Automatic Alignment of Sequential Monte Carlo Inference in Higher-Order Probabilistic Programs

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Abstract. Probabilistic programming is a programming paradigm for expressing flexible probabilistic models. Implementations of probabilistic programming languages employ a variety of inference algorithms, where sequential Monte Carlo methods are commonly used. A problem with current state-of-the-art implementations using sequential Monte Carlo inference is the alignment of program synchronization points. We propose a new static analysis approach based on the 0-CFA algorithm for automatically aligning higher-order probabilistic programs. We evaluate the automatic alignment on a phylogenetic model, showing a significant decrease in runtime and increase in accuracy.

1 Introduction

Probabilistic programming\textsuperscript{7,8,9,14,24} is a programming paradigm for expressing probabilistic models. A probabilistic programming language (PPL) includes two constructs: one for sampling from probability distributions, and one for conditioning on data. We use a construct called weight for the latter, which simply adds its argument to a logarithmic weight attached to the current execution. This is commonly done for numerical stability.

One motivation for using probabilistic programming is greater expressive power compared to classical approaches to probabilistic modeling, such as Bayesian networks. This increase in expressive power comes from two properties: stochastic branching, i.e. that control flow can depend on randomness, and recursion. A PPL with these two properties is called a universal PPL\textsuperscript{7}.

The most important component of a PPL is its inference algorithm, which is loosely analogous to the execution semantics of ordinary programming languages. Sequential Monte Carlo (SMC) methods\textsuperscript{11} are commonly used as such inference algorithms\textsuperscript{8,14,24}. They perform inference by executing a number of instances of a probabilistic program in parallel, pausing the executions when they encounter a conditioning on data. When all executions have been paused, the algorithm looks at the weights of the different executions given the data,
and resamples the set of executions proportional to these weights. That is, more probable executions are replicated, and less probable executions are discarded. This process repeats until the program has reached its end. There are, however, problems with this approach. The toy program in Fig. 1 encodes a probability distribution over booleans using a stochastic branch. The different executions in SMC inference for the program will encounter a different number of calls to weight, either three or two. Furthermore, they will not always align at the same weight statements simultaneously—it is possible that one execution can pause at line 3, while another pauses at line 7. In Fig. 1 if we are only running a moderate number of executions in total (say 10000), with overwhelmingly high probability, all executions ending up at line 3 will be discarded; this is because of their low weight ($e^{5+10}$) relative to the other weight at line 7 ($e^{5+95}$). We can clearly see, however, that in the end both branches should be equally weighted.

The problem illustrated in Fig. 1 is not handled optimally by a direct implementation of SMC. Such implementations are, for instance, available in WebPPL [8] and Anglican [24]. When performing SMC inference on an equivalent program in WebPPL, the algorithm performs inference without any visible errors, but only returns true. In Anglican, an error is given at runtime, stating that some observe statements are not global. This error is given for all programs where different executions do not have the same number of calls to weight.

It is possible for users to manually align unaligned programs, taking care to only place calls to weight where they are aligned. However, for larger programs, manual alignment can become an error-prone process, and a nuisance for the programmer. In this paper, we propose an automatic solution for aligning higher-order probabilistic programs using static analysis. The static analysis is used to find all dynamic terms in a program—that is, terms that may be reached from within a stochastic branch. In Fig. 1 all terms within both branches of the if

5 Anglican uses a different construct for conditioning on data called observe.
expression are dynamic, since the condition is random. In particular, the calls to `weight` on lines 3, 4, and 7 are dynamic, and hence unaligned. The call to `weight` on line 1 is not dynamic, however, and is therefore aligned. By identifying all unaligned `weight` calls, we can handle these specially when running SMC, making the SMC inference aligned. The contributions are:

- A static analysis algorithm, based on 0-CFA \[21,22\], for discovering dynamic terms in higher-order probabilistic programs (Section 3).
- An application of the above analysis, where the resulting dynamic terms are used to automatically align SMC inference for higher-order probabilistic programs (Section 4).
- An evaluation of our automatic alignment approach for SMC inference, compared to the unaligned SMC implementation, as found in WebPPL\[6]. This evaluation is performed through a case study on a model from phylogenetics (Section 5).

Before describing our contributions in detail, Section 2 will provide some necessary background.

2 Preliminaries

In this section, we give a brief introduction to a classical SMC method for Bayesian networks. This background is needed to understand the inference semantics of the PPL presented in the later sections.

**Bayesian networks.** A Bayesian network \[18\] is a directed acyclic graph where the vertices are random variables and the edges direct dependencies between them. An example of a Bayesian network is given in Fig. 2. The random variables \(X_i\) are the exact positions of some moving object at time \(i\). The random variables \(Y_1, Y_2,\) and \(Y_3\) are noisy observations of the positions with values given in the figure (shaded in the graph). For more details on probability theory and Bayesian networks, see e.g., Bishop \[3\].

\[6\] We compare to the SMC algorithm found in WebPPL, since the Anglican SMC algorithm does not handle unaligned programs.

\[p(x_1) = \mathcal{N}(0, 2^2)\]
\[p(x_i | x_{i-1}) = \mathcal{N}(x_{i-1} + 4, 1^2), \ i \in \{2, 3, 4\}\]
\[p(y_i | x_i) = \mathcal{N}(x_i, 1^2), \ i \in \{1, 2, 3\}\]

**Fig. 2.** A Bayesian network representation of a simple linear Gaussian state space model. The symbol \(\mathcal{N}\) is a notation for the ubiquitous normal distribution.
Observe $Y_1$ | Observe $Y_2$ | Observe $Y_3$ | Result
---|---|---|---
$X_1 \approx -2.5$ | $X_2 \approx 8.9$ | $X_3 \approx 11.5$ | $X_4 \approx 15.9$
$X_1 \approx 4.7$ | $X_2 \approx 8.0$ | $X_3 \approx 12.3$ | $X_4 \approx 16.1$
$X_1 \approx 4.6$ | $X_2 \approx 9.2$ | $X_3 \approx 11.9$ | $X_4 \approx 15.4$
$X_1 \approx -3.2$ | $X_2 \approx 8.1$ | $X_3 \approx 12.1$ | $X_4 \approx 18.0$
$X_1 \approx -2.8$ | $X_2 \approx 9.9$ | $X_3 \approx 11.8$ | $X_4 \approx 15.7$

Fig. 3. A resampling illustration for a bootstrap particle filter with 5 simulations. The nodes are colored according to their weight—the darker nodes indicate more likely samples given the observation. The lines indicate how simulations survive, and possibly replicate, to the next step. No lines means a simulation is discarded. In the result, all samples of $X_4$ have the same weight, because there is no $Y_4$ observation.

**Sequential Monte Carlo.** Consider again the example of a Bayesian network given in Fig. 2. We are now interested in inferring the marginal probability distribution $p(x_4 \mid y_1, y_2, y_3)$—that is, the distribution over the next location of the moving object given all of our observations up until this point. For this particularly simple model, we can compute the exact solution in closed form by using standard results from probability theory applied to the equations in Fig. 2. In more complex probabilistic models, an exact solution is most often not available. Instead, approximate inference such as SMC [11] or Markov chain Monte Carlo (MCMC) [10, 12] methods must be used. A basic Monte Carlo method is likelihood weighting—simply simulate the model repeatedly, and weigh each simulation based on the observed variables. This does not perform well for most models of interest, and we can instead use an SMC method—the **bootstrap particle filter** [9]. The key idea in the bootstrap particle filter is that we run many simulations in parallel, and resample simulations whenever encountering an observation. Intuitively, resampling means that less likely simulations are discarded and replaced by more likely simulations. This is illustrated in Fig. 3 for the model in Fig. 2. The resampling is especially obvious when encountering the first observation $Y_1$—only two simulations of $X_1$ make sense according to $Y_1$, and these simulations are the only two surviving to the next step. In general, we can always run SMC inference on a Bayesian network by finding a topological ordering over the random variables in the network, and then simulating the network in that order. SMC is, however, not always the preferred method of inference, depending on the network structure. MCMC is, for instance, sometimes a better alternative for networks where observed nodes do not occur sequentially enough throughout the network.

Fig. 4 shows a histogram of the samples produced by running the bootstrap particle filter with 10 000 simulations (also known as particles) on the model in Fig. 2. We are only interested in some of the unobserved random variables.
Fig. 4. The result of running a bootstrap particle filter with 10,000 simulations for the model in Fig. 2. The normalized histogram shows the samples from the particle filter, and the dashed line shows the exact solution, which is available for this particular model.

```plaintext
1 function sim(stop, lambda) {
2 t = sample(exponential(lambda))
3 if t <= stop then {
4    weight(2.0)
5    sim(stop-t, lambda+0.1)
6 } else t
7 }
8
9 lambda = sample(gamma(1.0, 1.0))
10 stop = sample(gamma(1.0, 1.0))
11 sim = sim(stop, lambda)
12 weight(sim+lambda)
13 lambda
```

Fig. 5. A probabilistic program, written in our own functional, higher-order PPL.

Fig. 2. Note that the exact solution \( p(x_4 \mid y_1, y_2, y_3) \) is shown with the dashed line. For more details on SMC, see e.g., Doucet et al. [6].

*Probabilistic programming: an example.* We gave a small toy example of a probabilistic program in Section 1. Here, we give a slightly bigger example, shown in Fig. 5. The language contains a construct `sample` for sampling from probability distributions, and a `weight` construct as seen before. The `sample` construct is equivalent to the unobserved random variables in a Bayesian network, and `weight` is related to the observed random variables in a network. The program is a smaller version of the phylogenetic model used for the case study in Section 5, but still demonstrates the alignment problem because `sim` recursively calls itself from a stochastic branch (line 5) and contains a call to `weight` (line 4). Hence, this call to `weight` should intuitively be marked dynamic, since it might not be properly aligned. Besides having stochastic branches and recursion, probabilistic programming languages also differ from Bayesian networks by defining an explicit ordering over random variables in the program. Such an ordering has to be provided separately for Bayesian networks before performing inference.

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8 Observing a random variable \( Y \) with probability distribution \( p(y) \) as in a Bayesian network can be expressed as \( \text{weight}(\log p(y)) \), where \( y \) is the concrete observation.
3 Discovering dynamic terms

As a first step, we perform a static analysis of our input program. The goal of this analysis is to, for every term in the program, decide whether or not this term can appear within a branch of an if expression with a stochastic condition. We say that such a term is dynamic. As we will see in Section 4, the information produced by the analysis is key for aligning the SMC inference correctly. We begin by introducing the target language of the analysis. After this, we outline the analysis with examples and give a formalization. Lastly, we discuss the limitations of the approach.

3.1 The target language

In order to simplify the presentation of the upcoming analysis, we begin by introducing a PPL with just enough constructs to make it universal. Fig. 6 states the abstract syntax for such a language, based on the untyped lambda calculus. Most importantly, the language contains sample and weight constructs. Furthermore, the language also includes if expressions, for which sampled values can be passed as the conditions. This, together with the inherent recursion available in the untyped lambda calculus, makes the language a minimal universal PPL. Extending the language to a more complete probabilistic programming language such as the language in Fig. 5 (which also contains various syntactic sugars) is straightforward, and has been done for the case study in Section 5.

For convenience when later defining our algorithm, we split the language into two production rules, e and t, where e is a labeled version of t. For all programs in the language, we assume a unique labeling of all expressions, and that all variables are bound in at most one place (which means that all variable names are unique). Any program can be transformed to fulfill this without any input from the programmer. The unique labels and variables are requirements for the static analysis.

Also included in the language is a set of constants C. We leave this set unspecified, with boolean, real numbers, and the unit element as exceptions. The reason for explicitly including boolean in the set of constants is because they are needed for if expressions. Additionally, real numbers are needed as
\[ v ::= c | \lambda x. t \]

\[ F ::= \square t_2 | v_1 \square | \text{fix} \square | \text{if} \square \text{then} t_2 \text{ else} t_3 | \text{sample} \square | \text{weight} \square \]

\[
\begin{align*}
& \frac{t \mid w \rightarrow t' \mid w'}{(\text{CONG})} \\
& \frac{F[t] \mid w \rightarrow F[t'] \mid w'}{(\text{APP})} \\
& \frac{\text{fix} (\lambda x. t_1) \mid w \rightarrow [x \mapsto \text{fix} (\lambda x. t_1)] t_1 \mid w}{(\text{FIX})} \\
& \frac{\text{if} \; \text{true} \; \text{then} \; t_2 \; \text{else} \; t_3 \mid w \rightarrow t_2 \mid w}{(\text{IFTRUE})} \\
& \frac{\text{if} \; \text{false} \; \text{then} \; t_2 \; \text{else} \; t_3 \mid w \rightarrow t_3 \mid w}{(\text{IFFALSE})} \\
& \frac{c \in D \hspace{1cm} \text{sample} \; c \mid w \rightarrow \text{sample}(c) \mid w}{(\text{SAMPLE})} \\
& \frac{c \in \mathbb{R} \hspace{1cm} \text{weight} \; c \mid w \rightarrow () \mid w + c}{(\text{Weight})}
\end{align*}
\]

Fig. 7. An evaluation relation \( \rightarrow \) for the language given in Fig. 6 with all labels ignored. The function \( \text{sample} \) correctly produces a sample from the provided distribution. All congruence rules are compactly described by \( \text{Cong} \), which specifies one rule for every case in \( F \). \( F[t] \) means that we replace the \( \square \) in one case in \( F \) with \( t \).

arguments for \( \text{weight} \), and the unit element as the result of a call to \( \text{weight} \). We also assume that various probability distributions \( \text{dist} \in D \) from which to sample are included in the set of constants, \( C \). We do, however, limit these distributions to not range over lambda abstractions, since this would complicate the analysis significantly.

Lastly, the language includes an explicit fixpoint operator \( \text{fix} \). Since we are dealing with the untyped lambda calculus, we could construct such an operator (the \( Y \) combinator) in the language itself. There is, however, an important difference between the two: the explicit fix point operator cannot be passed around as a value—it must be applied directly. As a consequence, we can make the analysis less conservative. That is, fewer terms will be marked as dynamic in comparison to using the \( Y \) combinator.

To give some more intuition for the language, we give a small-step operational semantics for it in Fig. 7. It is an ordinary call-by-value semantics for the untyped lambda calculus, with a weight \( w \) added in the evaluation relation. This weight is updated at calls to \( \text{weight} \), which is reflected in the rule \( \text{Weight} \). This semantics corresponds to obtaining a single sample from the distribution encoded by the program in a likelihood weighting inference algorithm. Likelihood weighting was briefly mentioned in Section 2. We will see how this semantics relates to SMC and resampling in Section 4.
3.2 The analysis

Finding dynamic terms is not straightforward, as can be seen from two simple examples. The first example is given by the following program (labels omitted):

\[(\lambda x. \text{if sample dist then } (x c_1) \text{ else } c_2) (\lambda y. y), \quad (1)\]

where \(\text{dist}\) is a distribution over booleans and \(c_1\) and \(c_2\) are constants. The analysis result for this program should, intuitively, be

\[(\lambda x. \text{if sample dist then } (\underline{x} c_1) \text{ else } \underline{c_2}) (\lambda y. y) \quad (2)\]

where the underlining shows all parts of the program which can appear within a stochastic branch. The right-hand side of the outermost application is bound by the left-hand side lambda abstraction, and can therefore appear in one of the branches. By regarding the entire program as a tree structure, we see that information has been propagated from the left-hand side of a node, to its right-hand side.

The reverse is also possible. Consider the following program:

\[(\lambda a. (\lambda b. a b) (\lambda c. c)) (\lambda d. \text{if sample dist then } (d c_1) \text{ else } c_2) \quad (3)\]

The analysis result for this program is given by

\[(\lambda a. (\lambda b. a b) (\underline{\lambda c. c})) (\lambda d. \text{if sample dist then } \underline{d} c_1 \text{ else } \underline{c_2}), \quad (4)\]

showing that information from the right-hand side of a node can propagate to its left-side.

We propose a solution for finding dynamic terms based on 0-CFA, a control-flow analysis algorithm for higher-order functional programming languages originally introduced by Shivers [21, 22]. The 0 in 0-CFA stands for context insensitivity. Many other, less conservative, approaches to control-flow in higher-order functional languages also exist [13]. We give details on the limitations of context insensitivity in Section 3.3 An example of a more accurate analysis is \(k\)-CFA, where \(k\) levels of context sensitivity are included in the analysis. This causes the analysis to run in exponential time, already for \(k = 1\). 0-CFA has worst-case time complexity \(O(n^3)\), where \(n\) is the size of the program. This is an upper bound, and might not affect how large programs can be handled in practice. The version of 0-CFA that we present here is based on Nielson et al. [17].

Generating the constraints. To give some intuition for the algorithm, we describe it with the program (1) as a running example. The first step is to assign each subterm a unique label:

\[
((\lambda x. (\text{if sample dist})^2 \text{ then } (x^3 c_1^4)^5 \text{ else } c_2^6)^7)^8 (\lambda y. y)^{910})^{11} \quad (5)
\]

As we will see, this labeling enables reasoning about possible flows of control in the program. We also define \(T = \{ (\lambda x. x)^8, (\lambda y. y)^{10} \}\), which is the set of all
lambda terms in the program. The bodies of the lambda terms are replaced by ·, since they are not required in the analysis. Next, we generate a set of constraints for the program. These constraints capture how both data and lambdas might flow between different locations in the program. Our goal is to find a minimal assignment to the unknown sets occurring in the constraints, such that the constraints are not violated. Such a solution is guaranteed to exist, and is key to finding all dynamic terms. The constraints generated for (5) are

\[\text{gen}(t) = \{ \begin{array}{l} \{\text{stoch}\} \subseteq S_2, \{(\lambda x.9)^{10}\} \subseteq S_{10}, \{(\lambda x.7)^8\} \subseteq S_8, \\ S_y \subseteq S_9, S_5 \subseteq S_7, S_6 \subseteq S_7, S_x \subseteq S_3, \\ \{(\lambda x.7)^8\} \subseteq S_8 \Rightarrow S_{10} \subseteq S_x, \{(\lambda x.7)^8\} \subseteq S_8 \Rightarrow S_7 \subseteq S_{11}, \\ \{(\lambda y.9)^{10}\} \subseteq S_8 \Rightarrow S_{10} \subseteq S_x, \{(\lambda y.9)^{10}\} \subseteq S_8 \Rightarrow S_9 \subseteq S_{11}, \\ \{(\lambda x.7)^8\} \subseteq S_3 \Rightarrow S_4 \subseteq S_x, \{(\lambda x.7)^8\} \subseteq S_3 \Rightarrow S_7 \subseteq S_3, \\ \{(\lambda y.9)^{10}\} \subseteq S_3 \Rightarrow S_4 \subseteq S_y, \{(\lambda y.9)^{10}\} \subseteq S_3 \Rightarrow S_9 \subseteq S_5 \end{array} \} \]

The variables \(S_1, S_2, \ldots, S_{11}, S_x, S_y\) denotes the unknown sets associated with each label or variable in the program. There are three types of constraints: direct, flow, and implication flow constraints. Direct constraints force a set \(S\) to contain a single abstract value \(av\), which can either be \text{stoch} or a lambda abstraction: \(av := \text{stoch} \mid (\lambda x.4)^i\). The first constraint in (6), \(\{\text{stoch}\} \subseteq S_2\), states that the term at label 2 in the program may be stochastic. By looking at (5), this is clearly true—the term at label 2 contains a sample from a distribution. We also have two other direct constraints, which states that lambda expressions may occur at the label where they syntactically originate. This must also clearly be true. The flow and implication flow constraints state how the abstract values flow between the sets. Flow constraints declare an immediate link between two sets. For instance, two of the flow constraints state that \(S_5\) and \(S_6\) must flow to \(S_7\), because the if expression at label 7 can evaluate to both its branches. Implication flow constraints, on the other hand, states that if an abstract value is in one set, this causes a flow between other sets. One such constraint is \(\{(\lambda y.9)^{10}\} \subseteq S_4 \Rightarrow S_4 \subseteq S_y\) which states that if the lambda with variable \(y\) occurs at the term with label 3, then the term at label 4 must flow to the variable \(y\). This is a simple consequence of how applications are evaluated. Formally, the constraints are given by

\[
\begin{align*}
\text{set} &:= S_l \mid S_x \\
\text{cstr} &:= \{av\} \subseteq \text{set} \quad \quad \quad \quad \quad \text{(Direct)} \\
&\mid \text{set}_1 \subseteq \text{set}_2 \\
&\mid \{av\} \subseteq \text{set}_1 \Rightarrow \text{set}_2 \subseteq \text{set}_3 \quad \text{(Implication flow)}
\end{align*}
\]

The constraint generation function \text{gen} is defined recursively in Fig. 8. The most intricate part of \text{gen} is the constraint generation for applications and fixpoints. Both produce two flow implication constraints for each lambda in \(T\), which we defined earlier. The application case is fairly intuitive: if a lambda
**Finding the dynamic terms.** The last step is to use the 0-CFA results to find dynamic terms. To do this, we do a depth-first left-to-right traversal of the program, flagging all terms (or, equivalently, their labels) occurring in the branch of
Algorithm 1 The final phase of the analysis. Uses the 0-CFA output to discover dynamic parts of the program. The input consists of the labeled program \(t\), and the results of the 0-CFA analysis \(S\) (that is, all the sets produced by the analysis). The function \(\text{labels}\) returns all labels within a term. The function \(\text{subexpr}\) returns all direct subexpressions of a term \(t\).

1: function \(\text{Dynamic}(t, S)\)  
2: \(\text{for } l' \in \text{labels}(t)\) do  
3: \(\text{Dyn}(l') \leftarrow \text{false}\) \triangleright Initialization  
4: \(\text{while } \text{mod} \) do  
5: \(\text{mod} \leftarrow \text{false}; \text{Recurse}(\text{false}, t')\) \triangleright Iterate until fixpoint  
6: \(\text{return } \{ l | l \in \text{labels}(t'), \text{Dyn}(l) = \text{true} \}\)  
7:  
8: function \(\text{Recurse}(\text{flag}, t')\)  
9: \(\text{if } \text{flag} \lor \text{Dyn}(l) \) then \(\triangleright \text{Mark dynamic terms}\)  
10: \(\text{if } \neg \text{Dyn}(l) \) then  
11: \(\text{Dyn}(l) \leftarrow \text{true}\)  
12: \(\text{mod} \leftarrow \text{true}\)  
13: \(\text{for } (\lambda x. l') l \in S_l \) do  
14: \(\text{if } \neg \text{Dyn}(l) \) then  
15: \(\text{Dyn}(l) \leftarrow \text{true}\)  
16: \(\text{mod} \leftarrow \text{true}\)  
17: \(\text{match } t \) with  
18: \(\text{if } t^1 \) then \(t^2\) else \(t^3\); \(\triangleright \text{Detect stochastic branches}\)  
19: \(\text{Recurse}(\text{flag}, t^1)\)  
20: \(\text{flag} \leftarrow \text{flag} \lor \text{stoch} \in S_l\)  
21: \(\text{Recurse}(\text{flag}, t^2); \text{Recurse}(\text{flag}, t^3)\)  
22: \(\lambda x. t^1; \) \(\triangleright \text{Detect previously marked lambdas}\)  
23: \(\text{Recurse}(\text{Dyn}(l) \lor \text{flag}, t^1)\)  
24: \(\text{otherwise: } \text{for } t^1 \in \text{subexpr}(t)\) do \(\text{Recurse}(\text{flag}, t^1)\)

a stochastic branch as dynamic. We can identify stochastic branches by checking if \text{stoch} is a member of \(S_l\), where \(l\) is the label of the condition term of an \text{if} expression. In (5), during traversal, we first go down the left branch of the outermost application and eventually reach

\[
(\text{if } (\text{sample dist}^1) \text{ then } (x^3 c_1^5 \text{ else } c_2^6))\text{.} \tag{9}
\]

We see that \text{stoch} is in \(S_2\), and the branch is therefore stochastic and we recursively flag the terms in the branches. Additionally, we flag the lambda term \((\lambda y. y^9)^{10}\), since it is in the set \(S_3\). Because of this, when we return to the outermost application and traverse down the right hand side, we can see that \((\lambda y. y^9)^{10}\) is flagged. Therefore, we also flag all terms enclosed in this lambda, which in this case is \(y^9\). To summarize, the result of performing this analysis on (5) with the help of (8) is \(\{3, 4, 5, 6, 9, 10\}\), which matches the result in (2) with the labels in (4). Note that \(y^9\) would not have been flagged if we would have done a right-to-left traversal. In general, we need to repeatedly traverse the program until
fixpoint, allowing all terms reachable from a stochastic branch to be flagged as
dynamic. The complete algorithm is shown in Algorithm\textsuperscript{1} We can reason about
the time complexity as follows: on every iteration, at least one label is flagged
or the program terminates. Since we have \( n \) labels, where \( n \) is the size of the
program, and every iteration is performed in \( n \) steps, it follows that the algo-
rithm (in the worst case) terminates in \( O(n^2) \) steps—less than the \( O(n^3) \) for the
0-CFA analysis. Therefore, the overall complexity is still \( O(n^3) \).

3.3 Limitations

The main limitation of the algorithm presented in this paper is the lack of con-
text sensitivity in the analysis. In practice, this will cause problems when reusing
functions in both stochastic and non-stochastic contexts—the non-stochastic
contexts will sometimes be unnecessarily marked as stochastic. As an exam-
ple, consider running the analysis on a program written in the same language as
in Fig. 1 and Fig. 5:

\begin{verbatim}
function plus(a, b) { a + b }
plus(sample(normal(0,1)), 2)
if plus(1, 3) < 5 then true else false
\end{verbatim}

Our analysis has marked the branches of the \texttt{if} expression as dynamic, even
though the condition is clearly not stochastic. This is because of context insen-
sitivity: the analysis cannot distinguish between the two applications of plus.
Since one of the applications produces a stochastic value, \textit{all} applications of plus
in the program are marked as stochastic—even if they are in fact not stochastic.
In this paper, we avoid this problem by using built in operators which cannot
be passed around the program as values in the same way as user-defined lambda
abstractions. This makes the analysis less conservative when using 0-CFA. An
obvious direction for future work is exploring other approaches to higher-order
control flow analysis that do take context into account\textsuperscript{13}.

4 Utilizing the Analysis Results for Sequential Monte
Carlo Inference

In this section, we use the analysis result from Section\textsuperscript{3} to transform the input
program, enabling \textit{aligned} SMC inference. Most importantly, we indicate how
to modify the semantics of Fig.\textsuperscript{7} to accommodate such inference, and also give
the aligned SMC algorithm for probabilistic programming. We use the program
from Section\textsuperscript{2} Fig.\textsuperscript{5} as a running example, assuming that the semantics include
proper extensions for arithmetic and comparison.

\textit{Transforming the program.} We begin by extending our language with one addi-
tional construct: \texttt{dweight} (dynamic weight). In contrast to \texttt{weight}, the \texttt{dweight}
construct will not cause resampling to be performed. By using the information
about dynamic terms from our static analysis, we do a simple transformation of our input program: we replace all dynamic weight terms with dweight (ignoring labels, since they are no longer required). The remaining calls to weight are now aligned—they are (1) always executed, and (2) always executed in the same order. This is a simple consequence of them not being reachable from stochastic branches. The transformation allows SMC inference to only resample at aligned calls to weight in the original program. As an example, for the program in Fig. 5, the call to weight at line 4 will be replaced by dweight, and the weight at line 13 will be untouched.

Modifying the semantics. Next, we modify our semantics to support SMC inference. In order to do this, we first need to do another program transformation to enable pausing and resuming executions when resampling. We will not go into detail about this transformation here, but the result is a program in continuation-passing style (CPS) \[2,23\]. Such a transformation is commonly used in PPLs, for instance in WebPPL and Anglican. The essential property of having the program in CPS is that functions never return. Instead, every function takes an additional argument, a continuation function, which is applied to the result of the function application in order to continue evaluation. The continuation can be thought of as a representation of the call stack that is explicitly available at each function call. In essence, this enables us to modify our evaluation relation \( \rightarrow \) so that we can pause and resume evaluation at calls to weight. To enable pausing, we explicitly add a pause term in our language. In the CPS transformed language, the weight, dweight, and pause terms all take one extra continuation argument \( t_c \). That is, \( t ::= \ldots | weight \ t_c \ t | dweight \ t_c \ t | pause \ t_c \). The key modification in the semantics for weight is shown in Fig. \[9\]. For dweight, we simply update the weight and take a step to \( t_1 \), the body of the continuation. This is a CPS equivalent of the previous rule for weight in Fig. \[7\]. For the new weight, we instead want to indicate to the inference algorithm that the program is paused. Therefore, we return a pause term, with the continuation as argument. There is no evaluation rule for pause, so the evaluation halts, and it is up to the SMC inference algorithm to decide the next course of action.

Aligned sequential Monte Carlo. The algorithm for aligned SMC is shown in Algorithm \[2\]. The intuition is quite simple: do \( n \) executions of the program using \( \rightarrow \) and stop whenever encountering an aligned weight to resample before continuing the executions by applying () to the continuations. Note that we use the alignment property at line 4, assuming that if \( r_1 \) is a pause term, then...
Algorithm 2 The algorithm for aligned SMC inference in probabilistic programs. The *eval* function repeatedly applies $\rightarrow$ on a program $t$ with weight $w$ until no evaluation rule is applicable. The input $n$ gives the number of executions, or particles.

1: function AlignedSMC($t, n$)  
2:     for $i \leftarrow 1$ to $n$ do $t_i \leftarrow t$ \hfill $\triangleright$ Create $n$ copies of $t$  
3:     for $i \leftarrow 1$ to $n$ do $r_i \leftarrow \text{eval}(t_i, 0)$  
4:         while $r_1 = \text{pause}(\lambda x. t) | w_1$ do \hfill $\triangleright$ Check if weight has been encountered.  
5:             for $i \leftarrow 1$ to $n$ do $(\text{pause} t_i | w_i) \leftarrow r_i$  
6:         $t_{1:n} \leftarrow \text{resample}(t_{1:n}, w_{1:n})$  
7:     for $i \leftarrow 1$ to $n$ do $r_i \leftarrow \text{eval}(t_i(), 0)$  
8:     for $i \leftarrow 1$ to $n$ do $(t_i | w_i) \leftarrow r_i$  
9:     $t_{1:n} \leftarrow \text{resample}(t_{1:n}, w_{1:n})$  
10: return $\{t_1, t_2, \ldots, t_n\}$

this will also be true for all other $r_i$. Also note that we set all weights to 0 after resampling. This is because resampling, by definition, produces a set of unweighted samples (in our case executions) from a set of weighted samples. When finished, the *eval* function will return a final value with an attached weight. After doing a final resample (the weights can have been modified by calls to *dweight* since the last resample), the values are returned as samples. For the program in Fig. 5, the algorithm would run all particles until encountering the single call to *weight* (line 13), accumulating the weights for each particle when encountering differing number of calls to *dweight* (line 6). Hence, there will only be two resamples: one at the *weight* at line 13, and one at the end of the program.

5 Case study

In this section, we give the details on a case study for a probabilistic model from phylogenetics, expressed as a probabilistic program. We begin by briefly describing the implementation of the analysis presented in Sections 3 and 4. This is followed by a description of the model, and the quantity of interest that we wish to estimate using SMC. Lastly, we present the results of the case study in the form of a comparison between aligned and unaligned SMC, and discuss the main limitations of our algorithms. All source code used in this case study is available at [https://github.com/miking-lang/pplcore](https://github.com/miking-lang/pplcore).

Implementation. The implementation language extends the abstract syntax and semantics of the language in Fig. 5 and Fig. 6 with various operators for arithmetic and comparison. Examples of the concrete syntax is given in Fig. 5 and Fig. 6. Our implementation of aligned SMC implements the analysis from Section 5 and follows Algorithm 2. Additionally, we implement unaligned SMC, based on the approach used in WebPPL 8]. In this version of SMC, dynamic
calls to weight also participate in resampling, as well as executions that have already terminated (which can occur since alignment is not guaranteed). We use systematic resampling \cite{5} for both versions of SMC. Everything is implemented in OCaml.

The model and the inference problem. We test the performance of the algorithms by using an example from statistical phylogenetics, in which a birth-death model is used to describe the rates of speciation and extinction in a group of organisms. Such models are of considerable interest to evolutionary biologists, as they can be used to study many important phenomena, such as the effects of various life-history traits or of environmental factors on net diversification rates \cite{16}. A famous research problem that can be addressed using birth-death models is the question of whether the extinction of dinosaurs at the end of the Cretaceous epoch caused an increased diversification rate in mammals \cite{19}.

In typical cases, we only have reliable observations of the extant species of the group, that is, the lineages that have survived until the present—the extinct lineages are unknown to us. From DNA sequence data and calibration fossils, we can reconstruct a time tree that describes how and when the extant lineages diverged from each other; this is known as a reconstructed tree \cite{15}. The task is now to estimate the speciation (birth) and extinction (death) rates from such a reconstructed time tree.

We focus on the basic task of estimating the normalizing constant for a particular set of birth and death rates and a given reconstructed time tree. That is, we force the model to always produce the same sample of the rates, and instead produce estimates of how likely this sample is given the data. The logarithm of this quantity can be estimated with SMC through

\[
\sum_{t=1}^{T} \left( \log \sum_{i=1}^{N} \exp(w_i^t) - \log N \right) \tag{10}
\]

where \( t \) ranges over all resampling points in the program, and \( w_i^t \) denotes the weight of execution \( i \) at resampling point \( t \). \( N \) is the total number of executions. The normalizing constant can be used for Bayesian model comparison of different scenarios; they can also be used in a nested particle MCMC approach, in which SMC is combined with MCMC to estimate a posterior distribution over birth and death rates.

Specifically, we use a consensus estimate of the divergence times of the 28 extant species of pitheciid monkeys provided by the TimeTree project \cite{1}. The tree has one trichotomy involving \textit{Chiropotes albinasus}. We resolve this ambiguity by assuming that \textit{C. albinasus} belongs to \textit{Chiropotes}, and that the stem lineage of \textit{Chiropotes} existed for 0.2 Ma before branching into extant species. This is similar to the shortest branch length observed in other parts of the tree. The birth rate is set to 0.2 Ma\(^{-1}\) and the death rate to 0.1 Ma\(^{-1}\).

In summary, the input data is a tree over which we simulate a birth-death process. Because of this, we have a mix of aligned and unaligned calls to \texttt{weight}—
aligned calls occur when traversing the nodes in the input tree, and unaligned calls occur when simulating along edges in the tree.

Result. The result of our case study is shown in Fig. 10 using box plots for 100 estimates produced from (10) on our phylogenetic model for different number of executions. The exact solution is available analytically for this model and is shown with the dashed line. We see that the aligned version gives better estimates in all cases. In addition, we measured aligned SMC to be approximately 1.66 times faster on average than unaligned SMC for this model.

Discussion. Looking back at the nonoptimal results for unaligned SMC in Section 7, the improvement of aligned over unaligned SMC (for the same number of executions) in this case study intuitively makes sense. However, it seems that, even when using the unaligned version, the result converges on the true value as the number of total executions increase. We can make the same observation for the example in Fig. 1 if we reduce the differences between the weights. By, for instance, setting weight(85) to weight(5), and weight(95) to weight(15), we do get approximately the same number of executions (taking the weights into account) for each branch when running enough executions in total. As long as a single execution from the false branch survives, it will have much higher weight in the end, thus offsetting the bias in the initial resampling. This implies that unaligned SMC is most likely correct, but that an enormous number of executions might be required, even for very simple models such as the model in Fig. 1.

The increase in speed from using aligned SMC most likely comes from simply doing less resampling while running the SMC algorithm.

6 Related work

Naturally, the work most closely related to ours can be found in papers on universal probabilistic programming languages using SMC, such as WebPPL [8].
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Anglican [24], and Birch [14]. Both WebPPL and Anglican are higher-order, functional PPLs, while Birch is an imperative, object-oriented PPL. Anglican includes many SMC algorithms, including different variations of particle MCMC [24]. Anglican also includes various MCMC methods. WebPPL includes fewer inference algorithms, but both SMC and MCMC methods are available. Birch performs SMC inference in combination with using closed-form optimizations at runtime, automatically yielding a more optimized version of SMC taking advantage of locally-optimal proposals and Rao–Blackwellization. None of the languages above, however, address the alignment issue presented in this article. In essence, the programmer needs to be aware of the internals of the SMC inference algorithm to write efficient models—the model and the inference algorithm have become coupled. Optimally, we would like the model and the inference to be as independent as possible. This is the goal of the work in this paper.

There also exists more theoretical work on SMC for probabilistic programming. One example is a recent denotational validation of SMC in probabilistic programming given by ´Scibior et al. [20]. This work also includes a denotational validation of trace MCMC, another common inference algorithm for PPLs. Trace MCMC has also been proven correct by Borgström et. al. [4] through an operational semantics for a probabilistic untyped lambda calculus.

7 Conclusion

In this paper, we have introduced an approach for aligning SMC inference in PPLs. This approach consists of performing a static analysis using 0-CFA, and using this analysis result to automatically align SMC inference through a program transformation. We have also evaluated this approach on a phylogenetic model, showing significant improvements. In conclusion, we have shown that alignment of SMC inference in probabilistic programming can be done automatically, and that it also has a significant effect on both execution time and accuracy.

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