Lazy object copy as a platform for population-based probabilistic programming

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Abstract

This work considers dynamic memory management for population-based probabilistic programs, such as those using particle methods for inference. Such programs exhibit a pattern of allocating, copying, potentially mutating, and deallocating collections of similar objects through successive generations. These objects may assemble data structures such as stacks, queues, lists, ragged arrays, and trees, which may be of random, and possibly unbounded, size. For the simple case of $N$ particles, $T$ generations, $D$ objects, and resampling at each generation, dense representation requires $O(DNT)$ memory, while sparse representation requires only $O(DT + D N \log DN)$ memory, based on existing theoretical results. This work describes an object copy-on-write platform to automate this saving for the programmer. The core idea is formalized using labeled directed multigraphs, where vertices represent objects, edges the pointers between them, and labels the necessary bookkeeping. A specific labeling scheme is proposed for high performance under the motivating pattern. The platform is implemented for the Birch probabilistic programming language, using smart pointers, hash tables, and reference-counting garbage collection. It is tested empirically on a number of realistic probabilistic programs, and shown to significantly reduce memory use and execution time in a manner consistent with theoretical expectations. This enables copy-on-write for the imperative programmer, lazy deep copies for the object-oriented programmer, and in-place write optimizations for the functional programmer.

1 Introduction

Probabilistic programming aims at better accommodating the workflow of probabilistic modeling and inference in general-purpose programming languages. Probabilistic programming languages (PPLs) support stochastic control flow, allow probability distributions to be expressed over rich data structures and higher-order functions, and are able to marginalize and condition random variables using various inference techniques.

Among various approaches to the design and implementation of PPLs, this work is most concerned with a category that might be called population-based. In a population-based PPL, multiple executions of a model are maintained at any one time, via an inference method such as the particle filter (see e.g. Doucet and Johansen [2011] or Sequential Monte Carlo (SMC) sampler (Del Moral et al., 2006). PPLs with support for such methods include LibBi (Murray, 2015), Biips (Todeschini et al., 2014), Venture (Mansinghka et al., 2014), Anglican (Tolpin et al., 2016), WebPPL (Goodman and Stuhlmüller, 2014), Figaro (Pfeffer, 2016), and Turing (Ge et al., 2018). The population-based approach contrasts with, for example, gradient-based approaches that make use of automatic differentiation to compute gradients for an inference method such as Hamiltonian Monte Carlo, maximum likelihood or variational inference. Some of the above languages support this approach also. Other popular languages with support for gradient-based inference include Stan (Stan Development Team, 2013) and Pyro (Bingham et al., 2019).

Recent efforts have targeted tensor-based systems such as PyTorch (Paszke et al., 2017) and TensorFlow (Abadi et al., 2015). PPLs such as Pyro (Bingham et al., 2019) and Probabilistic Torch (Siddharth et al., 2017) use the former, Edward (Tran et al., 2017) and TensorFlow Probability (Dillon et al., 2017) the latter. These platforms are well-established for deep learning, offer dense representations and automatic differentiation, and are well-suited to gradient-based methods on models of bounded size. They are less suited to population-based methods on models of potentially unbounded size, which may use stochastic control flow in a way that causes multiple executions to diverge, and be difficult to vectorize. Furthermore, they may use data structures such as stacks, lists, trees, and ragged arrays, the size of which may be unbounded and even random; they may grow or shrink as the program executes and require dynamic memory allocation and deallocation. Tensor-based platforms are not ideal for these data structures.

To better illustrate the memory usage pattern of a population-based probabilistic program, consider a state-space model of $T$ time steps with hidden states $x_{0:T}$ and observations $y_{1:T}$. The relationships between these are...
Figure 1: The state-space model as a directed graphical model, where arrows represent conditional dependencies, unfilled nodes represent latent variables, and filled nodes represent observed variables.

Figure 2: Example of a tree formed during execution of a particle filter. Time $t = 1, \ldots, T$ progresses from left to right. Each column represents a population of particles $x^{1:N}_t$ as circles, their areas proportional to $w^{1:N}_t$, each connected to its parent $x^{a_{t-1}}_t$ at the previous generation, chosen during resampling. The subtree reachable from the final generation is shown in black, the remainder in grey.

represented mathematically via the joint distribution:

$$p(x_0:T, y_1:T) = p(x_0) \prod_{t=1}^{T} p(y_t | x_t)p(x_t | x_{t-1}).$$

The model is represented graphically in Figure 1. We will consider the different ways in which this model might be represented programmatically, i.e. as a computer program, below.

A standard inference task for a PPL is, given observations $y_1:T$, to compute the posterior distribution $p(x_1:T | y_1:T)$. Various approaches are available based on exact or approximate inference. Consider the bootstrap particle filter (Gordon et al., 1993), a building block for more elaborate methods that include SMC as a generalization (Del Moral et al., 2006), particle Markov chain Monte Carlo (Andrieu et al., 2010) methods, which iterate a single filter, and SMC² (Chopin et al., 2013) methods, which run multiple filters simultaneously. Recent variational approaches also use particle filters to estimate objectives (Maddison et al., 2017; Naesseth et al., 2018). The bootstrap particle filter maintains $N$ number of weighted particles, each corresponding to an execution of the model:

1. For $n = 1, \ldots, N$, initialize particle $x^n_0 \sim p(x_0)$ and weight $w^n_0 = 1$.

2. For $t = 1, \ldots, T$ and $n = 1, \ldots, N$:
   
   (a) Resample $a^n_t \sim C(w^{1:N}_{t-1})$.
   
   (b) Propagate $x^n_t \sim p(x_t | x^{a^n_{t-1}}_{t-1})$.
   
   (c) Weight $w^n_t = p(y_t | x^n_t)$.

Here, $C(w^{1:N}_{t-1})$ represents the categorical distribution on $\{1, \ldots, N\}$ with associated unnormalized probabilities $\{w^{1:N}_1, \ldots, w^{1:N}_{N}\}$. At each step $t$, the particles $x^{1:N}_t$ with weights $w^{1:N}_t$ approximate the distribution $p(x_t | y_{1:t})$. The particles form a tree via the resampling step, as depicted in Figure 2 where for $t > 0$ each particle $x^n_t$ has $x^{a^n_{t-1}}_{t-1}$ as its parent.

For many models, $x^n_t \in \mathbb{R}^D$, for $D$ number of dimensions. A new generation is added at each time step, and previous generations are immutable, such that $x^{1:N}_t$ may be stored in a dense $D \times N \times T$ array (often called a tensor). To reduce memory use it is preferable, however, to make use of the ancestor indices $a^{1:N}_{1:T}$ to remove
entries that are not reachable from the latest generation. This is the case with LibBi [Murray 2015], for which 
the simple algorithm described and studied in [Jacob et al. 2015] was developed, which essentially uses a sparse 
representation for the dimension of the array associated with $T$. Jacob et al. (2015) establishes that the number 
of particles reachable from the $t$th generation is bounded above by $t + cN \log N$, for some constant $c$. This means 
that the dense approach requires $DNT$ storage, while the sparse approach requires at most $DT + cDN \log DN$. 
These are often interpreted for fixed $N$ and increasing $T$, where the memory saving approaches the constant 
factor $N$. In practice, where $T$ is known and an estimate of the likelihood $p(y_{1:T})$ is required, one typically 
chooses $N = O(T)$ to control the variance of that estimate. One rule-of-thumb to achieve this is to perform 
pilot runs with small $T$ and choose an appropriate $N$ by trial and error; then, one gradually increases $T$, and 
$N$ in proportion to it, until the full data set is accommodated or computational limits reached. Taking this 
perspective, the memory use for a task of size $T$ becomes more like $O(T^2)$ for the dense representation, reduced 
to $O(T \log T)$ for the sparse.

Models where $x^n_t$ is of some fixed type and size $D$ are the simplest case. Amongst the models evaluated in 
Section 4, $x^n_t$ includes stacks and ragged arrays of variable dimension, binary trees, accumulators of sufficient 
statistics for variable elimination, and mutation of previous states. All of these data structures are better 
represented sparsely, or with multiple memory allocations that can be separately deallocated, to enable the 
fastest algorithms for adding, deleting and updating elements. The purpose of this work is to easily enable such representations via a lazy object copy-on-write platform. The platform must, of course, produce correct results, but should also maximize object sharing, minimize object copying, and minimize the bookkeeping required to achieve this. The motivating usage pattern of tree-structured copies is used to direct design choices.

Immutable objects offer another paradigm. These are common in functional programming languages, but also 
occur in imperative languages such as Swift. Under this paradigm, in place of modifying an object, a program 
creates a new object with the desired alteration. Because this can greatly increase the number of object copies 
performed by a program, good performance relies on either the use of persistent data structures (see e.g. [Okasaki] 
1999) that create the appearance of incremental mutation without the computational expense, or copy elimination 
and in-place mutation as a compiler optimization (see e.g. [Gopinath and Hennessy] 1989). In a sense, immutable 
objects pose the converse problem to that of mutable objects: to determine when a copy is unnecessary, rather 
than when a copy is necessary. While not the focus of the present work, the proposed platform may be useful for 
this converse problem, allowing, for example, a compiler to aggressively apply copy elimination and in-place 
mutation, while deferring to runtime copy-on-write for correctness.

The operating system offers another alternative, as virtual memory pages are typically copy-on-write in modern 
operating systems. Paige and Wood (2014) make use of this facility, running particles as separate processes that 
fork and terminate during resampling. The approach proposed in the present work is finer-grained, working 
with individual objects rather than pages, and a single process (with multiple threads) rather than many. This 
increases the opportunity for sharing.

Section 2 provides a formal treatment of the ideas using directed labeled multigraphs. This is intended to make 
the motivation and correctness clear. In Section 3 a concrete implementation for the Birch PPL is sketched using 
smart pointers, hash tables, and reference-counting garbage collection. In Section 4 the approach is evaluated on 
a number of realistic probabilistic programs. Section 5 concludes.

2 Methods

The proposed approach develops in three steps, defining:

1. $F$ as a directed multigraph, where vertices represent objects, and edges the pointers between them, to 
demonstrate shallow and deep copies.

2. $G$ as a labeled directed multigraph that encodes one or more ongoing lazy copies, edges labeled with lists 
to identify them.

3. $H$ as another labeled directed multigraph, edges now labeled with single items to identify lazy copies 
within tree-structured patterns, with eager copies outside of these patterns.

Algorithms are provided to map $H$ to $G$ to $F$, making the equivalence and correctness of the latter two 
representations clear.
2.1 Shallow and deep copies

Definition 1. Let $F = (V, E, s, t, b)$ be a directed multigraph, where:

- $V$ is a set of vertices,
- $E$ is a set of edges,
- $s : E \rightarrow V$ maps each edge to its source vertex,
- $t : E \rightarrow V$ maps each edge to its target vertex,
- $b : V \rightarrow \cdot$ maps each vertex to its payload data, which will be of some composite type as defined by a class; these types need no be defined.

Vertices represent objects and edges the pointers between them. One particular vertex is the root vertex, which, rather than representing an object, encapsulates variables in global and local scopes. All vertices are reachable from the root vertex by a directed path. If a vertex becomes unreachable from the root vertex, it is assumed to be deleted by garbage collection. Each vertex has some payload data that does not require a formal specification, except to say that it contains pointers, which establish the out-edges. Changes to these pointers will change the out-edges accordingly, and so determine $s$ and $t$.

A copy (qualified, if necessary, to shallow copy) is applied to an edge $e \in E$. The effect is to create a new vertex $v$ with a copy of the payload data $b(t(e))$; this also copies the out-edges of $t(e)$. A pointer is then created in some other vertex $u$, creating a new edge $d$ with $s(d) = u$ and $t(d) = v$.

A deep copy is likewise applied to an edge $e \in E$. The effect is to copy the entire subgraph reachable from that edge, not just the immediate target vertex of the edge. This proceeds recursively. The first step is a shallow copy of $e$ to create a new vertex $v$, the next step is a shallow copy applied to each out-edge of $v$, and so on. The caveat is that each reachable vertex should be copied only once. This requires keeping a record of objects that have already been copied.

Figure 3 illustrates the effect of shallow and deep copy operations.

2.2 Lazy copies

The aim is to preserve the appearance of a deep copy, while eliminating unnecessary operations. Unnecessary copies occur when a deep copy is performed, but not all vertices in the reachable subgraph will need to be written, or even read, before they become unreachable. Lazy copies are proposed to achieve this, where multiple deep copies can be underway concurrently, and vertices are only copied when a write is necessary. This requires some bookkeeping, represented by a labeling scheme on the graph.

Definition 2. Let $G = (V, E, s, t, b, R, L, m, f, g)$ be a labeled directed multigraph, where $V$, $E$, $s$, $t$ and $b$ are as before, with new components:

- $R \subseteq V$ is a set indicating read-only vertices,
- $L$ is a set of labels, each of which identifies a distinct deep copy operation,
- $m : V \times L \nrightarrow V$ is a partial function that maps vertex and label pairs to another vertex, providing a memo of object copies,
- $f : V \rightarrow L$ assigns, to each vertex, a label identifying the deep copy operation that created it,
- $g : V \rightarrow [L]$ assigns, to each edge, a sequence of labels identifying the deep copy operations through which the target vertex is yet to be propagated.

Condition 1. Any vertex $v \in V$ that has been copied has also been marked read-only, i.e. for all $(v, l) \in \text{dom} \ m$, $v \in R$.

The graph $G$ is a compressed representation of $F$, combining identical vertices. The additional components can be seen as the bookkeeping necessary to restore $F$ from $G$. Algorithm $\square$ provides the means to restore $F$ from $G$, Figure $\square$ illustrates its application with examples.
Figure 3: Illustration of shallow and deep copy operations. On the left is the original graph. In the middle is the result of applying a shallow copy to the single out-edge of the root. On the right is the result of applying a deep copy to the same edge.

Figure 4: Two illustrations of restoring $F$ from $G$ using Algorithm 1. From left to right, an edge with a non-empty label is chosen (shown in color) and expanded to form the next state.

Algorithm 1. Repeating the following procedure restores $F$ from $G$:

1. Choose an edge $e \in E$ such that $|g(e)| > 0$ and $e$ is reachable from the root through a path in which each edge, $d$, along that path has $|g(d)| = 0$.

2. Let $v = t(e)$ and $l = \text{head}(g(e))$. If $(v, l) \in \text{dom} m$ then let $u = m(v, l)$, otherwise let $u$ be a copy of $v$ (i.e. $b(u) = b(v)$, implying updates to $s$ and $t$ also) with $f(u) = l$. Update $t(e) \leftarrow u$ and $g(e) \leftarrow \text{tail}(g(e))$.

Algorithm 1 can be applied on demand to read or write any desired vertex. Condition 2 establishes the interface to make the graph $G$ look like $F$ from the outside.

Condition 2. To read or write the data $b(v)$ of some vertex $v \in V$, that $v$ must be reachable from the root through a path in which each edge $e$ has $|g(e)| = 0$. Algorithm 1 can be applied to achieve this.

2.3 Lazy copies on a tree

The graph $G$ provides a straightforward way to reason about lazy copies, but for implementation, labeling edges with lists adds significant overhead. The motivating usage pattern suggests that copies tend to be tree-structured, and that edge labels in $G$ will be paths on this tree. Paths on trees can be represented more efficiently.

Definition 3. Let $H = (V, E, s, t, b, R, L, m, f, h, a)$ be a labeled directed multigraph where all but the last two components are as for $G$. Function $g$ is replaced with the function $h$ and a new partial function $a$:

- $h : V \rightarrow L$ assigns, to each edge, a single label,
- $a : L \rightarrow L$ is a partial function that assigns a parent to each label other than a particular label designated the root, and so arranging them in a tree.
Condition 3. For all $e \in E$, there exists an $n \geq 0$ such that $a^n(h(e)) = f(t(e))$, with the interpretation $a^0(l) = l$.

That is, the single label on each edge $e \in E$ is traced back through $a$ until arriving at the label of its target vertex $f(t(e))$. This restores a list that would be the equivalent label in $G$.

Algorithm 2. To restore $G$ from $H$, for each $e \in E$:

- if $h(e) = f(t(e))$, $g(e) = \emptyset$,
- otherwise, set $g(e) = [a^{n-1}(h(e)), \ldots, a(h(e)), h(e)]$ where $a^n(h(e)) = f(t(e))$.

The labeling scheme of $H$ requires only a single label per edge, which does not add much overhead, certainly compared to a list. It is not as expressive as the labeling scheme of $G$, which can accommodate arbitrary relationships between copy operations. The situations where this generality is required are uncommon in the motivating usage pattern, however, and when they occur, the proposed approach is to simply forego the lazy copy and trigger an eager deep copy.

2.4 Dynamics

The graph $H$ represents only a snapshot in time of the memory state. Of course, a program is dynamic, creating new vertices, writing data to create and delete edges between them, and garbage collecting vertices and edges that become unreachable. It is necessary to understand how it evolves dynamically as a program executes. A number of new concepts are necessary.

Definition 4. A thread of execution is considered to have a current context. This is a particular label $c \in L$, set as follows:

1. At the start of the program, it is set to some arbitrary label, considered the root context. This is also the root of the tree defined by $a$.
2. For some vertex $v \in V$, whenever its data $b(v)$ is being modified or a member function (sometimes called a method) of $v$ is executing, the current context is set to the label of that vertex, i.e. $c = f(v)$.

Condition 4. When a new vertex $v$ or new edge $e$ is created, its label is set to the current context, i.e. $f(v) = c$ or $g(e) = c$.

This means, for example, that if a member function of some vertex $v \in V$ is executing, any new vertices that it creates along the way are assigned the same label, $f(v)$. The current context can be maintained using a stack, initialized with the root label, pushing and popping labels as required by the above circumstances, and taking the top of the stack as the current context at any time. In a multithreaded environment, each thread requires its own context, and so maintains its own stack.

For convenience, the memo $m$ is partitioned by labels $l \in L$, where each $m_l$ contains all the entries of $m$ pertaining to $l$ and all of its ancestors. Flattening in this way makes it unnecessary to maintain the function $a$. We return to the motivation behind this in Section 3.

Definition 5. For $l \in L$, define $m_l : V \rightarrow V := \{u \mapsto v \in V : \exists k \in a^+(l)((u, k) \mapsto v \in m)\}$, where $a^+$ is the transitive closure of $a$.

Below, pseudocode for operations on the graph $H$ is provided, with worked examples of how real code triggers these operations as it executes. The basic links between the two are that a deep copy operation in real code, e.g. $y \leftarrow \text{deep\_copy}(x)$;

will trigger a Deep-Copy($x$) operation, as defined in pseudocode. Dereferencing an object to obtain the value of a member variable for reading, e.g. $\text{value} \leftarrow x.\text{value};$

will trigger a Pull($x$) operation, while for writing, e.g. $x.\text{value} \leftarrow \text{value};$

will trigger a Get($x$) operation.
As a simplification for pseudocode, assume that the sets $V$, $E$ and $L$ are automatically updated as objects are created, copied, modified, and garbage collected. For example, when a new object $v$ is created, the update $V \leftarrow V \cup \{v\}$ is implied, and likewise, if its payload data $b(v)$ is modified, $E$, $s$ and $t$ are updated accordingly.

For some function or partial function $\varphi$, the notation $\varphi(x) \leftarrow y$ is used to insert a new entry $x \mapsto y$, possibly replacing existing entries, i.e. $\varphi(x) \leftarrow y$ means exactly $\varphi \leftarrow \varphi \setminus \{x \mapsto \beta : \beta \in \text{ran } \varphi\} \cup \{x \mapsto y\}$.

A deep copy is initialized on an edge:

**Algorithm 3.**

```
DEEP-COPY(e ∈ E)
  Freeze(e)
  let $l$ be a new label
  set $m_l \leftarrow m_{h(e)}$
```

The `Freeze` is a recursive operation that marks reachable vertices as read-only; it is defined later.

Read access to a vertex requires repeated application of Algorithm 1 to a single edge until it cannot be applied further without creating a new vertex. This is encoded by the `Pull` operation:

**Algorithm 4.**

```
Pull(e ∈ E)
  let $v = t(e)$
  let $l = h(e)$
  while $(v, l) \in \text{dom } m$
    $v \leftarrow m_l(v)$
    update $t(e) \leftarrow v$
```

After application, $t(e)$ targets the correct vertex for reading. The pre-condition of Algorithm 1 is implicitly satisfied by the fact that the program could not have discovered the edge $e$ without having first acquired its source vertex $s(e)$ via a `Pull` operation, and so on recursively, back to the root vertex.

Write access to a vertex is encoded by the `Get` operation, which begins with `Pull`, but if the resulting vertex is frozen, it must be copied before writing:

**Algorithm 5.**

```
Get(e ∈ E)
  Pull(e)
  let $v = t(e)$
  let $l = h(e)$
  if $v \in R$
    let $u = \text{Copy}(e)$
    update $t(e) \leftarrow u, m_l(v) \leftarrow u$
```

After application, $t(e)$ targets the correct vertex for writing. The operation `Get` also has an implicit forwarding effect: write attempts on a read-only vertex are forwarded to a copy.

An optimization is possible here. In many cases, there is only a single in-edge to a vertex. There is no need to enter such vertices in $m_l$ when copied, as $m_l$ will never need to be queried for them.

**Remark 1 (Single-reference optimization).** Let $v \in R$ be such that:

1. at the time of being frozen, the in-degree of $v$ is 1 and $v \notin \text{ran } m$, and
2. at the time of being copied, all the in-edges of $v$ have distinct labels.

When copying such a $v$, for any $l$, it is not necessary to update $m_l$.

The first condition requires not only that the in-degree of $v$ is one, but also that it does not appear in the output of a memo. This is because its appearance in a memo may compactly represent more than one in-edge in the expanded graph. The condition is sufficient, but not necessary, for the optimization to be valid. A sufficient and necessary condition would require an expensive graph search. This optimization is particularly important, and its effect evaluated separately in Section 4.

The `Get` operation requires a shallow copy operation, which proceeds as follows:
Algorithm 6.

\text{COPY}(e \in E) \rightarrow V

\begin{align*}
& \text{let } v = t(e) \\
& \text{for } d \in \{ i \in E \mid s(i) = v \} \\
& \quad \text{if } h(d) \neq f(v) \\
& \quad \text{FINISH}(d) \\
& \quad \text{FREEZE}(d) \\
& \text{let } u \text{ be a new vertex with } b(u) = b(v) \\
& \text{return } u
\end{align*}

The conditional triggers an eager deep copy for usage patterns outside that of a tree. This occurs when copying some edge \(d \in E\) where \(h(d) \neq f(v)\). We call such edges cross references. Cross references are precisely those that are outside the tree-structured usage pattern, and can be represented in the labeling scheme of \(G\), but not \(H\).

The two operations \text{FINISH} and \text{FREEZE} have similar recursive structures. The first ensures that all vertices in the subgraph reachable from an edge are read-only, i.e. put in the set \(R\):

Algorithm 7.

\text{FREEZE}(e \in E)

\begin{align*}
& \text{let } v = t(e) \\
& \text{if } v \not\in R \\
& \quad R \leftarrow R \cup \{v\} \\
& \quad \text{for } d \in \{ i \in E \mid s(i) = v \} \\
& \quad \quad \text{FREEZE}(d)
\end{align*}

The second ensures that all lazy copies in the subgraph have been completed:

Algorithm 8.

\text{FINISH}(e \in E)

\begin{align*}
& \text{let } v = t(e) \\
& \text{if } h(e) \neq f(v) \\
& \quad \text{GET}(e) \\
& \quad \text{for } d \in \{ i \in E \mid s(i) = v \} \\
& \quad \quad \text{FINISH}(d)
\end{align*}

The intent is that real code will trigger the above operations, given in pseudocode, as it executes. Consider, first, the following class, intended to serve as the type of nodes in a singly-linked list of integers:

```java
class Node {
    value: Integer;
    next: Node;
}
```

The member variables \text{value} and \text{next} hold the value of the current node and a pointer to the next node, respectively. Assume that variables of primitive types like \text{Integer} are kept as values, while variables of class types like \text{Node} hold pointers to those objects, dynamically allocated.

This basic class is sufficient to explain how real code triggers the pseudocode operations. Table \text{I} provides an example of the standard usage pattern, where deep copy operations relate as a tree. Table \text{II} gives an example outside of the standard usage pattern, where there exists a cross reference, and an incorrect result would be produced if not for the special treatment of cross references in Algorithm \text{VI}.

3 Implementation

The proposed approach has been implemented for Birch [Murray and Schön 2018], an imperative and object-oriented language with copyable (multi-shot) coroutines and specialized operators that provide ergonomic support.
| Code | Operations | State | Commentary |
|------|------------|-------|------------|
| x1:Node; y1:Node; z1:Node; x1.next <- y1; y1.next <- z1; x2:Node <- deep_copy(x1); | DEEP-COPY($x_1$) | | A new label 2 is created, and a new edge, but no new vertex. |
| value <- x2.value; | PULL($x_2$) | | Read-only access, copy not required, state unchanged. |
| x2.value <- value; | GET($x_2$) ↲ COPY($x_1$) | | Write access, copy required. |
| y2:Node <- x2.next; z2:Node <- y2.next; | GET($y_2$) GET($z_2$) ↲ COPY($y_1$) ↲ COPY($z_1$) | | As each node in the list is accessed it must be copied, as write access is potentially required to update its next pointer. |
| value <- z2.value; | PULL($z_2$) | | Read-only access, copy not required, state unchanged. |
| z2.value <- value; | GET($z_2$) ↲ COPY($z_1$) | | Write access, copy required. |

Table 1: Example of the standard use case of several lazy deep copy operations related as a tree. As the program in the first column executes it triggers the operations indicated in the second column, updating the state of the multigraph depiction of the memory state in the third column.
| Code | Operations | State | Commentary |
|------|------------|-------|------------|
| `x1:Node;`<br>`x1.value <- 1;` |  |  |  |
| `x2:Node <- deep_copy(x1);`<br>`DEEP-COPY(x_1)` |  |  |  |
| `x2.value <- 2;`<br>`COPY(x_1)` |  |  |  |
| `x2.next <- x1;` |  |  |  |
| `x3:Node <- deep_copy(x2);`<br>`DEEP-COPY(x_2)` |  |  |  |
| `x3.value <- 3;`<br>`COPY(x_1) to y_3`<br>`FINISH(y_3)` |  |  |  |
| `y3:Node <- x3.next;`<br>`print(y3.value);`<br>`PULL(y_1)` |  |  |  |
| `x3.value <- 3;`<br>`COPY(x_2)` |  |  |  |
| `y3:Node <- x3.next;`<br>`print(y3.value);`<br>`PULL(y_1)` |  |  |  |

This establishes a cross reference: the vertex `x_2` has an outgoing edge with a different label (= 1) to itself (= 2).

Table 2: Example of a use case outside the standard, where assignment creates a cross reference, and a `FINISH` operation is triggered for correctness. The second last row depicts the correct behaviour, the last row depicts a counterfactual that would produce an incorrect result.
Another issue is that memos may keep objects reachable longer than necessary. This occurs when the only

Although not detailed here, atomic operations are used judiciously to ensure thread safety.

Finally, the choice to use $m_l$, given in Definition 5, requires some justification. As well as simplifying the

Reference counting facilitates the single-reference optimization described in Remark 1. The chosen implementation is to flag an object that meets the condition at time of freezing. It is allowed that reference counts on the object subsequently change, as long as each in-edge has a distinct label. This is violated only if an assignment occurs that creates an identical in-edge. In this situation GET is triggered on the edge, maintaining distinct labels.

The single-reference optimization avoids the update of a memo according to an object having only a single reference at the time of being frozen. This is different to copy elimination for an object having only a single reference at the time of being copied. This latter optimization is also used. It requires that a frozen object can be thawed for reuse.

Although not detailed here, atomic operations are used judiciously to ensure thread safety.
4 Evaluation

The implementation is evaluated with regards to execution time and memory use across a number of realistic probabilistic models and inference methods. Each test case is run for two tasks:

1. performing inference with a given data set, and
2. performing simulation with no data set.

No copies occur in the second task; its purpose is to isolate the additional resource requirements of lazy pointers. For each task there are three configurations:

1. eager copy,
2. lazy copy, and
3. lazy copy with the single-reference optimization.

These are compile-time configurations that compile away unnecessary bookkeeping. The problems are as follows:

1. **RBPF** A mixed linear-nonlinear state-space model as described in Lindsten and Schön (2010), with a Rao–Blackwellized particle filter via delayed sampling (Murray et al., 2018), with \( N = 2048 \) and \( T = 500 \) for both inference and simulation.

2. **PCFG** A probabilistic context-free grammar model (unpublished) with an auxiliary particle filter (Pitt and Shephard 1999) with custom proposal, \( N = 16384 \), \( T = 3262 \) for inference, and \( T = 2000 \) for simulation.

3. **VBD** A vector-borne-disease model as described in Murray et al. (2018), with dengue data set from Micronesia as in Funk et al. (2016), with a marginalized particle Gibbs method as described in Wigren et al. (2019) for 3 iterations, \( N = 4096 \), \( T = 182 \) for inference, and \( T = 400 \) for simulation. With this method, there is a deep copy of a single particle between iterations that must be completed eagerly, as it is outside the tree pattern.

4. **MOT** A multi-object tracking model for an unknown number of objects with linear-Gaussian dynamics, as described in Murray and Schön (2018), with simulated data, \( N = 4096 \), \( T = 100 \) for inference, and \( T = 300 \) for simulation.

5. **CRBD** A constant rate birth-death model over a tree with an alive particle filter (Del Moral et al., 2015) and delayed sampling as described in Kudlicka et al. (2019), with data set of cetacean phylogeny (Steeman et al., 2009), \( N = 5000 \) and \( T = 173 \) for both inference and simulation.

All combinations of task, configuration, and problem are compiled and run for 20 repetitions, on a system with two Intel Xeon E5-2680 CPUs (each 12 cores, 30 MiB cache) and 64 GiB memory. The C++ compiler used is GCC 9.1.0. The propagation and weighting of particles is parallelized across 24 threads, one bound to each hardware core, using OpenMP with static scheduling. Random number seeds are matched across configurations, using a different seed for each repetition. For each task and problem, the output is expected to match regardless of the configuration; a comparison of output files confirms that this is the case.

Figure 5 reports execution time and peak memory use. On the inference task (with the exception of the PCFG problem, discussed below), significant reductions are apparent when using lazy copies compared to eager copies, with even greater reductions when the single-reference optimization is applied. For the simulation task, comparable execution time and increased memory use is apparent, as expected. This additional memory use is attributed to an extra 8 bytes per pointer and 12 bytes per object to support lazy copies, even if unused.

For the PCFG problem, the implementation of the model keeps only the latest state, \( x_t \), in memory, rather than the full chain, \( x_{0:t−1} \). Lazy copies are not expected to offer more than a constant factor improvement for this, which may be outweighed by overhead. Nonetheless, an improvement in execution time is apparent, with only a small increase in memory use.

The theoretical results described in Section 1 suggest that the ratio between the memory use of the eager and lazy strategies will eventually increase with \( t \) for all but the PCFG and CRBD problems (for the reasons given above). Figure 7 shows execution time and memory use over \( t \) for the inference task on each problem. While complexity cannot be established empirically, the results at least seem consistent with such an interpretation, especially with the single-reference optimization enabled.
Figure 5: Execution time (left) and peak memory use (right) for the inference task. Heights indicate median, and error bars the interquartile range, across 20 runs.

Figure 6: Execution time (left) and peak memory use (right) for the simulation task. Heights indicate median, and error bars the interquartile range, across 20 runs. This task isolates the overhead of lazy copies when unused in a program.

5 Discussion and conclusion

This work has considered population-based probabilistic programs and the specialization of dynamic memory management to their particular usage patterns. The problem and proposed solution was formalized using labeled directed multigraphs. Whereas, in the general case, the labeling scheme requires that each edge is assigned a list of labels, for tree-structured copies a single label is sufficient, which significantly reduces bookkeeping. This single label can be used to accommodate these common tree-structured copies lazily, while handling other copies eagerly.

The key impact of the approach is enabling mutability of objects while increasing object sharing and reducing memory use. Mutability is necessary for imperative programming, but may also facilitate in-place write optimizations for functional programming. It does not, of course, alleviate the programmer from making sensible choices. Where mutability is the sensible choice, however, the platform accommodates this; examples include where an in-place algorithm is optimal, where contiguous storage is required for cache efficiency, and where incremental modifications to data structures are not well-accommodated by immutable objects.

Empirically, the approach has been shown to offer significant improvements in terms of execution time and memory use across a number of realistic probabilistic programs.

6 Supplementary materials

The platform is implemented in C++ as part of LibBirch, the support library for the Birch probabilistic programming language, available at birch-lang.org.
Figure 7: Elapsed time and memory use across \( t = 1, \ldots, T \). Results are consistent with the theoretical expectation that the eager copy configuration should exhibit quadratic execution time and linear memory use in \( t \), while the lazy copy configurations exhibit linear execution time and slower linear memory use in \( t \), except for the PCFG example, discussed in the text.
References

M. Abadi, A. Agarwal, P. Barham, E. Brevdo, Z. Chen, C. Citro, G. S. Corrado, A. Davis, J. Dean, M. Devin, S. Ghemawat, I. Goodfellow, A. Harp, G. Irving, M. Isard, Y. Jia, R. Jozefowicz, L. Kaiser, M. Kudlur, J. Levenberg, D. Mané, R. Monga, S. Moore, D. Murray, C. Olah, M. Schuster, J. Shlens, B. Steiner, I. Sutskever, K. Talwar, P. Tucker, V. Vanhoucke, V. Vasudevan, F. Viégas, O. Vinyals, P. Warden, M. Wattenberg, M. Wicke, Y. Yu, and X. Zheng. TensorFlow: Large-scale machine learning on heterogeneous systems, 2015. URL https://www.tensorflow.org/.

C. Andrieu, A. Doucet, and R. Holenstein. Particle Markov chain Monte Carlo methods. Journal of the Royal Statistical Society B, 72:269–302, 2010. doi: 10.1111/j.1467-9868.2009.00736.x.

E. Bingham, J. P. Chen, M. Jankowiak, F. Obermeyer, N. Pradhan, T. Karaletsos, R. Singh, P. Szerlip, P. Horsfall, and N. D. Goodman. Pyro: Deep universal probabilistic programming. Journal of Machine Learning Research, 20(28):1–6, 2019.

N. Chopin, P. Jacob, and O. Papaspiliopoulos. SMC²: An efficient algorithm for sequential analysis of state space models. Journal of the Royal Statistical Society B, 75:397–426, 2013. doi: 10.1111/j.1467-9868.2012.01046.x.

P. Del Moral, A. Doucet, and A. Jasra. Sequential Monte Carlo samplers. Journal of the Royal Statistical Society B, 68:441–436, 2006. doi: 10.1111/j.1467-9868.2006.00553.x.

P. Del Moral, A. Jasra, A. Lee, C. Yau, and X. Zhang. The alive particle filter and its use in particle Markov chain Monte Carlo. Stochastic Analysis and Applications, 33(6):943–974, 2015. doi: 10.1080/07362994.2015.1060892.

J. V. Dillon, I. Langmore, D. Tran, E. Brevdo, S. Vasudevan, D. Moore, B. Patton, A. Alemi, M. Hoffman, and R. A. Saurous. TensorFlow Distributions. 2017. URL https://arxiv.org/abs/1711.10604.

A. Doucet and A. M. Johansen. A tutorial on particle filtering and smoothing: fifteen years later, chapter 24, pages 656–704. Oxford University Press, 2011.

S. Funk, A. J. Kucharski, A. Camacho, R. M. Eggo, L. Yakob, L. M. Murray, and W. J. Edmunds. Comparative analysis of dengue and Zika outbreaks reveals differences by setting and virus. PLOS Neglected Tropical Diseases, 10(12):1–16, 2016. doi: 10.1371/journal.pntd.0005173.

H. Ge, K. Xu, and Z. Ghahramani. Turing: A language for flexible probabilistic inference. In Proceedings of the Twenty-First International Conference on Artificial Intelligence and Statistics, volume 84 of Proceedings of Machine Learning Research, pages 1682–1690, 2018.

N. D. Goodman and A. Stuhlmüller. The design and implementation of probabilistic programming languages. http://dippl.org, 2014. Accessed: 2015-7-15.

K. Gopinath and J. L. Hennessy. Copy elimination in functional languages. In Proceedings of the 16th ACM SIGPLAN-SIGACT Symposium on Principles of Programming Languages, POPL ’89, pages 303–314, New York, NY, USA, 1989. ACM. ISBN 0-89791-294-2. doi: 10.1145/75277.75304.

N. Gordon, D. Salmond, and A. Smith. Novel approach to nonlinear/non-Gaussian Bayesian state estimation. IEE Proceedings-F, 140:107–113, 1993. doi: 10.1049/ip-f-2.1993.0015.

P. E. Jacob, L. M. Murray, and S. Rubenthaler. Path storage in the particle filter. Statistics and Computing, 25(2):487–496, 2015. doi: 10.1007/s11222-013-9445-x.

J. Kudlicka, L. M. Murray, F. Ronquist, and T. B. Schön. Probabilistic programming for birth-death models of evolution using an alive particle filter with delayed sampling. Uncertainty in Artificial Intelligence, 2019.

F. Lindsten and T. B. Schön. Identification of mixed linear/nonlinear state-space models. In 49th IEEE Conference on Decision and Control (CDC), pages 6377–6382, 2010.

C. J. Maddison, D. Lawson, G. Tucker, N. Hesser, M. Norouzi, A. Mnih, A. Doucet, and Y. W. Teh. Filtering variational objectives. In Proceedings of the 31st International Conference on Neural Information Processing Systems, pages 6576–6586, 2017.

V. K. Mansinghka, D. Selsam, and Y. N. Perov. Venture: a higher-order probabilistic programming platform with programmable inference. arXiv abs/1404.0099, 2014.

L. M. Murray. Bayesian state-space modelling on high-performance hardware using LibBi. Journal of Statistical Software, 67(10):1–36, 2015. doi: 10.18637/jss.v067.i10.
L. M. Murray and T. B. Schö̈n. Automated learning with a probabilistic programming language: Birch. *Annual Reviews in Control*, 46:29–43, 2018. ISSN 1367-5788. doi: 10.1016/j.arcontrol.2018.10.013.

L. M. Murray, D. Lundén, J. Kudlicka, D. Broman, and T. B. Schö̈n. Delayed sampling and automatic Rao–Blackwellization of probabilistic programs. In *Proceedings of the 21st International Conference on Artificial Intelligence and Statistics (AISTATS)*, Lanzarote, Spain, 2018. URL [arxiv.org/abs/1708.07787](http://arxiv.org/abs/1708.07787).

C. Naesseth, S. Linderman, R. Ranganath, and D. Blei. Variational sequential Monte Carlo. In *Proceedings of the Twenty-First International Conference on Artificial Intelligence and Statistics*, volume 84 of *Proceedings of Machine Learning Research*, pages 968–977, 2018.

C. Okasaki. *Purely Functional Data Structures*. Cambridge University Press, 1999.

B. Paige and F. Wood. A compilation target for probabilistic programming languages. *31st International Conference on Machine Learning (ICML)*, 2014.

A. Paszke, S. Gross, S. Chintala, G. Chanan, E. Yang, Z. DeVito, Z. Lin, A. Desmaison, L. Antiga, and A. Lerer. Automatic differentiation in PyTorch. In *NIPS Autodiff Workshop*, 2017.

A. Pfeffer. *Practical Probabilistic Programming*. Manning, 2016.

M. Pitt and N. Shephard. Filtering via simulation: Auxiliary particle filters. *Journal of the American Statistical Association*, 94:590–599, 1999.

N. Siddharth, B. Paige, J.-W. van de Meent, A. Desmaison, N. D. Goodman, P. Kohli, F. Wood, and P. Torr. Learning disentangled representations with semi-supervised deep generative models. In *Advances in Neural Information Processing Systems 30*, pages 5927–5937, 2017.

Stan Development Team. Stan: A C++ library for probability and sampling, 2013. URL [http://mc-stan.org](http://mc-stan.org).

M. E. Steeman, M. B. Hebsgaard, R. E. Fordyce, S. Y. Ho, D. L. Rabosky, R. Nielsen, C. Rahbek, H. Glenner, M. V. Sørensen, and E. Willerslev. Radiation of extant cetaceans driven by restructuring of the oceans. *Systematic Biology*, 58(6):573–585, 2009.

A. Todeschini, F. Caron, M. Fuentes, P. Legrand, and P. Del Moral. Biips: Software for Bayesian inference with interacting particle systems. *arXiv abs/1412.3779*, 2014.

D. Tolpin, J. van de Meent, H. Yang, and F. Wood. Design and implementation of probabilistic programming language Anglican. *arXiv abs/1608.05263*, 2016.

D. Tran, M. D. Hoffman, R. A. Saurous, E. Brevdo, K. Murphy, and D. M. Blei. Deep probabilistic programming. In *International Conference on Learning Representations*, 2017.

A. Wigren, R. S. Risuleo, L. M. Murray, and F. Lindsten. Parameter elimination in particle Gibbs sampling. *Advances in Neural Information Processing Systems 32 (NeurIPS 2019)*, 2019.