))
if b == 1 then
    m = sample("mu", Normal(0., 1.))
else
    m = 1
x = sample("x", Normal(m, s))

N = Assign(x = ...)

V_s^N(tr) = tr("s")
V_m^N(tr) = δ_{tr("b")} · tr("mu") + (1 - δ_{tr("b")}) · 1

```

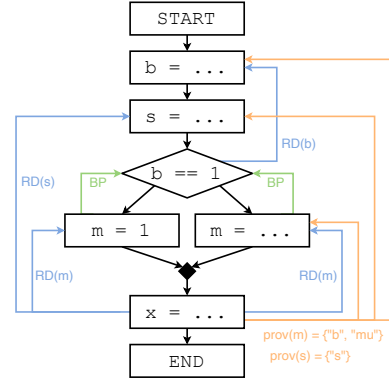


Fig. 1. Reaching definitions, branch parents, and the provenance set for a simple example. The evaluation functions introduced in Section 3.2.1 are also given for node  $N$ .

We get a clearer sense of the introduced definitions and Algorithm 1. by considering a simple program in Fig. 1. On the right you can see examples for reaching definitions and branch parents for several nodes drawn as arrows. These arrows illustrate how Algorithm 1 computes the provenance of variables  $m$  and  $s$  at the sample node for  $x$ . Note that if we were to change the if statement to `(if (b == 1) then (m = 1) else (m = 1))`, then the provenance calculation would be unchanged. This illustrates that the presented algorithm can only over-approximate the provenance and not compute it exactly.

Lastly, we list properties of the provenance set that will become useful in subsequent proofs.

LEMMA 1. *prov has following properties:*

- For all nodes  $N, N'$ , and variable  $x$  it holds that

$$\text{RD}(N, x) = \text{RD}(N', x) \implies \text{prov}(N, x) = \text{prov}(N', x). \quad (1)$$

- If  $N' \in \text{RD}(N, x)$  is an assignment node,  $N' = \text{Assign}(x = E)$ , then

$$\text{prov}(N', E) = \bigcup_{y \in \text{vars}(E)} \text{prov}(N', y) \subseteq \text{prov}(N, x). \quad (2)$$

- if  $N' \in \text{RD}(N, x)$  is a sample node,  $N' = \text{Assign}(x = \text{sample}(E_0, \dots))$ , then

$$\text{prov}(N', E_0) \subseteq \text{prov}(N, x) \quad \text{and} \quad \text{addresses}(N') \subseteq \text{prov}(N, x). \quad (3)$$



- For all  $N' \in \text{RD}(N, x)$  it holds that for all branch parents  $N_{bp} = \text{Branch}(E_{N_{bp}}) \in \text{BP}(N')$  we have  $\text{prov}(N_{bp}, E_{N_{bp}}) \subseteq \text{prov}(N, x)$  and

$$\begin{aligned} \bigcup_{N_{bp} \in \text{BP}(N')} \text{prov}(N_{bp}, E_{N_{bp}}) = \\ \bigcup_{N_{bp} \in \text{BP}(N')} \bigcup_{y \in \text{vars}(E_{N_{bp}})} \text{prov}(N_{bp}, y) \subseteq \text{prov}(N, x). \end{aligned} \quad (4)$$

PROOF. If  $(N', y)$  is pushed into the queue, then  $\text{prov}(N', y) \subseteq \text{prov}(N, x)$  as the algorithm for computing  $\text{prov}(N', y)$  starts with only  $(N', y)$  in the queue. With this fact the properties follow directly from the definition of the algorithm.  $\square$

**3.2.1 Soundness.** Recall that the purpose of finding the provenance of variable  $x$  at node  $N$  is to determine which addresses contribute to the computation of its value. To prove that Algorithm 1 indeed finds the correct set of addresses, first, we have to precisely defined what we mean that a set of addresses contribute to the computation. Suppose that there is a function  $f$  that maps a trace  $\text{tr}$  to a value  $v$ . The set of addresses  $A$  contribute to the computation of value  $v$ , if any other trace  $\text{tr}'$  that has the same values as  $\text{tr}$  for all addresses  $\alpha \in A$ , gets mapped to the same value  $f(\text{tr}') = v$ . In other words, if we change the trace  $\text{tr}$  at an address  $\beta \in \text{Strings} \setminus A$ , the value of  $f(\text{tr})$  remains unchanged. Or equivalently, if  $f(\text{tr}) \neq f(\text{tr}')$ , then there must be an address  $\alpha \in A$  such that  $\text{tr}(\alpha) \neq \text{tr}'(\alpha)$ .

DEFINITION 6. For a function from traces to an arbitrary set  $B$ ,  $f : \mathcal{T} \rightarrow B$ , we write  $f \in [\mathcal{T}|_A \rightarrow B]$ , if and only if

$$\forall \alpha \in A : \text{tr}(\alpha) = \text{tr}'(\alpha) \implies f(\text{tr}) = f(\text{tr}').$$

That is, changing the values of  $\text{tr}$  at addresses  $\beta \in \text{Strings} \setminus A$  does not change the value  $f(\text{tr})$ .

The next lemma states that we can always over-approximate the set of addresses that contribute to the computation of the values  $f(\text{tr})$ .

LEMMA 2. If  $A \subseteq A'$  and  $f \in [\mathcal{T}|_A \rightarrow B]$ , then  $f \in [\mathcal{T}|_{A'} \rightarrow B]$ . Thus

$$A \subseteq A' \implies [\mathcal{T}|_A \rightarrow B] \subseteq [\mathcal{T}|_{A'} \rightarrow B]. \quad (5)$$

PROOF. Let  $f \in [\mathcal{T}|_A \rightarrow B]$ . Assume  $\forall \alpha \in A' : \text{tr}(\alpha) = \text{tr}'(\alpha)$ . In particular, this holds for the smaller set  $A$ ,  $\forall \alpha \in A : \text{tr}(\alpha) = \text{tr}'(\alpha)$ , which implies  $f(\text{tr}) = f(\text{tr}')$ . Thus,  $f \in [\mathcal{T}|_{A'} \rightarrow B]$ .  $\square$

If we combine two functions with provenance  $A_1$  and  $A_2$  respectively, then the resulting function has provenance  $A_1 \cup A_2$ . This is shown in the following lemma.

LEMMA 3. Let  $f_1 \in [\mathcal{T}|_{A_1} \rightarrow B_1]$ ,  $f_2 \in [\mathcal{T}|_{A_2} \rightarrow B_2]$ ,  $h : B_1 \times B_2 \rightarrow C$ . Then

$$\text{tr} \mapsto h(f_1(\text{tr}), f_2(\text{tr})) \in [\mathcal{T}|_{A_1 \cup A_2} \rightarrow C].$$

PROOF. Assume  $\forall \alpha \in A_1 \cup A_2 : \text{tr}(\alpha) = \text{tr}'(\alpha)$ . Thus,  $f_i(\text{tr}) = f_i(\text{tr}')$  and  $h(\text{tr}) = h(\text{tr}')$ .  $\square$

This brings us to the main soundness proof of Algorithm 1. Proposition 2 states that we can equip each CFG node  $N$  with evaluation functions that depend on the addresses determined by  $\text{prov}$  in the sense of Definition 6. The evaluation functions directly map the trace  $\text{tr}$  to the values of variables at node  $N$  such that the values agree with the small-step CFG semantics relation  $\xrightarrow{\text{tr}}$ . Importantly, while the operational semantics are defined for each individual trace, the evaluation functions work for all traces. In Fig. 1, you can see concrete examples of these evaluation functions for a simple program.

PROPOSITION 2. For each node  $N$  in the CFG  $G$  and variable  $x$ , there exists an evaluation function

$$V_x^N \in [\mathcal{T}|_{\text{prov}(N,x)} \rightarrow \mathcal{V}],$$

such that for all traces  $\text{tr}$  with  $\sigma_0 = (x_i \mapsto \text{null}, \mathbf{p} \mapsto 1)$  and execution sequence

$$(\sigma_0, \text{START}) \xrightarrow{\text{tr}} \dots \xrightarrow{\text{tr}} (\sigma_i, N_i) \xrightarrow{\text{tr}} \dots \xrightarrow{\text{tr}} (\sigma_l, \text{END})$$

we have

$$\sigma_i(x) = V_x^{N_i}(\text{tr}).$$

Intuitively,  $V_x^N$  computes the value of  $x$  before executing  $N$ . These evaluation functions  $V_x^N$  can be lifted to evaluation functions for expressions  $V_E^N$ :

$$V_c^N(\text{tr}) = c, \quad V_{g(E_1, \dots, E_n)}^N(\text{tr}) = g(V_{E_1}^N(\text{tr}), \dots, V_{E_n}^N(\text{tr})).$$

By Lemma 3, if  $V_y^N \in [\mathcal{T}|_{\text{prov}(N,y)} \rightarrow \mathcal{V}]$  for all  $y \in \text{vars}(E)$ , then  $V_E^N \in [\mathcal{T}|_{\text{prov}(N,E)} \rightarrow \mathcal{V}]$ .

PROOF.

**Step 1. Defining  $V_x^N$  and proving  $V_x^N \in [\mathcal{T}|_{\text{prov}(N,x)} \rightarrow \mathcal{V}]$ .**

We begin by defining  $V_x^N$  inductively by noting that every node  $N \neq \text{START}$  has exactly one predecessor except for join nodes which have two predecessors. Further, the CFG  $G$  is a directed acyclic graph with a single root node which makes mathematical induction possible.

**Base case.** For  $((x_i \mapsto \text{null}, \mathbf{p} \mapsto 1), \text{START})$ , let  $V_{\mathbf{p}}^{\text{START}}(\text{tr}) = 1$  and  $V_x^{\text{START}}(\text{tr}) = \text{null}$  for all variables  $x$ . We have  $V_x^{\text{START}} \in [\mathcal{T}|_{\emptyset} \rightarrow \mathcal{V}]$ .

**Induction step.**

**Case 1.** Let  $N$  be a node with single predecessor  $N'$  ( $N$  is not a join node). We define  $V_x^N$  based on the node type of  $N'$ , for which we make the induction assumption that the evaluation functions  $V_x^{N'} \in [\mathcal{T}|_{\text{prov}(N',x)} \rightarrow \mathcal{V}]$  exist for all variables.

- **Case 1.1.**  $N'$  is an assignment node,  $N' = \text{Assign}(x = E)$ . Define

$$V_y^N(\text{tr}) = \begin{cases} V_E^{N'}(\text{tr}) & \text{if } x = y \\ V_y^{N'}(\text{tr}) & \text{otherwise.} \end{cases}$$

By assumption  $V_y^{N'} \in [\mathcal{T}|_{\text{prov}(N',y)} \rightarrow \mathcal{V}]$  for all  $y$  and thus,  $V_E^{N'} \in [\mathcal{T}|_{\text{prov}(N',E)} \rightarrow \mathcal{V}]$ .

For  $y \neq x$ ,  $\text{RD}(N, y) = \text{RD}(N', y)$  and by Eq. (1) we have  $\text{prov}(N, y) = \text{prov}(N', y)$ , implying that  $V_y^N \in [\mathcal{T}|_{\text{prov}(N,y)} \rightarrow \mathcal{V}]$ .

For  $x$ ,  $N' \in \text{RD}(N, x)$  since  $N'$  is the single predecessor of  $N$  and assigns  $x$ . By Eq. (2)  $\text{prov}(N', E) \subseteq \text{prov}(N, x)$ , and by Eq. (5)

$$V_x^N = V_E^{N'} \in [\mathcal{T}|_{\text{prov}(N',E)} \rightarrow \mathcal{V}] \subseteq [\mathcal{T}|_{\text{prov}(N,x)} \rightarrow \mathcal{V}].$$

- **Case 1.2.**  $N'$  is a sample node,  $N' = \text{Assign}(x = \text{sample}(E_0, f(E_1, \dots, E_n)))$ . Define

$$V_y^N(\text{tr}) = \begin{cases} \text{tr}(V_{E_0}^{N'}(\text{tr})) & \text{if } x = y \\ V_y^{N'}(\text{tr}) & \text{otherwise.} \end{cases}$$

As before, for  $x \neq y$ ,  $V_y^N \in [\mathcal{T}|_{\text{prov}(N,y)} \rightarrow \mathcal{V}]$ .

For  $x$ , by definition  $V_{E_0}^{N'}(\text{tr}) \in \text{addresses}(N')$ . Since  $N' \in \text{RD}(N, x)$  it follows from Eq. (3) that  $\text{addresses}(N') \subseteq \text{prov}(N, x)$  and by Eq. (3)  $\text{prov}(N', E_0) \subseteq \text{prov}(N, x)$ . Lastly, by Eq. (5)

$$V_x^N \in [\mathcal{T}|_{\text{addresses}(N') \cup \text{prov}(N', E_0)} \rightarrow \mathcal{V}] \subseteq [\mathcal{T}|_{\text{prov}(N,x)} \rightarrow \mathcal{V}].$$

- **Case 1.3.**  $N'$  is a branch or join node. Define  $V_y^N = V_y^{N'}$  for all variables  $y$ .

**Case 2.** Let  $J$  be a join node with two predecessor nodes,  $N'_1 = \text{predcons}(N)$ ,  $N'_2 = \text{predalt}(N)$ . Let  $B = \text{Branch}(E)$  be the corresponding branching node,  $(B, J) \in \text{BranchJoin}(G)$ .

For each variable  $x$ , there are two cases:

- (1) There exists a reaching definition  $N' \in \text{RD}(J, x)$  on a path  $(B, \dots, N', \dots, J)$ . Define  $V_x^1$  and  $V_x^2$  depending on the node type of  $N'_1$  and  $N'_2$  as above. The functions  $V_x^i$  compute the value of  $x$  after executing  $N'_i$ . Similar to before one can see that  $V_x^i \in [\mathcal{T}|_{\text{prov}(J, x)} \rightarrow \mathcal{V}]$ . Let

$$V_x^J(\text{tr}) := \delta_{V_E^B(\text{tr})} V_x^1(\text{tr}) + (1 - \delta_{V_E^B(\text{tr})}) V_x^2(\text{tr}).$$

Since  $B \in \text{BP}(N')$ , by Eq. (4)  $\text{prov}(B, E) \subseteq \text{prov}(N, x)$  and thus  $V_x^J \in [\mathcal{T}|_{\text{prov}(J, x)} \rightarrow \mathcal{V}]$ .

- (2) All reaching definitions of  $x$  (if there are any) are predecessors of  $B$ . Then,  $\text{RD}(J, x) = \text{RD}(B, x)$  and by Eq. (1)  $\text{prov}(J, x) = \text{prov}(B, x)$ . Define  $V_x^J := V_x^B$ .

**Step 2: Proving that  $\sigma_i(x) = V_x^{N_i}(\text{tr})$ .**

Having defined the evaluation functions, we now have to prove that they indeed compute the correct values. For trace  $\text{tr}$  let the corresponding execution sequence be

$$(\sigma_0, \text{START}) \xrightarrow{\text{tr}} \dots \xrightarrow{\text{tr}} (\sigma_i, N_i) \xrightarrow{\text{tr}} \dots \xrightarrow{\text{tr}} (\sigma_l, \text{END}).$$

We will prove that  $\sigma_i(x) = V_x^{N_i}(\text{tr})$  by induction.

**Base case.** The base case immediately follows from the definition  $\sigma_0(x) = V_x^{\text{START}}(\text{tr})$ .

**Induction step.** For transition  $(\sigma_i, N_i) \xrightarrow{\text{tr}} (\sigma_{i+1}, N_{i+1})$  the assumption is that  $\sigma_j(x) = V_x^{N_j}(\text{tr})$  holds for all variables  $x$  and  $j \leq i$ .

If  $N_{i+1}$  is not a join node, then  $\sigma_{i+1}(x) = V_x^{N_{i+1}}(\text{tr})$  follows directly from the CFG semantics and definition of  $V_x^{N_{i+1}}$  in case 1 of step 1.

Lastly, we consider the case when  $N_{i+1}$  is a join node with branching node  $N_j = \text{Branch}(E)$ ,  $(N_j, N_{i+1}) \in \text{BranchJoin}(G)$ ,  $j \leq i$ . Let  $N'_1 = \text{predcons}(N_{i+1})$ ,  $N'_2 = \text{predalt}(N_{i+1})$ .

By the semantics of if statements,  $V_E^B(\text{tr}) = \text{true}$  iff  $N_i = N'_1$  and  $V_E^B(\text{tr}) = \text{false}$  iff  $N_i = N'_2$ . If there is a node  $N'$  between  $N_j$  and  $N_{i+1}$  in the execution sequence that assigns  $x$ ,  $N' \in \text{RD}(N_{i+1}, x)$ , then by definitions of  $V_x^1$ ,  $V_x^2$ , and  $V_x^{N_{i+1}}$  we have

$$\sigma_{i+1}(x) = \delta_{V_E^B(\text{tr})} V_x^1(\text{tr}) + (1 - \delta_{V_E^B(\text{tr})}) V_x^2(\text{tr}) = V_x^{N_{i+1}}(\text{tr}).$$

If there is no such  $N'$ , then

$$\sigma_{i+1}(x) = \sigma_j(x) = V_x^{N_j}(\text{tr}) = V_x^{N_{i+1}}(\text{tr}).$$

□

### 3.3 Static Factorisation Theorem for Programs Without Loops

With Proposition 2, we can prove the first factorisation theorem by combining the evaluation functions  $V_x^N$  to express the program density  $p$  in a factorised form.

**THEOREM 1.** Let  $G$  be the CFG for a program  $S$  without while loop statements. Let  $N_1, \dots, N_K$  be all sample nodes in  $G$ . For each sample node  $N_k = \text{Assign}(x = \text{sample}(E_0, f(E_1, \dots, E_n)))$ , let

$$A_k = \text{addresses}(N_k) \cup \bigcup_{i=0}^n \text{prov}(N_k, E_i) \cup \bigcup_{N' \in \text{BP}(N_k)} \text{prov}(N', E_{N'}).$$

Then, there exist functions  $p_k \in [\mathcal{T}|_{A_k} \rightarrow \mathbb{R}_{\geq 0}]$  such that if  $p_S(\text{tr}) \neq \text{undefined}$ , then

$$p_S(\text{tr}) = p_G(\text{tr}) = \prod_{k=1}^K p_k(\text{tr}).$$

PROOF. For each sample node  $N_k$ , define  $b_k(\text{tr}) := \prod_{N' \in \text{BP}(N_k)} V_{E_{N'}}^{N'}(\text{tr})$  where

$$b_k \in [\mathcal{T} | \bigcup_{N' \in \text{BP}(N_k)} \text{prov}(N', E_{N'}) \rightarrow \{\text{true}, \text{false}\}].$$

Above,  $V_{E_{N'}}^{N'}(\text{tr})$  are precisely the evaluations of the branch conditions for node  $N_k$ . Thus,  $b_k(\text{tr}) = \text{true}$  if  $N_k$  is in the execution sequence for  $\text{tr}$  else false. Define the factor  $p_k$  as

$$p_k(\text{tr}) := \delta_{b_k(\text{tr})} \text{pdf}_f \left( \text{tr}(V_{E_0}^{N_k}(\text{tr})); V_{E_1}^{N_k}(\text{tr}) \dots, V_{E_n}^{N_k}(\text{tr}) \right) + (1 - \delta_{b_k(\text{tr})}).$$

By construction,  $p_k \in [\mathcal{T} |_{A_k} \rightarrow \mathbb{R}_{\geq 0}]$ . □

For the example program in Fig. 1, the density factorises like below:

$$\begin{aligned} p(\text{tr}) &= \text{pdf}_{\text{Bernoulli}}(\text{tr}(\text{"b"}); 0.5) && \in [\mathcal{T} |_{\{\text{"b"}\}} \rightarrow \mathbb{R}_{\geq 0}] \\ &\times \text{pdf}_{\text{InverseGamma}}(\text{tr}(\text{"s"}); 1, 1) && \in [\mathcal{T} |_{\{\text{"s"}\}} \rightarrow \mathbb{R}_{\geq 0}] \\ &\times (\delta_{\text{tr}(\text{"b"})} \text{pdf}_{\text{Normal}}(\text{tr}(\text{"mu"}); 0, 1) + (1 - \delta_{\text{tr}(\text{"b"})})) && \in [\mathcal{T} |_{\{\text{"b"}, \text{"mu"}\}} \rightarrow \mathbb{R}_{\geq 0}] \\ &\times \text{pdf}_{\text{Normal}}(\text{tr}(\text{"x"}); V_m^N(\text{tr}), V_s^N(\text{tr})) && \in [\mathcal{T} |_{\{\text{"x"}, \text{"b"}, \text{"mu"}, \text{"s"}\}} \rightarrow \mathbb{R}_{\geq 0}] \end{aligned}$$

This is exactly the factorisation obtained from Theorem 1. However, if we would replace the if-statement with a nonsensical one, (if (b == 1) then (m = 1) else (m = 1)), then the fourth factor is in  $[\mathcal{T} |_{\{\text{"b"}, \text{"s"}\}} \rightarrow \mathbb{R}_{\geq 0}]$  with  $V_m^N(\text{tr}) = \delta_{\text{tr}(\text{"b"})} \cdot 1 + (1 - \delta_{\text{tr}(\text{"b"})}) \cdot 1 = 1$ . Thus, the static analysis over-approximates the true provenance with the spurious dependency on "b".

**3.3.1 Equivalence to Bayesian Networks.** If we restrict the way sample statements are used in our PPL, we can establish an equivalence to Bayesian networks. A Bayesian network [Koller and Friedman 2009] is a directed acyclic graph  $\mathcal{G}$  over a finite set of nodes  $X_1, \dots, X_n$  which represent random variables, such that the joint distribution factorises according to the graph  $\mathcal{G}$ ,

$$P(X_1, \dots, X_n) = \prod_{i=1}^n P(X_i \mid \text{parents}_{\mathcal{G}}(X_i)).$$

If we assume that all sample statements of a program have a constant unique address,  $N_k = \text{Assign}(x = \text{sample}(\alpha_k, f(E_1, \dots, E_n)))$ , then we can identify each factor  $p_k \in [\mathcal{T} |_{A_k} \rightarrow \mathbb{R}_{\geq 0}]$  of Theorem 1 with the unique address  $\alpha_k \in \text{Strings}$ . We construct the Bayesian network  $\mathcal{G}$  by mapping each address to a random variable  $X_{\alpha_k}$ . Since  $\alpha_k$  is unique,  $p_k$  is the only relevant factor for  $X_{\alpha_k}$  and can be interpreted as conditional density function of  $X_{\alpha_k}$ . To see this, rewrite

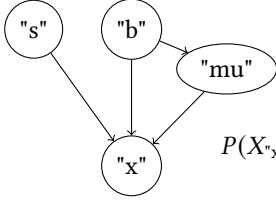
$$p_k(\text{tr}) = \delta_{b_k(\text{tr})} \text{pdf}_f \left( \text{tr}(\alpha_k); V_{E_1}^{N_k}(\text{tr}) \dots, V_{E_n}^{N_k}(\text{tr}) \right) + (1 - \delta_{b_k(\text{tr})}) \mathbf{1}_{\text{null}}(\text{tr}(\alpha_k)),$$

where the function  $\mathbf{1}_{\text{null}}(v)$  equals 1 if  $v = \text{null}$  else 0. If the node  $N_k$  is not executed, then the value of  $X_{\alpha_k}$  can be assumed to be null. As  $\text{pdf}_f$  is a probability density function and  $\mathbf{1}_{\text{null}}$  is the density of a Dirac distribution centered at null, the factor  $p_k$  is also a density function for each choice of values in  $\text{tr}$  at addresses  $\alpha \in A_k \setminus \{\alpha_k\}$ . Thus, we introduce the edge  $\alpha_j \rightarrow \alpha_k$  if  $\alpha_j \in A_k \setminus \{\alpha_k\}$ , such that  $\text{parents}_{\mathcal{G}}(X_{\alpha_k}) = A_k \setminus \{\alpha_k\}$  and

$$P(X_{\alpha_k} \mid \text{parents}_{\mathcal{G}}(X_{\alpha_k})) = p_k(\{\alpha_j \mapsto X_j : \alpha_j \in A_k\}).$$

In the above construction, it is important that each sample statement has an *unique* address. This guarantees no cyclic dependencies and a well-defined conditional probability distributions.

Below you can see the Bayesian network equivalent to the example program of Fig. 1. Since the value of the program variable `m` depends on which program branch is taken during execution, the random variable  $X_{\text{"x"}}$  not only depends on  $X_{\text{"mu"}}$ , but also on  $X_{\text{"b"}}$ .



$$\begin{aligned}
 P(X_{\text{"b"}}) &= \text{pdf}_{\text{Bernoulli}}(X_{\text{"b"}}; 0.5) \\
 P(X_{\text{"s"}}) &= \text{pdf}_{\text{InverseGamma}}(X_{\text{"s"}}; 1, 1) \\
 P(X_{\text{"mu"}} | X_{\text{"b"}}) &= \delta_{X_{\text{"b"}}} \text{pdf}_{\text{Normal}}(X_{\text{"mu"}}; 0, 1) + (1 - \delta_{X_{\text{"b"}}}) \mathbf{1}_{\text{null}}(X_{\text{"mu"}}) \\
 P(X_{\text{"x"}} | X_{\text{"b"}}, X_{\text{"mu"}}, X_{\text{"s"}}) &= \text{pdf}_{\text{Normal}}(X_{\text{"x"}}; \delta_{X_{\text{"b"}}} X_{\text{"mu"}} + (1 - \delta_{X_{\text{"b"}}}) 1, X_{\text{"s"}})
 \end{aligned}$$

**3.3.2 Equivalence to Markov Networks.** If the sample addresses are not unique or not constant, then the factorisation is in general not a Bayesian network. However, we can show equivalence to the more general Markov networks. A Markov network [Koller and Friedman 2009] is an *undirected* graph  $\mathcal{H}$  over random variables  $X_i$  that represents their dependencies. We consider Markov networks where the joint distribution of  $X_i$  factorises over  $\mathcal{H}$ :

$$P(\vec{X}) = \prod_{D \in \text{cliques}(\mathcal{H})} \phi_D(D).$$

We again identify a random variable  $X_\alpha$  for each address  $\alpha \in \bigcup_{k=1}^K A_k$  and construct a Markov network  $\mathcal{H}$  by connecting node  $X_\alpha$  to  $X_\beta$  if  $\alpha \in A_k \wedge \beta \in A_k$  for any  $k$ . Thus,  $D_k = \{X_\alpha : \alpha \in A_k\}$  forms a clique and  $p_S$  factorises over  $\mathcal{H}$  with  $\phi_{D_k}(D_k) = p_k(\{\alpha_j \mapsto X_j : \alpha_j \in A_k\})$ .

Consider the program with constant but non-unique sample addresses in Listing 2. With nine sample statements we get a Markov network over  $\{X_{\text{"F"}}, X_{\text{"P0"}}, X_{\text{"P1"}}, X_{\text{"D0"}}, X_{\text{"D1"}}\}$  shown in Fig. 2. The nine factors correspond to the address sets  $\{\text{"F"}\}$ ,  $\{\text{"F"}, \text{"P0"}\}$ ,  $\{\text{"F"}, \text{"P1"}\}$ ,  $\{\text{"F"}, \text{"D0"}, \text{"P1"}\}$ ,  $\{\text{"F"}, \text{"D1"}, \text{"P0"}\}$ ,  $2 \times \{\text{"F"}, \text{"P0"}, \text{"D0"}\}$ , and  $2 \times \{\text{"F"}, \text{"P1"}, \text{"D1"}\}$ . In the consequent branch of the program the distribution in the sample statement with address "P1" depends on "D0", while in the alternative branch, the distribution of "P0" depends on "D1". Thus, there is the dependency cyclic  $\text{"P0"} \rightarrow \text{"D0"} \rightarrow \text{"P1"} \rightarrow \text{"D1"} \rightarrow \text{"P0"}$ , which means there is no Bayesian network representation for the program. If we rewrite the model with dynamic addresses shown in Listing 3, the red dashed edges are introduced in the Markov network in Fig. 2 and we have one factor for address set  $\{\text{"F"}\}$ , one for set  $\{\text{"F"}, \text{"P0"}, \text{"P1"}\}$ , and three factors for address set  $\{\text{"F"}, \text{"P0"}, \text{"P1"}, \text{"D0"}, \text{"D1"}\}$ .

Listing 2. Probabilistic program for the hurricane example of [Milch et al. 2005].

```

first_city_ixs = sample("F", Bernoulli(0.5))
if first_city_ixs == 0 then
  prep_0 = sample("P0", Bernoulli(0.5))
  damage_0 = sample("D0", Bernoulli(if prep_0 == 1 then 0.2 else 0.8))
  prep_1 = sample("P1", Bernoulli(if damage_0 == 1 then 0.75 else 0.5))
  damage_1 = sample("D1", Bernoulli(if prep_1 == 1 then 0.2 else 0.8))
else
  prep_1 = sample("P1", Bernoulli(0.5))
  damage_1 = sample("D1", Bernoulli(if prep_1 == 1 then 0.2 else 0.8))
  prep_0 = sample("P0", Bernoulli(if damage_1 == 1 then 0.75 else 0.5))
  damage_0 = sample("D0", Bernoulli(if prep_0 == 1 then 0.2 else 0.8))

```

Lastly, while the programs considered up until this point were equivalent to finite Bayesian networks or finite Markov networks, the small program in Listing 4 is equivalent to a Markov network with an infinite number of nodes.

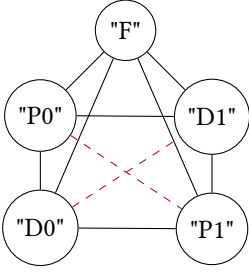


Fig. 2. Markov network of the hurricane model.

Listing 3. Second version of program in Listing 2 with dynamic addresses.

```

first_city_ixs = sample("F", Bernoulli(0.5))
first = str(first_city_ixs)
second = str(1 - first_city_ixs)

prep_first = sample("P"+first, Bernoulli(0.5))
damage_first = sample("D"+first,
    Bernoulli(if prep_first == 1 then 0.2 else 0.8))
prep_second = sample("P"+second,
    Bernoulli(if damage_first == 1 then 0.75 else 0.5))
damage_second = sample("D"+second,
    Bernoulli(if prep_second == 1 then 0.2 else 0.8))

```

Listing 4. Probabilistic program equivalent to a Markov network with an infinite number of variables.

```

n = sample("n", Poisson(5))
x = sample("x"+str(n), Normal(0., 1.))

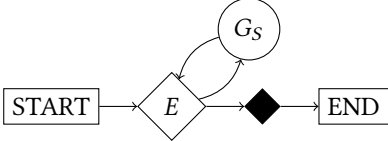
```

## 4 STATIC FACTORISATION FOR PROGRAMS WITH LOOPS

In this section, we describe how the argument for proving the factorisation theorem for programs without loops, can be extended to generalise the result to programs with loops.

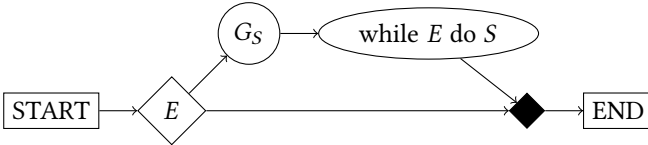
### 4.1 Unrolled Control-Flow-Graph

The translation rules for programs to their CFG can be extended to support while loops as follows. Let  $G_S$  be the sub-CFG of statement  $S$ . The CFG of (while  $E$  do  $S$ ) is given by



For this CFG,  $\text{prov}(N, x)$  is still well-defined by Algorithm 1, but the proof of Proposition 2 does not work anymore since it requires a directed acyclic graph.

To establish Proposition 2 for programs with while loops, we introduce a second type of control-flow graph, the *unrolled CFG*. All translation rules are as before except for while loops, which is given below.



This is a recursive definition, which we will describe in more detail. The resulting graph  $G$  contains for every  $i \in \mathbb{N}$  branch nodes  $B_i$ , join nodes  $J_i$ , and *copies* of the sub-CFG  $G_i$  of statement  $S$ . The edges are given by

- $\text{START} \rightarrow B_1, J_1 \rightarrow \text{END}$
- $B_i \rightarrow \text{successor}(\text{START}_{G_i}), \text{predecessor}(\text{END}_{G_i}) \rightarrow B_{i+1}, B_i \rightarrow J_i, J_{i+1} \rightarrow J_i$

This definition implies that the number of nodes of  $G$  is countable. Furthermore, since the unrolled CFG consists only of start, end, branch, join, and assign nodes, we can equip it with the same semantics as the standard CFG. Again, the semantics are equivalent.

PROPOSITION 3. For all program  $S$  with CFG  $H$  and unrolled CFG  $G$ , it holds that for all traces  $\text{tr}$

$$p_S(\text{tr}) = p_H(\text{tr}) = p_G(\text{tr}).$$

PROOF. See Appendix A.2.  $\square$

As mentioned, Algorithm 1 still works for the unrolled CFG. However, since the unrolled CFG contains an infinite number of nodes, in practice, we run this algorithm on the standard CFG with a finite number of nodes. We will show that both computations produce the same provenance set, but first, we define the connection between the two graph types.

DEFINITION 7. Let  $H$  be the CFG and  $G$  the unrolled CFG of program  $S$ . For each node  $M \in G$ , we define  $\iota_{\text{cfg}}(M) \in H$  as the node from which  $M$  was copied in the construction of  $G$ .

The definition of  $\iota_{\text{cfg}}$  is best understood when considering the example in Fig. 3, where you can see the CFG and unrolled CFG of a program with the mapping  $\iota_{\text{cfg}}$ .

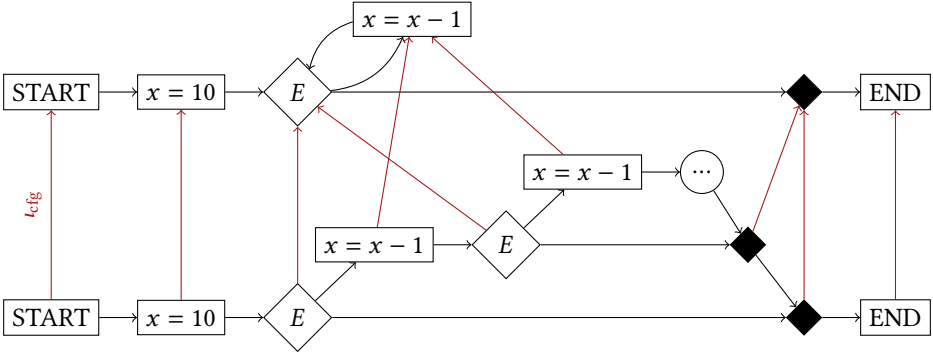


Fig. 3. CFG and unrolled CFG for program  $(x = 10; \text{ while } (x < 10) \text{ do } (x = x - 1))$  and their connection via the map  $\iota_{\text{cfg}}$  shown with red edges.

The next lemma states that we can compute the provenance set for variable  $x$  at node  $M$  in the unrolled CFG by applying Algorithm 1 to the corresponding node  $\iota_{\text{cfg}}(M)$  in the standard CFG.

LEMMA 4. Let  $H$  be the CFG and  $G$  the unrolled CFG of program  $S$ . For each node  $M \in G$  following equations hold.

$$\{\iota_{\text{cfg}}(M') : M' \in \text{RD}(M, x)\} = \text{RD}(\iota_{\text{cfg}}(M), x) \quad (6)$$

$$\{\iota_{\text{cfg}}(M') : M' \in \text{BP}(M)\} = \text{BP}(\iota_{\text{cfg}}(M)) \quad (7)$$

$$\text{prov}(M, x) = \text{prov}(\iota_{\text{cfg}}(M), x) \quad (8)$$

PROOF. This follows from the fact that the standard CFG and unrolled CFG of while loops produce paths that are compatible regarding reaching definitions and branch parents. The former produces paths of form  $\text{START}, B, \bar{S}_1, B, \bar{S}_2, \dots, \dots, \bar{S}_n, B, J, \text{END}$ , while the latter produces paths of form  $\text{START}, B_1, \bar{S}_1, B_2, \bar{S}_2, \dots, \dots, \bar{S}_n, B_{n+1}, J_{n+1}, J_n, \dots, J_1, \text{END}$ , where  $\bar{S}_i$  are paths in the sub-CFGs. The full proof is given in Appendix A.3.  $\square$

## 4.2 Static Factorisation Theorem for Programs With Loops

The unrolled CFG has the important property that it is a directed acyclic graph with a potentially infinite number of nodes, but with a single root node. Further, each node  $N \neq \text{START}$  still has exactly one predecessor except for join nodes which have two predecessors. Therefore, Proposition 2 can be generalised to unrolled CFGs without having to modify the proof.

PROPOSITION 4. *For each node  $M$  in the unrolled CFG  $G$  and variable  $x$ , there exists an evaluation function*

$$V_x^M \in [\mathcal{T}|_{\text{prov}(M,x)} \rightarrow \mathcal{V}],$$

*such that for all traces  $\text{tr}$  with  $\sigma_0 = (x_i \mapsto \text{null}, \mathbf{p} \mapsto 1)$  and execution sequence*

$$(\sigma_0, \text{START}) \xrightarrow{\text{tr}} \dots \xrightarrow{\text{tr}} (\sigma_i, M_i) \xrightarrow{\text{tr}} \dots \xrightarrow{\text{tr}} (\sigma_l, \text{END})$$

*we have*

$$\sigma_i(x) = V_x^{M_i}(\text{tr}).$$

As before, Proposition 4 allows us to explicitly construct the factorisation of the program density. However, since there is a potentially infinite number of sample nodes in the unrolled CFG, in the proof we will group their contribution to the density to get a factorisation over a finite number of terms. The factorisation theorem for programs with loops reads exactly the same as the theorem for programs without loops.

THEOREM 2. *Let  $H$  be the CFG for a program  $S$ . Let  $N_1, \dots, N_K$  be all sample nodes in  $H$ . For each sample node  $N_k = \text{Assign}(x = \text{sample}(E_0, f(E_1, \dots, E_n)))$ , let*

$$A_k = \text{addresses}(N_k) \cup \text{prov}(N_k, E_0) \cup \bigcup_{i=1}^n \text{prov}(N_k, E_i) \cup \bigcup_{N' \in \text{BP}(N_k)} \text{prov}(N', E_{N'}).$$

*Then, there exist functions  $p_k \in [\mathcal{T}|_{A_k} \rightarrow \mathbb{R}_{\geq 0}]$  such that if  $p_S(\text{tr}) \neq \text{undefined}$ , then*

$$p_S(\text{tr}) = p_H(\text{tr}) = \prod_{k=1}^K p_k(\text{tr}).$$

PROOF. Let  $G$  be the *unrolled* CFG of program  $S$  and let  $M_j$  be all sample nodes in  $G$  (countably many). Like in the proof of Theorem 1, define for each  $M_j$ ,  $b_j(\text{tr}) := \prod_{M' \in \text{BP}(M_j)} V_{E_{M'}}^{M'}(\text{tr})$  where

$$b_j \in [\mathcal{T}|_{\bigcup_{M' \in \text{BP}(M_j)} \text{prov}(M', E_{M'})} \rightarrow \{\text{true}, \text{false}\}].$$

Again,  $b_j(\text{tr}) = \text{true}$  if  $M_j$  is in the execution sequence for  $\text{tr}$  else false. Define

$$\tilde{p}_j(\text{tr}) := \delta_{b_j(\text{tr})} \text{pdf}_f\left(\text{tr}(V_{E_0}^{M_j}(\text{tr})); V_{E_1}^{M_j}(\text{tr}), \dots, V_{E_n}^{M_j}(\text{tr})\right) + (1 - \delta_{b_j(\text{tr})}).$$

We have  $\tilde{p}_j \in [\mathcal{T}|_{\tilde{A}_j} \rightarrow \mathbb{R}_{\geq 0}]$ , for

$$\tilde{A}_j = \text{addresses}(M_j) \cup \bigcup_{i=0}^n \text{prov}(M_j, E_i) \cup \bigcup_{M' \in \text{BP}(M_j)} \text{prov}(M', E_{M'}).$$

Finally, we group the nodes  $M_j$  by their corresponding CFG node.

$$p_k = \prod_{j: \iota_{\text{cfg}}(M_j) = N_k} \tilde{p}_j$$

If  $\iota_{\text{cfg}}(M_j) = N_k$ , then  $\tilde{A}_j = A_k$ , since by Eq. (8) for  $i = 0, \dots, n$

$$\text{prov}(M_j, E_i) = \text{prov}(\iota_{\text{cfg}}(M_j), E_i) = \text{prov}(N_k, E_i)$$

and by Eq. (7)

$$\{\iota_{\text{cfg}}(M') : M' \in \text{BP}(M_j)\} = \text{BP}(\iota_{\text{cfg}}(M_j)) = \text{BP}(N_k)$$



such that

$$\begin{aligned} \bigcup_{M' \in \text{BP}(M_j)} \text{prov}(M', E_{M'}) &= \bigcup_{M' \in \text{BP}(M_j)} \text{prov}(\iota_{\text{cfg}}(M'), E_{\iota_{\text{cfg}}(M')}) \\ &= \bigcup_{N' \in \text{BP}(N_k)} \text{prov}(N', E_{N'}). \end{aligned}$$

Thus,  $\tilde{p}_j \in [\mathcal{T}|_{A_k} \rightarrow \mathbb{R}_{\geq 0}]$  for all  $j$ , such that  $\iota_{\text{cfg}}(M_j) = N_k$ , which implies  $p_k \in [\mathcal{T}|_{A_k} \rightarrow \mathbb{R}_{\geq 0}]$ .  $\square$

**4.2.1 Equivalence to Markov Networks.** As in Section 3.3.2, Theorem 2 implies that a program  $S$  with  $K$  sample statements is equivalent to a Markov network  $\mathcal{H}$  with nodes  $\{X_\alpha : \alpha \in \bigcup_{k=1}^K A_k\}$  even if it contains loops. Again, the sets  $D_k = \{X_\alpha : \alpha \in A_k\}$  form cliques in  $\mathcal{H}$  and  $p_S$  factorises over  $\mathcal{H}$  with  $\phi_{D_k}(D_k) = p_k(\{\alpha_j \mapsto X_j : \alpha_j \in A_k\})$ ,

$$P(\vec{X}) = \prod_{D \in \text{cliques}(\mathcal{H})} \phi_D(D) = \prod_{k=1}^K \phi_{D_k}(D_k).$$

Consider the program in Listing 5. After starting at a random position in  $[0, 3]$ , the iteration takes random steps in either direction until travelling a distance of 10 units or until reaching the origin 0. In this process, an unbounded number of random variables may be instantiated. While the sample statement with address "step\_t" has seemingly no dependencies, the provenance analysis tells us that it depends on all variables with a "step" address and the "start" variable through the while loop condition. This is an over-approximation since, in fact, the variable with address "step\_t" depends only on the variables from previous iterations, i.e. variables with address "step\_k" for  $k < t$ , and the "start" variable. Note that due to the fact that this program only contains three sample statements, the factorisation obtained from Theorem 2 is close to being trivial, i.e. one factor equal to the whole program density depending on all sample addresses.

Listing 5. Pedestrian example adapted from [Mak et al. 2021].

```
start = sample("start", Uniform(0,3))
t = 0
position = start
distance = 0.0
while position > 0 and distance < 10:
    step = sample("step_" + str(t), Uniform(-1,1))
    distance = distance + abs(step)
    position = position + step
    t = t + 1
sample("final_distance", Normal(1.1, 0.1), obs=distance)
```

## 5 CASE STUDY: SPEEDING-UP POSTERIOR INFERENCE

In this section, we demonstrate a practical application of our theoretical results. In particular, we discuss how the dependency structure obtained by the static provenance analysis can be used to speed-up posterior inference.

Consider the Gaussian mixture model in Listing 6. For the sake of eligibility, we introduce arrays and for loops. For constant integer  $K$ , a for loop (for  $(x \text{ in } 1 : K) S$ ) is *syntactic sugar* for the statement  $(S_1; \dots; S_K)$ , where  $S_i$  is a modification of statement  $S$  with all occurrences of variable  $x$  being replaced with the integer  $i$ . To formally include arrays in our language we could define functions `get(a, i)` and `a = put(a, i, v)` for retrieving or modifying the value of array  $a$  at index  $i$ . For simplicity, we use the more common bracket notation in the presented example instead.

Listing 6. GMM adapted from [Matheos et al. 2020].

```

w = sample("w", fill( $\delta$ , K))
means = array(K)
vars = array(K)
for k in 1:K
    means[k] = sample("mu_" + str(k),
        Normal( $\xi$ , 1/sqrt( $\kappa$ )))
    vars[k] = sample("var_" + str(k),
        InverseGamma( $\alpha$ ,  $\beta$ ))
z = array(N)
i = 1
while i <= N (or for i in 1:N)
    z[i] = sample("z_" + str(i),
        Categorical(w))
    y[i] = sample("y_" + str(i),
        Normal(means[z[i]], sqrt(vars[z[i]])))
    i = i + 1 (or skip)

```

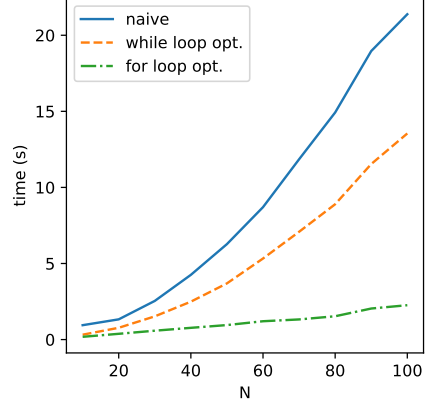


Fig. 4. Posterior inference time for the GMM by the size of observations and optimisation strategy.

We consider the single-site Metropolis Hastings algorithm [van de Meent et al. 2018; Wingate et al. 2011] to infer the most likely clusters for data set  $y$ , as well as the most probable allocation of each data point  $y_i$  to one cluster  $z_i \in [1, K]$ . We fix the number of clusters to  $K = 4$ . The inference algorithm works by selecting a single address  $\alpha$  in each iteration at random and proposing a new value  $v$  according to the kernel  $v \sim Q_\alpha(v)$ . The proposed trace  $\text{tr}' = \text{tr}[\alpha \mapsto v]$  is then accepted with probability

$$A = \min \left( 1, \frac{p(\text{tr}') \times Q_\alpha(\text{tr}(\alpha))}{p(\text{tr}) \times Q_\alpha(\text{tr}'(\alpha))} \right).$$

Since we only change  $\text{tr}$  at one address, we can make use of the factorisation theorems to more efficiently compute  $p(\text{tr}')/p(\text{tr})$ . That is, if we update at address  $\alpha$ , we only need to recompute the factors corresponding to the sample statements where  $\alpha$  is in the provenance set.

For instance, if we change the value for the center of cluster 1, "mu\_1", we only need to update the contributions of  $y$  to  $p$ . We do not have to recompute the contributions of the variables with address "w", "var\_k" or "z\_i". If we update one of the allocations "z\_i", we have to be careful. In the presented implementation a while loop is used and the array  $z$  is read at a "dynamic" index  $i$ . From the static perspective of Algorithm 1, we do not know which element of  $z$  is used in sample statement for "y\_j", i.e. we do not know the value of program variable  $i$ . Therefore, we have to recompute the contributions to the density of variables "y\_j" for all  $1 \leq j \leq N$ . (Note that in this simple case, we could modify the algorithm with heuristics to infer that  $i = j$  in the sample statement of "y\_j").

However, in this program, we could also simply replace the while loop with a for loop. This is *syntactically* equivalent to unrolling the loop by copying its body  $N$  times and replacing  $i$  with a constant integer increasing by each copy, as described before.

```

z[1] = sample("z_" + str(1), Categorical(w))
y[1] = sample("y_" + str(1), Normal(means[z[1]], sqrt(vars[z[1]])))
z[2] = sample("z_" + str(2), Categorical(w))
y[2] = sample("y_" + str(2), Normal(means[z[2]], sqrt(vars[z[2]])))
...

```

Note that this is different to the *mathematical* unrolling of while loops in Section 4.1. For the modified program, all sample addresses are constant and we statically know that if we update " $z_i$ " we only need to recompute the contribution of the single data point " $y_i$ ".

In Fig. 4, you can see how the optimisations described above influence the runtime of the single-site Metropolis Hastings inference algorithm. Using the provenance information of the unmodified program with a while loop results in a 2x speed-up. This is explained by the fact that as we increase the data size  $N$ , in most iterations we update at an address " $z_i$ ". Instead of reusing the contributions of variables " $z_j$ ",  $j \neq i$ , and only recomputing at addresses " $y_j$ " ( $N$  computations), the naive implementation computes  $p(\text{tr}')$  from scratch ( $2N + 2K + 1$  computations), thus doubling the runtime. Modifying the program by unrolling the while loop and using its provenance information decreases the runtime by a factor of 10 for  $N = 100$ . The reason is that now in most iterations only the contributions of variables " $z_i$ " and " $y_i$ " for a single  $1 \leq i \leq N$  have to be computed.

## 6 RELATED WORK

### 6.1 Semantics of Probabilistic Programming Languages

One of the first works to formally define the semantics of a probabilistic programming language was [Kozen 1979]. Operational semantics were given in form of machine-state transitions, where the state contains two infinite stacks of continuous and discrete random choices. When executing a sample statement an element will be popped from these stacks. In the same work, denotational semantics were also presented, where the program state is modelled as a probability distribution and a program is interpreted as an operator on distributions. Derivatives of this semantics can be found throughout literature, e.g. see [Hur et al. 2015] and [Dwyer et al. 2017].

In recent years, a lambda calculus for probabilistic programming was presented [Borgström et al. 2016]. This work and a domain theoretic approach for probabilistic programming [Vákár et al. 2019] had an influence on the development of the statistical PCF [Mak et al. 2021] (programming computable functions), which was used to prove differentiability of terminating probabilistic programs. Probabilistic programming was also examined from a categorical perspective [Heunen et al. 2017] and the semantics of higher order probabilistic programs is actively researched [Dahlqvist and Kozen 2019; Staton et al. 2016].

Semantics for probabilistic programming languages are also developed for specific applications like approximate inference [Huang et al. 2021] or handling exceptions [Bichsel et al. 2018].

As already mentioned, the semantics presented in this work generalise those of [Gorinova et al. 2019] which formalises the core language constructs of Stan by interpreting a program as a function over a fixed set of finite variables. In our semantics, we interpret programs as functions over traces which are mappings from addresses to values similar to dictionaries. Another dictionary based approach to probabilistic programming can be found in [Cusumano-Towner et al. 2020].

### 6.2 Graphical Representations and Static Analysis

The advantages of representing a probabilistic model graphically are well-understood [Koller and Friedman 2009]. For this reason, some PPLs like PyMC [Salvatier et al. 2016] or Infer.NET [Minka 2012] require the user to explicitly define their model as a graph. Modifying the Metropolis Hastings algorithm to exploit the structure of the model is also common practice, e.g. see [Nori et al. 2014; van de Meent et al. 2018].

While the connection of simple probabilistic programs to Bayesian networks is known [van de Meent et al. 2018], our approach shows how to *statically* determine a non-trivial factorisation and show equivalence to Markov networks even for programs containing while loops. Previous work

extended Bayesian networks to so-called contingent Bayesian networks in order to support models with an infinite number of random variables or cyclic dependencies [Milch et al. 2005].

The probabilistic dependency structure of programs has also been exploited in previous work. [Baah et al. 2008] use it for fault diagnosis, [Hur et al. 2014] designed an algorithm for slicing probabilistic programs, and [Bernstein et al. 2020] extract the factor graph of programs to automate model checking for models implemented in Stan.

However, in general, the field of static analysis for probabilistic programming is young and under-explored [Bernstein 2019]. We list a few recent advances. In 2014, [Sampson et al. 2014] introduced probabilistic assertion statements and an evaluation approach to either statically or dynamically verify them. In 2018, [Hoffman et al. 2018] presented a method to automatically analyse the source code of density functions for conjugacy structure and leveraged the structure for improved inference.

Stan has received the most attention with regards to static analysis. In 2018, SlicStan [Gorinova et al. 2019], a compositional version of the probabilistic programming language, was published. In this work, a semantics-preserving translation to Stan was developed. In the following years, Stan was also extended with a pedantic compilation mode [Bernstein 2023] statically checking for frequent programming mistakes. Lastly, a compilation scheme was designed to translate a Stan program to a generative PPL [Baudart et al. 2021].

Most recently [Wang et al. 2021] developed a type system to enforce absolute continuity of Pyro guide programs and [Li et al. 2023] presented an automatic approach to generate sound guide programs for a given Pyro program.

## 7 CONCLUSION

In this work, we introduced address-based operational semantics for a formal probabilistic programming language. Our semantics are better suited to reason about PPLs which make use of user-defined sample addresses like Gen, Pyro, or PyMC. We presented a sound static analysis that approximates the dependency structure of random variables in the program and used this structure to factorise the implicitly defined program density. The factorisation allowed us to show equivalence of programs to either Bayesian or Markov networks. Lastly, we demonstrated that we can speed-up a single-site Metropolis Hastings algorithm by a factor of 10 by deriving an optimised computation of the program density from the dependency structure.

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## A PROOFS

### A.1 Proof of Proposition 1

STATEMENT. For all programs  $S$  with control-flow-graph  $G$ , it holds that for all traces  $\text{tr}$

$$p_S(\text{tr}) = p_G(\text{tr}).$$

PROOF. With structural induction we prove the more general equivalence:

$$(\sigma, S) \Downarrow^{\text{tr}} \sigma' \iff (\sigma, \text{START}) \xrightarrow[S]{\text{tr}} \dots \xrightarrow[S]{\text{tr}} (\sigma', \text{END}).$$

We write  $\xrightarrow[S]{\text{tr}}$  to indicate that the predecessor-successor relationship follow the CFG of program  $S$ .

For programs consisting of a single skip, assignment, or sample statement, the equality can be seen by directly comparing the operational semantic rules to the graph semantics.

For sequence  $S = (S_1; S_2)$ , by induction assumption we have

$$\begin{aligned} (\sigma, S_1) \Downarrow^{\text{tr}} \sigma' &\iff (\sigma, N_{\text{start}}^1) \xrightarrow[S_1]{\text{tr}} \dots \xrightarrow[S_1]{\text{tr}} (\sigma'_1, N^1) \xrightarrow[S_1]{\text{tr}} (\sigma', N_{\text{end}}^1) \\ (\sigma', S_2) \Downarrow^{\text{tr}} \sigma'' &\iff (\sigma', N_{\text{start}}^2) \xrightarrow[S_2]{\text{tr}} (\sigma', N^2) \xrightarrow[S_2]{\text{tr}} \dots \xrightarrow[S_2]{\text{tr}} (\sigma'', N_{\text{end}}^2) \end{aligned}$$

By comparing the recursive definition of the CFG of  $S$ , we see that

$$(\sigma, S) \Downarrow^{\text{tr}} \sigma'' \iff (\sigma, N_{\text{start}}^1) \xrightarrow[S]{\text{tr}} \dots \xrightarrow[S]{\text{tr}} (\sigma'_1, N^1) \xrightarrow[S]{\text{tr}} (\sigma', N^2) \xrightarrow[S]{\text{tr}} \dots \xrightarrow[S]{\text{tr}} (\sigma'', N_{\text{end}}^2)$$

In a similar way, we proof the result for if statements  $S = (\text{if } E \text{ then } S_1 \text{ else } S_2)$  by considering the two cases  $\sigma(E) = \text{true}$  and  $\sigma(E) = \text{false}$ .

$$(\sigma, S) \Downarrow^{\text{tr}} \sigma' \iff (\sigma, N_{\text{start}}) \xrightarrow[S]{\text{tr}} (\sigma, \text{Branch}(E)) \xrightarrow[S]{\text{tr}} \dots \xrightarrow[S]{\text{tr}} (\sigma', N_{\text{join}}) \xrightarrow[S]{\text{tr}} (\sigma', N_{\text{end}})$$

Depending on the case, we replace the dots with the path of  $S_i$  without the start and end nodes. Note that in our notation in both cases  $(\sigma, S_i) \Downarrow^{\text{tr}} \sigma'$ .  $\square$

### A.2 Proof of Proposition 3

STATEMENT. For all program  $S$  with CFG  $H$  and unrolled CFG  $G$ , it holds that for all traces  $\text{tr}$

$$p_S(\text{tr}) = p_H(\text{tr}) = p_G(\text{tr}).$$

PROOF. We continue the proof of Proposition 1 for a while statement. Note the well-known equivalence for while statements in terms of the operational semantics:

$$(\sigma, \text{while } E \text{ do } S) \Downarrow^{\text{tr}} \sigma' \iff (\sigma, \text{if } E \text{ then } (S; \text{while } E \text{ do } S) \text{ else skip}) \Downarrow^{\text{tr}} \sigma'$$

Thus, if the program terminates for  $\text{tr}$ , it is equivalent to  $S; \dots; S$  ( $S$  repeated  $n$  times), where  $\sigma_0 = \sigma$ ,  $(\sigma_i, S) \Downarrow^{\text{tr}} \sigma_{i+1}$ ,  $\sigma_n = \sigma'$ , such that  $\sigma_i(E) = \text{true}$  for  $i < n$ ,  $\sigma_n(E) = \text{false}$ .

In this case, it can be shown that the (unrolled) CFG of  $S; \dots; S$  is also equivalent to the (unrolled) CFG of the while statement.

If the program does not terminate, then  $p_S(\text{tr}) = p_H(\text{tr}) = p_G(\text{tr}) = \text{undefined}$ .  $\square$

### A.3 Proof of Lemma 4

STATEMENT. Let  $H$  be the CFG and  $G$  the unrolled CFG of program  $S$ . For each node  $M \in G$  following equation holds.

$$\{\iota_{\text{cfg}}(M') : M' \in \text{RD}(M, x)\} \subseteq \text{RD}(\iota_{\text{cfg}}(M), x) \quad (9)$$

PROOF. We will prove following Lemma by structural induction:

LEMMA. For every path  $\vec{M} = (M', \dots, M)$  in the unrolled CFG  $G$ , there is a path in the CFG  $H$ ,  $\vec{N} = (N', \dots, N)$ , such that

$$\iota_{\text{cfg}}(M') = N', \quad \iota_{\text{cfg}}(M) = N,$$

$$\text{AssignNodes}(\vec{N}, x) = \{\iota_{\text{cfg}}(M_i) : M_i \in \text{AssignNodes}(\vec{M}, x)\} = \text{AssignNodes}_{\text{cfg}}(\vec{M}, x),$$

for all variables  $x$ , where  $\text{AssignNodes}(\vec{N}, x)$  is the set of all CFG nodes that assign  $x$  in path  $\vec{N}$  and  $\text{AssignNodes}_{\text{cfg}}(\vec{M}, x)$  is the set of all assign nodes in path  $\vec{M}$  mapped to  $H$  with  $\iota_{\text{cfg}}$ .

With this lemma we can prove the statement:

Let  $M' \in \text{RD}(M, x)$ . Thus, there exists a path  $\vec{M} = (M', \dots, M)$ , such that  $M'$  is the only assign node for  $x$  before  $M$ . By the lemma, there is a path in the CFG  $\vec{N} = (N', \dots, N)$ , such that  $\iota_{\text{cfg}}(M') = N'$  and  $\iota_{\text{cfg}}(M) = N$ .

Further, since  $\text{AssignNodes}(\vec{N}, x) = \text{AssignNodes}_{\text{cfg}}(\vec{M}, x) \subseteq \{\iota_{\text{cfg}}(M'), \iota_{\text{cfg}}(M)\} = \{N', N\}$ , the node  $N'$  is also the only node in the path  $\vec{N}$  before  $N$  that assigns  $x$ .

Thus,  $\iota_{\text{cfg}}(M') = N' \in \text{RD}(N, x) = \text{RD}(\iota_{\text{cfg}}(M), x)$ .

PROOF OF LEMMA. By structural induction.

For CFGs only consisting of a single assign node, the unrolled CFGs are identical and the statement follows.

For a sequence of two statements  $(S_1; S_2)$ , let  $H$  be the CFG with sub-graphs  $H_1$  and  $H_2$  for statements  $S_1$  and  $S_2$  respectively. Let  $G$  the unrolled CFG with sub-graphs  $G_1$  and  $G_2$ . We consider the only interesting case where  $M' \in G_1$  and  $M \in G_2$ :

$$\vec{M} = (\underbrace{M, \dots, M_i}_{\in G_1}, \underbrace{M_{i+1}, \dots, M}_{\in G_2}),$$

For sub-paths  $\vec{M}_1 := (M, \dots, M_i, \text{END})$  and  $\vec{M}_2 := (\text{START}, M_{i+1}, \dots, M)$  we apply the induction assumption to get two paths  $\vec{N}_1 = (N', \dots, N_1, \text{END})$ ,  $\vec{N}_2 = (\text{START}, N_2, \dots, N)$ , with  $\iota_{\text{cfg}}(M') = N'$  and  $\iota_{\text{cfg}}(M) = N$ . The corresponding CFG path is  $\vec{N} := (N', \dots, N_1, N_2, \dots, N)$  as

$$\begin{aligned} \text{AssignNodes}_{\text{cfg}}(\vec{M}, x) &= \text{AssignNodes}_{\text{cfg}}(\vec{M}_1, x) \cup \text{AssignNodes}_{\text{cfg}}(\vec{M}_2, x) \\ &= \text{AssignNodes}(\vec{N}_1, x) \cup \text{AssignNodes}(\vec{N}_2, x) = \text{AssignNodes}(\vec{N}, x). \end{aligned}$$

For an if statement, let  $H$  be the CFG with branch node  $\tilde{B}$ , join node  $\tilde{J}$ , and sub-graphs  $H_1, H_2$ . Let  $G$  be the unrolled CFG with corresponding  $B, J, G_1$ , and  $G_2$ . We only show the statement for the case

$$\vec{M} = (B, \underbrace{M', \dots, M}_{\in G_i}, J).$$

Again, we apply the induction assumption to  $\vec{M}_i := (\text{START}, M', \dots, M, \text{END})$  and get a CFG path  $\vec{N}_i = (\text{START}, N', \dots, N, \text{END})$ . Since  $\iota_{\text{cfg}}(B) = \tilde{B}$ ,  $\iota_{\text{cfg}}(J) = \tilde{J}$ , which are not assign nodes, and  $\text{AssignNodes}(\vec{N}_i) = \text{AssignNodes}_{\text{cfg}}(\vec{M}_i)$ , the statement follows for the path  $(\tilde{B}, N', \dots, N, \tilde{J})$ .



Lastly, for a while loop, let  $H$  be the CFG with branch node  $\tilde{B}$ , join node  $\tilde{J}$ , and sub-graph  $H_S$ . Let  $G$  be the unrolled CFG with  $B_i$  branch nodes,  $J_i$  join nodes, and  $G_i$  sub-graphs. For the sake of brevity we consider three cases:

- For  $M' \in G_i$  and  $M \in G_j$

$$\vec{M} = (\underbrace{M', \dots, M_i}_{\in G_i}, B_{i+1}, \dots, B_j, \underbrace{M_j, \dots, M}_{\in G_j})$$

we apply the induction assumption to the sub-paths and construct the path

$$\vec{N} = (\underbrace{N', \dots, N_i}_{\in H_S}, B, \dots, B, \underbrace{N_j, \dots, N}_{\in H_S})$$

where  $B$ ,  $B_i$ , and  $J_i$  are not assign nodes.

- For  $M' \in G_i$  and  $J_k$

$$\vec{M} = (\underbrace{M', \dots, M_i}_{\in G_i}, B_{i+1}, \dots, B_l, J_l, J_{l-1}, \dots, J_k)$$

we construct the path

$$\vec{N} = (\underbrace{N', \dots, N_i}_{\in H_S}, B, \dots, B, J)$$

- For the path  $\vec{M} = (B_l, J_l, \dots, J_k)$  the path in the CFG is  $\vec{N} = (B, J)$ .

□

STATEMENT. Let  $H$  be the CFG and  $G$  the unrolled CFG of program  $S$ . For each node  $M \in G$  following equation holds.

$$\{\iota_{\text{cfg}}(M') : M' \in \text{RD}(M, x)\} \supseteq \text{RD}(\iota_{\text{cfg}}(M), x) \quad (10)$$

PROOF. Like for the reverse inclusion, it is sufficient to prove the following lemma.

LEMMA. For every path  $\vec{N} = (N', \dots, N)$  in the CFG  $H$ , there is a path in the unrolled CFG  $G$ ,  $\vec{M} = (M', \dots, M)$ , such that

$$\iota_{\text{cfg}}(M') = N', \quad \iota_{\text{cfg}}(M) = N,$$

$$\text{AssignNodes}(\vec{N}, x) = \{\iota_{\text{cfg}}(M_i) : M_i \in \text{AssignNodes}(\vec{M}, x)\} = \text{AssignNodes}_{\text{cfg}}(\vec{M}, x)$$

As in the proof of the last statement, this is proven by induction and finding equivalent paths in the CFG and unrolled CFG.

Let  $N' \in \text{RD}(\iota_{\text{cfg}}(M), x)$ . Thus, there is a path  $\vec{N} = (N', \dots, \iota_{\text{cfg}}(M))$  with  $\text{AssignNodes}(\vec{N}, x) \subseteq \{N', \iota_{\text{cfg}}(M)\}$ . We can find a path  $\vec{M} = (M', \dots, M)$  such that  $\iota_{\text{cfg}}(M') = N'$  and

$$\text{AssignNodes}_{\text{cfg}}(\vec{M}, x) = \text{AssignNodes}(\vec{N}, x) \subseteq \{\iota_{\text{cfg}}(M'), \iota_{\text{cfg}}(M)\}.$$

Therefore, in the path  $\vec{M}$ , node  $M'$  is the only node that assigns  $x$  before  $M$  and hence we have  $M' \in \text{RD}(M, x)$ . □

STATEMENT. Let  $H$  be the CFG and  $G$  the unrolled CFG of program  $S$ . For each node  $M \in G$  the following equation holds.

$$\text{BP}_{\text{cfg}}(M) := \{\iota_{\text{cfg}}(M') : M' \in \text{BP}(M)\} = \text{BP}(\iota_{\text{cfg}}(M)) \quad (11)$$

PROOF. We prove this statement by structural induction.

For CFGs only consisting of a single assign node, the unrolled CFGs are identical, there are no branch parents, and the statement follows.

The sequencing of two statements  $(S_1; S_2)$  does not change the branch parents of any node.

For an if statement, let  $H$  be the CFG with branch node  $\tilde{B}$ , join node  $\tilde{J}$ , and sub-graphs  $H_1, H_2$ . Let  $G$  be the unrolled CFG with corresponding  $B, J, G_1$ , and  $G_2$ . Every node  $M$  in  $G_i$  has branch parents  $(\text{BP}(M) \cap G_i) \cup \{B\}$ .

By induction assumption  $\text{BP}_{\text{cfg}}(M) \cap H_i = \text{BP}(\iota_{\text{cfg}}(M)) \cap H_i$  and thus

$$\begin{aligned} \text{BP}_{\text{cfg}}(M) &= \{\iota_{\text{cfg}}(M') : M' \in \text{BP}(M) \cap G_i\} \cup \{\iota_{\text{cfg}}(B)\} \\ &= (\text{BP}(\iota_{\text{cfg}}(M)) \cap H_i) \cup \{\tilde{B}\} = \text{BP}(\iota_{\text{cfg}}(M)). \end{aligned}$$

Nodes  $B, \tilde{B}, J$ , and  $\tilde{J}$  do not have branch parents.

Lastly, for a while loop, let  $H$  be the CFG with branch node  $\tilde{B}$ , join node  $\tilde{J}$ , and sub-graph  $H_S$ . Let  $G$  be the unrolled CFG with  $B_i$  branch nodes,  $J_i$  join nodes, and  $G_i$  sub-graphs.

Every node  $M$  in  $G_i$  has branch parents  $(\text{BP}(M) \cap G_i) \cup \{B_1, \dots, B_i\}$ .

The CFG node  $\iota_{\text{cfg}}(M) \in H_S$  has branch parents  $(\text{BP}(\iota_{\text{cfg}}(M)) \cap H_S) \cup \{\tilde{B}\}$ .

Since  $\iota_{\text{cfg}}(B_j) = \tilde{B}$  and by induction assumption  $\text{BP}_{\text{cfg}}(M) \cap H_S = \text{BP}(\iota_{\text{cfg}}(M)) \cap H_S$ , we get

$$\begin{aligned} \text{BP}_{\text{cfg}}(M) &= \{\iota_{\text{cfg}}(M') : M' \in \text{BP}(M) \cap G_i\} \cup \{\iota_{\text{cfg}}(B_1), \dots, \iota_{\text{cfg}}(B_i)\} \\ &= (\text{BP}(\iota_{\text{cfg}}(M)) \cap H_S) \cup \{\tilde{B}\} = \text{BP}(\iota_{\text{cfg}}(M)). \end{aligned}$$

□

STATEMENT. Let  $H$  be the CFG and  $G$  the unrolled CFG of program  $S$ . For each node  $M \in G$  the following equation holds.

$$\text{prov}(M, x) = \text{prov}(\iota_{\text{cfg}}(M), x) \quad (12)$$

PROOF. Follows directly from the two equalities  $\{\iota_{\text{cfg}}(M') : M' \in \text{RD}(M, x)\} = \text{RD}(\iota_{\text{cfg}}(M), x)$  and  $\{\iota_{\text{cfg}}(M') : M' \in \text{BP}(M)\} = \text{BP}(\iota_{\text{cfg}}(M))$ , since  $\text{prov}(M, x)$  is defined in terms of RD and BP. □

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