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Efficient Extensional Binary Tries

Andrew W. Appel · **Xavier Leroy**

Abstract Lookup tables (finite maps) are a ubiquitous data structure. In pure functional languages they are best represented using trees instead of hash tables. In pure functional languages within constructive logic, without a primitive integer type, they are well represented using binary tries instead of search trees.

In this work, we introduce *canonical binary tries*, an improved binary-trie data structure that enjoys a natural extensionality property, quite useful in proofs, and supports sparseness more efficiently. We provide full proofs of correctness in Coq.

We provide microbenchmark measurements of canonical binary tries versus several other data structures for finite maps, in a variety of application contexts; as well as measurement of canonical versus original tries in two big, real systems. The application context of *data structures contained in theorem statements* imposes unusual requirements for which canonical tries are particularly well suited.

1 Introduction

Lookup tables—finite maps from identifiers to bindings—are a central data structure in many kinds of programs. We are particularly interested in programs that are proved correct—compilers, static analyzers, program verifiers. Those programs are often written in pure functional languages, since the proof theory of functional programming is more tractable than those of imperative or object-oriented languages. Thus we focus on applications written in the functional languages internal to the logics of Coq or HOL. Such programs *may* be

There are no conflicts of interest. Code is available at https://github.com/xavierleroy/canonical-binary-tries/tree/v2.

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"extracted" to programming languages such as OCaml, Standard ML, or Haskell, and compiled with optimizing compilers for those languages; the CompCert C compiler [13] and the Verasco static analyzer [11] are examples. On the other hand, some programs, such as the Verified Software Toolchain program verifier [2], don't use extraction: those programs are reduced within the logic of a proof assistant, so that the program verifier can gracefully interact with user-driven interactive proof in the ambient logic.

Many proved-correct programs of this kind deliberately use an impoverished set of primitives, so that fewer axioms need to be assumed (or equivalently, fewer lines of proof-checker kernel code need to be trusted). In particular, there may be no primitive integer type implemented in a machine word. Instead, integers (or whatever type is used for *keys,* the domain of the finite maps) may be constructed from the inductive data types of the logic. Consequently, we cannot assume that a less-than comparison of two keys takes constant time; it will be logarithmic in the magnitude of the numbers.

These criteria led to a preliminary design for a data structure and its algebraic interface: binary tries, also called positive trees (for reasons that will become clear). This data structure was used in the CompCert C compiler, the Verified Software Toolchain (VST), the Verasco verified static analyzer, and in other applications. In the process, we have learned to demand more and more criteria of efficiency and provability from them:

Core Requirements

1. Basic operators: empty (the finite map with an empty domain), get (the lookup operator), and set (the update operator).
2. Proofs[1] of basic laws: $\mathsf{get}\ i\ \mathsf{empty} = \mathsf{None}$, $\mathsf{get}\ i\ (\mathsf{set}\ i\ v\ m) = \mathsf{Some}\ v$, $i \neq j \ \rightarrow \mathsf{get}\ i\ (\mathsf{set}\ j\ v\ m) = \mathsf{get}\ i\ m$.
3. A purely functional implementation (which rules out hash tables, for example).
4. A *persistent* semantics, so that $\mathsf{set}\ j\ v\ m$ does not destroy m; this arises naturally from the purely functional implementation.
5. Efficient representation of keys.
6. Efficient asymptotic time complexity of get and set operations, as extracted to OCaml.
7. Linear-time computation of the list of key-binding pairs of a finite-map, in sorted order by key, with proofs of its properties.
8. Linear-time combining two finite maps m_1 and m_2 with function f yielding a map m such that, at any key i, $m(i) = f(m_1(i), m_2(i))$; with proofs of its properties.

Extended Requirements

9. Efficiency in the face of sparseness: that is, if the magnitude of individual keys is much greater than the number of keys bound in the map.
10. Efficiency not only as extracted to OCaml (i.e., with proofs erased), but also as represented in Coq and computed within Coq (i.e., without proof erasure).
11. Extensionality: the property that $(\forall i.\ m_1(i) = m_2(i)) \ \rightarrow\ m_1 = m_2$. This allows Leibniz equality to be used in proofs about the larger systems in which the finite maps are embedded; otherwise, equivalence relations must be used, which is less convenient.

The *Core Requirements* were all satisfied by a simple binary-trie data structure, implemented in CompCert and used 2005–2021 [16]. In section 2 we will present the data structure and its operations, and discuss the proofs.

In more recent applications, the *Extended Requirements* have been needed. Section 4 describes a new variant of the data structure that has the extensionality property, handles

[1] All proofs mentioned in this paper are machine-checked unless explicitly noted otherwise.

sparseness better, and is significantly more efficient within Coq and somewhat more efficient as extracted to OCaml. It has been integrated in CompCert in 2021 [15]. Source code for implementations and proofs may also be found in the Coq development accompanying this article [14].

Extensionality could be achieved in other ways, such as sigma-types in Coq (the dependent pair of a data structure with a proof of its canonicity). We describe alternative implementations in section 6. Our benchmark measurements (section 7) show that our new variant, "canonical binary tries" performs well in all contexts, while each of the alternatives is problematic in at least some contexts.

Related work. Many lookup-table data structures have been implemented and proved correct in proof assistants. The books *Verified Functional Algorithms* [3] and *Functional Algorithms Verified* [18] each describe several pure-functional tree data structures with proofs of correctness (in Coq and Isabelle/HOL, respectively). They describe binary search trees, red-black trees, 2-3 trees, AVL trees, Braun trees, binary tries, Patricia tries. Of these,

- Only Braun trees, binary tries, and Patricia tries avoid the assumption that comparisons are constant-time.
- Only red-black trees, 2-3 trees, AVL trees, and Patricia tries (but not Braun trees) handle sparseness efficiently.
- Only Braun trees have the extensionality property. Braun trees support certain other operations, not supported by the other data structures (or by ours), useful for priority queues but not part of our core requirements.

That is, none of the standard data structures satisfy our Core and Extended Requirements.

A different approach would be to build single-threaded mutable arrays into the kernel of the logic, as was done long ago in ACL2 [7] and more recently in Coq. These do not satisfy *persistence,* except in a very inefficient way, nor sparseness.

2 PTree: simple binary tries keyed by positive numbers

A simple and efficient data structure for lookup tables (finite maps on integer or string keys) is the *hash table*. But this is not suitable for purely functional implementations, since the update operation is destructive.[2]

Therefore one turns naturally to trees—for example, binary search trees. The lookup operator in a balanced BST takes $\log N$ comparisons, and achieves asymptotic complexity of $\log N$ per operation only if comparison takes constant time. But Coq does not have a primitive integer type with constant-time comparisons.[3]

Coq's logic, the Calculus of Inductive Constructions (CiC) encourages the *construction* of types and operations, instead of *axiomatization*. For example, the natural numbers, and addition upon them, are constructed as,

[2] *Persistent arrays* give a functional semantics layered on an imperative (destructive-update) implementation, but these are not suitable because they would require extending the logic's kernel of axioms.

[3] In fact, no programming language has a primitive integer type with constant-time comparisons; they typically have a *range-limited* integer type $-2^k \leq i < 2^k$ or a *modular* integer type $(i \bmod 2^k)$. Most versions of Coq 2005-present have not had a built-in integer type with fast comparisons; and relying on them would increase the size of the trusted base, that is, Coq kernel code, Coq axioms, Coq extraction to OCaml, and OCaml operations upon which we rely.

```
Inductive nat := O : nat | S : nat → nat.

Fixpoint add (n m : nat) : nat := match n with O ⇒ m | S p ⇒ S (add p m) end.
```

and then properties such as the associativity of add are proved as lemmas instead of being axiomatized.

But this representation of natural numbers is not suitable for use as the keys of efficient lookup tables, because it is essentially a *unary* notation, in which representing the number n takes space proportional to n, comparing $n < m$ takes time proportional to $\min(n,m)$, and so on. Therefore users of Coq often use a *binary* representation of integers, constructed as follows:

```
Inductive positive :=  xI : positive → positive  |  xO : positive → positive  |  xH : positive.

Inductive Z :=  Z0 : Z  |  Zpos : positive → Z  |  Zneg : positive → Z.
```

The "meaning" of xH is the positive number 1; $\mathsf{xO}(p)$ represents $2p+0$, and $\mathsf{xI}(p)$ represents $2p+1$. Therefore the number $13_{10} = 1101_2 = \mathsf{xI}(\mathsf{xO}(\mathsf{xI}\ \mathsf{xH}))$, and the number 0 is unrepresentable—these numbers truly are *positive*, not merely nonnegative.

That means that the Z type (of binary unbounded signed integers) has the property of *extensionality*—no two data structures of type Z represent the same mathematical integer. But the Z type is of no further concern in this paper; we will use positive as the type of keys for lookup tables.

The number p, represented as a positive, is represented with $\Theta(\log p)$ constructors. When extracted to OCaml, this really means $\log p$ two-word records (in which the first word contains the constructor tag xI/xO/xH and the second word is a pointer to the remainder). That's a lot more than the single word in which a native OCaml program or a C++ program might use to represent an integer key, but it is *efficient enough* in practice, for the CompCert compiler and similar applications.

The positive number p, represented within Coq, also has $\log p$ constructors, but each Coq construction is represented within the Coq kernel as two OCaml constructions that *describe* the Coq constructor. So the number p occupies $5\log p$ words (or $8 \cdot 5\log p$ bytes on a 64-bit machine). In practice this is usually efficient enough.[4]

Given that Coq has this natural way to represent binary numbers using inductive data types, it is natural to use *binary tries* to implement lookup tables. A *trie* is a directed tree in which every edge is labeled from a finite alphabet; a *word* (such as "cat") is looked up by traversing the path of edges labeled sequentially with the letters of the word (such as "c" then "a" then "t"); and the *nodes* contain values of the range type of the lookup table. A *binary* trie is one in which the alphabet is $\{0,1\}$.

The implementation of binary tries, with *positive* keys, is straightforward in Coq:

```
Inductive option (A: Type) := Some : A → option A | None : option A.

Inductive tree (A : Type) := Leaf : tree A | Node : tree A → option A → tree A → tree A.

Definition empty {A : Type} : tree A := Leaf.

Fixpoint get {A : Type} (i : positive) (m : tree A) : option A :=
```

[4] In OCaml, an arity-k constructor applied to arguments takes $k+1$ words, including one for the constructor-tag. In Coq, an arity-k constructor is represented as one arity-2 OCaml construction plus one length-k array, which take (respectively) 3 words and $k+1$ words as represented in OCaml within the Coq kernel. The arity-2 OCaml construction also points to a description of the constructor, but that description is shared among all its uses so we don't count it.

```
  match m with
  | Leaf ⇒ None
  | Node l o r ⇒ match i with xH ⇒ o | xO i' ⇒ get i' l | xI i' ⇒ get i' r end
  end.

Fixpoint set {A : Type} (i : positive) (v : A) (m : tree A) : tree A :=
  match m, i with
  | Leaf, xH ⇒ Node Leaf (Some v) Leaf
  | Leaf, xO i' ⇒ Node (set i' v Leaf) None Leaf
  | Leaf, xI i' ⇒ Node Leaf None (set i' v Leaf)
  | Node l o r, xH ⇒ Node l (Some v) r
  | Node l o r, xO i' ⇒ Node (set i' v l) o r
  | Node l o r, xI i' ⇒ Node l o (set i' v r)
  end.
```

That is, each node of the tree is either a Leaf, meaning that *no extension of the key leading to this node is in the domain of the map*, or an internal Node with left subtree l, optional binding-at-this-node o, and right subtree r. If $o =$ None then the key leading to this node is not in the domain of the map, but some extensions of it might be. If $o =$ Some v then the key leading to this node is mapped to v, and extensions of the key might also be mapped (in l and r). The edge from this node to subtree l is implicitly labeled by 0 (or xO), and the edge to subtree r is implicitly labeled by 1 (or xI).

Looking up a key p in a trie takes time proportional to the number of constructors representing the key, which is about $\log_2 p$; update is similarly efficient; this is *efficient enough* for many important applications, including CompCert.

From these definitions it is easy to prove the important algebraic properties of maps:

```
Theorem gempty: (* ''get−empty'' *)
    ∀(A: Type) (i: positive), get i (empty A) = None.
Proof. induction i; simpl; auto. Qed.

Theorem gss: (* ''get−set−same'' *)
  ∀(A: Type) (i: positive) (x: A) (m: tree A), get i (set i x m) = Some x.
Proof. induction i; destruct m; simpl; auto. Qed.

Theorem gso: (* ''get−set−other'' *)
    ∀(A: Type) (i j: positive) (x: A) (m: tree A), i <> j → get i (set j x m) = get i m.
Proof. induction i; intros; destruct j; destruct m; simpl;
        try rewrite <− (gleaf A i); auto; try apply IHi; congruence.
Qed.
```

As usual in machine-checked proof scripts, the reader is not necessarily expected to read and understand the proofs; but the *theorem statements* should be clear, and induction i; destruct m suggests that the proof is by induction on the positive number i and then case analysis on m.

In less than 50 lines of Coq we have accomplished the first 6 of the core requirements: the operators empty, get, set, proofs of the algebraic laws, a purely functional implementation with a persistent semantics, an efficient-enough representation of keys, and efficient-enough asymptotic time complexity for many programs extracted to OCaml.

Deletion (the remove operation) is similar to insertion (the set operation) but runs into an issue: empty subtrees can be represented in several different ways, and the most compact representation (namely, the Leaf constructor) should be favored.

```
Fixpoint remove {A: Type} (i: positive) (m: tree A) : tree A :=
  match m, i with
  | Leaf, _ ⇒ Leaf
  | Node l o r, xH ⇒ Node' l None r
```

```
  | Node l o r, xO i' ⇒ Node' (remove i' l) o r
  | Node l o r, xI i' ⇒ Node' l o (remove i' r)
  end.
```

In the second case, if l and r are both Leaf, we do not want to build a useless empty subtree Node Leaf None Leaf. This could also happen in the third and fourth cases if the recursive call to remove returns Leaf. Empty nonleaf subtrees are not *wrong,* but they waste memory. So the solution is to use a Node' pseudoconstructor function, as follows:

```
Definition Node' {A: Type} (l: tree A) (o: option A) (r: tree A): tree A :=
  match l, o, r with Leaf, None, Leaf ⇒ Leaf | _, _, _ ⇒ Node l x r end.
```

Crucially, the pseudoconstructor Node' behaves like the actual constructor Node with respect to the get operation:

```
Lemma gNode':
  ∀(A: Type) (i: positive) (l: tree A) (o: option A) (r: tree A),
  get i (Node' l o r) = match i with xH ⇒ x | xO i' ⇒ get i' l | xI i' ⇒ get i' r end.
Proof.
  intros. destruct l, x, r; simpl; auto. destruct i; auto.
Qed.
```

This makes it easy to prove get-remove algebraic properties similar to the get-set properties.

To produce an association list of the key-binding pairs, one *could* write a function such as,

```
Fixpoint elements {A} (m: tree A) (i: positive) : list (positive * A) :=
 match m with
 | Leaf ⇒ nil
 | Node l o r ⇒
     elements l (xO i)
    ++ match o with None ⇒ nil | Some x ⇒ (prev i, x)::nil end
    ++ elements r (xI i)
    end.
```

where prev is positive-reversal, so prev(xI (xI (xO (xH))) = xO (xI (xI xH)). However, this implementation is inefficient: since list-concatentation ++ takes time proportional to the length of its first argument, this function will take about $N \log N$ time for a tree containing N elements. So instead, one implements elements by accumulating the list to the right of the current tree, costing time exactly linear in the number of nodes in the tree. We will not show the details.

Proofs of the properties of the elements function are reasonably straightforward, though more complex than the gso theorem.

It is easy to define collective operations such as "map" and "filter" that transform a finite map into another finite map. For example, here is a map_filter f operation that applies a function f: $A \to$ option B to every value a contained in a tree A map, discarding the value if $f\ a =$ None.

```
Fixpoint map_filter {A B} (f: A → option B) (m: tree A) : tree B :=
  match m with
  | Leaf ⇒ Leaf
  | Node l None r ⇒ Node' (map_filter f l) None (map_filter f r)
  | Node l (Some a) r ⇒ Node' (map_filter f l) (f a) (map_filter f r)
  end.
```

As in remove, we use the pseudoconstructor Node' to avoid generating empty subtrees Node Leaf None Leaf.

Many applications wish to combine two finite maps m_1 : tree A, m_2 : tree B with a user-supplied function f: option $A \to$ option $B \to$ option C. We assume that f None None = None, and we require that combine m_1 $m_2 = m$ if and only if $\forall i, f(m_1(i))(m_2(i)) = m(i)$.

One might propose an implementation something like this:

```
Fixpoint combine (m1: tree A) (m2: tree B) : tree C :=
 match m1, m2 with
 | Leaf, Leaf ⇒ Leaf
 | Leaf, Node l2 o2 r2 ⇒ Node' (combine Leaf l2) (f None o2) (combine Leaf r2)
 | Node l1 o1 r1, Leaf ⇒ Node' (combine l1 Leaf) (f o1 None) (combine r1 Leaf)
 | Node l1 o1 r1, Node' l2 o2 r2 ⇒ Node (combine l1 l2) (f o1 o2) (combine r1 r2)
 end.
```

but there is a problem here. Some of the recursive calls use substructures of m_1 while others use substructures of m_2, so this is not actually legal in Coq. The solution is that once a Leaf is reached on either side, we can traverse the other side using map_filter, which is recursive on just one tree.

```
Fixpoint combine (m1: tree A) (m2: tree B) : tree C :=
  match m1, m2 with
  | Leaf, _ ⇒ map_filter (fun b ⇒ f None (Some b)) m2
  | _, Leaf ⇒ map_filter (fun a ⇒ f (Some a) None) m1
  | Node l1 o1 r1, Node l2 o2 r2 ⇒ Node' (combine l1 l2) (f o1 o2) (combine r1 r2)
end.
```

This combine function is quite general and reasonably efficient. It takes time linear in the total sizes of the input trees. Proofs of its properties are straightforward, for example,

```
Theorem gcombine: ∀(m1: tree A) (m2: tree B) (i: positive),
      get i (combine m1 m2) = f (get i m1) (get i m2).
```

The proof is only 6 lines of Coq.

Summary of Section 2. Binary tries, with keys that are constructive binary positive numbers, are a simple data structure with an easy implementation and reasonably straightforward proofs. They are efficient enough in practice for many useful applications, especially as extracted into OCaml.

3 The need for extensionality

Extensionality is a property of equality in formal logics. It says that two objects are equal if they have the same external properties. For example, the extensionality property for functions says that two functions f and g are equal as soon as they have the same domain and satisfy $\forall x,\ f(x) = g(x)$. This extensionality property holds in set theory but not in Coq's type theory.

For finite maps, the extensionality property says that two maps are equal if they are equivalent, that is, if they map equal keys to equal values. Like most popular implementations of finite maps, binary tries (represented as in Section 2) are not extensional. That is, equivalent tries are not necessarily equal, as shown by the following example.

m_1	$\cdot\ 1\ ((\cdot\ 2\ \cdot) \circ (\cdot\ 2\ \cdot))$	$\cdot$ represents Leaf
m_2	$(\cdot \circ \cdot)\ 1\ ((\cdot\ 2\ \cdot) \circ (\cdot\ 2\ \cdot))$	$\circ$ represents None

Here, m_1 and m_2 are equivalent (for any i, $\mathsf{get}\ i\ m_1 = \mathsf{get}\ i\ m_2$), but m_2 has an extra empty left subtree $\mathsf{Node\ Leaf\ None\ Leaf}$ where m_1 has just Leaf.

This is not an insurmountable problem. One can reason using equivalence rather than equality. Coq has support for such "Setoid" reasoning; but it's still inconvenient, and a truly canonical representation of tries would simplify many definitions and proofs. For example, consider the following two algebraic laws of finite maps:

$$\mathsf{set}\ k\ v\ m = m \qquad \text{if } \mathsf{get}\ k\ m = \mathsf{Some}\ v$$
$$\mathsf{set}\ k_1\ v_1\ (\mathsf{set}\ k_2\ v_2\ m) = \mathsf{set}\ k_2\ v_2\ (\mathsf{set}\ k_1\ v_1\ m) \qquad \text{if } k_1 \neq k_2$$

If the representation of m were canonical (which the binary tries of Section 2 are not), then these laws would be trivial consequences of extensionality. In the absence of extensionality, these laws require specific proofs, using the definition of set and induction over m.

More generally, a large Coq development might have types that contain finite maps, such as a type for "program modules" in which finite maps represent bindings of names to definitions. If the finite maps do not support Leibnitz equality, and one must therefore use setoids, then equality reasoning about "program modules" must also use setoids.

Coq proofs with setoids are larger and slower than proofs with Leibnitz equality. Extensional tries (permitting Leibnitz equality) could perform much faster in Coq proofs. And indeed they do; see section 9.

One might think, "extra empty subtrees will never arise in practice, since the set operation cannot produce them." But then one would have to maintain the invariant that a given trie was produced by a sequence of set operations.

One might think, "we'll maintain that invariant using dependent types containing proofs that the tree has no empty subtrees." Section 6 describes two attempts along this line and the efficiency problems they cause.

Therefore, what we want is a *first-order, naturally extensional representation* of tries.

4 Canonical binary tries

For a first-order naturally extensional representation that handles sparseness better, our solution is to make an inductive datatype that *cannot* represent an empty mapping. The data structure is as follows:

```
Inductive tree' (A: Type) : Type :=
 | Node001: tree' A → tree' A                    (* only a right subtree *)
 | Node010: A → tree' A                          (* only a middle value *)
 | Node011: A → tree' A → tree' A                (* only middle and right *)
 | Node100: tree' A → tree' A                    (* only a left subtree *)
 | Node101: tree' A → tree' A → tree' A          (* left, right, no middle *)
 | Node110: tree' A → A → tree' A                (* only left and middle *)
 | Node111: tree' A → A → tree' A → tree' A.     (* left, middle, right *)

Inductive tree (A: Type) : Type :=
  | Empty : tree A
  | Nodes: tree' A → tree A.
```

Each of the three digits in the name of a node constructor represents the presence or absence of the left, middle, or right components of the node. Thus, $\mathsf{Node101}\ l\ r$ represents a node with left and right subtrees but no middle, and $\mathsf{Node011}\ x\ r$ represents what would have been written (in our previous representation) as $\mathsf{Node\ Leaf\ (Some}\ x\mathsf{)}\ r$.

A crucial property of this data structure is *canonicity*: for any finite set S of (key, value) bindings, there is only one value of type tree that represents this set. If S is empty, it is represented by Empty, and cannot be represented by Nodes t, as a value t of type tree' always contains at least one (key, value) binding. If S is not empty, it can only be represented by Nodes t. The head constructor of t is uniquely determined by whether the sets

$$S_h = \{(\mathsf{xH}, v) \mid (\mathsf{xH}, v) \in S\} \quad S_o = \{(i, v) \mid (\mathsf{xO}\ i, v) \in S\} \quad S_i = \{(i, v) \mid (\mathsf{xI}\ i, v) \in S\}$$

are empty or not. Induction on the size of S shows that the subtrees of t, if any, are uniquely determined.

Canonicity implies extensionality, of course: two values of type tree that represent the same set of (key, value) pairs are equal. In addition, canonicity improves computational efficiency compared with the noncanonical binary tries from section 2: no memory is consumed to represent empty left, middle, or right components of a node. As the experimental evaluation in sections 7, 8 and 9 shows, the gains in memory usage and execution times are significant, especially for sparse maps.

Defining the lookup and update functions is not quite as simple as before:

```
Definition empty (A : Type) := (Empty : tree A).

Fixpoint get' {A} (p: positive) (m: tree' A) : option A :=
  match p, m with
  | xH, Node001 _ ⇒ None
  | xH, Node010 x ⇒ Some x
  | xH, Node011 x _ ⇒ Some x
  | xH, Node100 _ ⇒ None
  | xH, Node101 _ _ ⇒ None
  | xH, Node110 _ x ⇒ Some x
  | xH, Node111 _ x _ ⇒ Some x
  | xO q, Node001 _ ⇒ None
  | xO q, Node010 _ ⇒ None
  | xO q, Node011 _ _ ⇒ None
  | xO q, Node100 m' ⇒ get' q m'
  | xO q, Node101 m' _ ⇒ get' q m'
  | xO q, Node110 m' _ ⇒ get' q m'
  | xO q, Node111 m' _ _ ⇒ get' q m'
  | xI q, Node001 m' ⇒ get' q m'
  | xI q, Node010 _ ⇒ None
  | xI q, Node011 _ m' ⇒ get' q m'
  | xI q, Node100 m' ⇒ None
  | xI q, Node101 _ m' ⇒ get' q m'
  | xI q, Node110 _ _ ⇒ None
  | xI q, Node111 _ _ m' ⇒ get' q m'
end.

Definition get {A} (p: positive) (m: tree A) : option A :=
  match m with Empty ⇒ None | Nodes m' ⇒ get' p m' end.
```

The get' function has 21 cases, handling each combination of one of the 3 positive constructors and one of the 7 node constructors.

The update function set follows the same pattern. An update to the empty tree is handled by the set0 function, which creates a nonempty tree with a single branch:

```
Fixpoint set0 {A} (p: positive) (x: A) : tree' A :=
match p with
| xH ⇒ Node010 x
| xO q ⇒ Node100 (set0 q x)
| xI q ⇒ Node001 (set0 q x)
```

```
end.
```

To update a nonempty tree, the function set' performs the same 21-case analysis as get':

```
Fixpoint set' {A} (p: positive) (x: A) (m: tree' A) : tree' A :=
match p, m with
| xH, Node001 r ⇒ Node011 x r
| xH, Node010 _ ⇒ Node010 x
| xH, Node011 _ r ⇒ Node011 x r
| xH, Node100 l ⇒ Node110 l x
| xH, Node101 l r ⇒ Node111 l x r
| xH, Node110 l _ ⇒ Node110 l x
| xH, Node111 l _ r ⇒ Node111 l x r
| xO q, Node001 r ⇒ Node101 (set0 q x) r
| xO q, Node010 y ⇒ Node110 (set0 q x) y
| xO q, Node011 y r ⇒ Node111 (set0 q x) y r
| xO q, Node100 l ⇒ Node100 (set' q x l)
| xO q, Node101 l r ⇒ Node101 (set' q x l) r
| xO q, Node110 l y ⇒ Node110 (set' q x l) y
| xO q, Node111 l y r ⇒ Node111 (set' q x l) y r
| xI q, Node001 r ⇒ Node001 (set' q x r)
| xI q, Node010 y ⇒ Node011 y (set0 q x)
| xI q, Node011 y r ⇒ Node011 y (set' q x r)
| xI q, Node100 l ⇒ Node101 l (set0 q x)
| xI q, Node101 l r ⇒ Node101 l (set' q x r)
| xI q, Node110 l y ⇒ Node111 l y (set0 q x)
| xI q, Node111 l y r ⇒ Node111 l y (set' q x r)
end.
```

```
Definition set {A} (p: positive) (x: A) (m: tree A) : tree A :=
match m with
| Empty ⇒ Nodes (set0 p x)
| Nodes m' ⇒ Nodes (set' p x m')
end.
```

Proofs of the fundamental theorems (such as gss and gso) are still short and easy: about 25 lines in all, including supporting lemmas.

Other functions that operate over a single tree remain reasonably easy to write. For example, here is the recursive part of the map_filter function that applies a function f: $A \to$ option B to a nonempty tree m: tree' A:

```
Fixpoint map_filter' {A B} (f: A → option B) (m: tree' A) : tree B :=
  match m with
  | Node001 r ⇒ Node Empty None (map_filter' f r)
  | Node010 x ⇒ Node Empty (f x) Empty
  | Node011 x r ⇒ Node Empty (f x) (map_filter' f r)
  | Node100 l ⇒ Node (map_filter' f l) None Empty
  | Node101 l r ⇒ Node (map_filter' f l) None (map_filter' f r)
  | Node110 l x ⇒ Node (map_filter' f l) (f x) Empty
  | Node111 l x r ⇒ Node (map_filter' f l) (f x) (map_filter' f r)
  end.
```

The Node function used in the definition above is similar to the Node constructor and the Node' pseudoconstructor of section 2: given a possibly empty left subtree, a possibly absent value, and a possibly empty right subtree, it returns the corresponding tree.

```
Definition Node {A} (l: tree A) (o: option A) (r: tree A) : tree A :=
  match l,o,r with
  | Empty, None, Empty ⇒ Empty
  | Empty, None, Nodes r' ⇒ Nodes (Node001 r')
  | Empty, Some x, Empty ⇒ Nodes (Node010 x)
```

```
  | Empty, Some x, Nodes r' ⇒ Nodes (Node011 x r')
  | Nodes l', None, Empty ⇒ Nodes (Node100 l')
  | Nodes l', None, Nodes r' ⇒ Nodes (Node101 l' r')
  | Nodes l', Some x, Empty ⇒ Nodes (Node110 l' x)
  | Nodes l', Some x, Nodes r' ⇒ Nodes (Node111 l' x r')
  end.
```

The case analysis performed by Node can be partially redundant. For instance, in the first case of the map_filter' function, we use Node with l = Empty and o = None; we would prefer to avoid discriminating over l and o in Node. This is easily achieved by asking Coq to unfold the definition of Node inside map_filter', then simplify using call-by-value evaluation:

```
Definition fast_map_filter' := Eval cbv [Node] in @map_filter'.
```

The resulting function performs the minimal number of case distinctions on the results of f and of recursive calls. Hence, it executes faster than map_filter', both within Coq and after extraction to OCaml. At the same time, fast_map_filter' is *convertible* with map_filter', since it is obtained by reductions, hence the two functions are definitionally equal, and all the results proved on the nicer-looking map_filter' hold for the faster fast_map_filter'.

Functions that operate over two trees, such as the combine function from Section 2, are more difficult to write because of the high number of cases. Consider the recursive case of the combine function, the one that operates on two nonempty trees in parallel.

```
Variables A B C: Type.
Variable f: option A → option B → option C.
Definition combine'_l := map_filter' (fun a ⇒ f (Some a) None).
Definition combine'_r := map_filter' (fun b ⇒ f None (Some b)).

Fixpoint combine' (m1: tree' A) (m2: tree B) {struct m1} : tree C :=
  match m1, m2 with
  | ...
  | Node101 l1 r1, Node011 x2 r2 ⇒ Node (combine'_l l1) (f None (Some x2)) (combine' r1 r2)
  | ...
  end.
```

A naive case analysis on m1 and m2 results in 49 cases. Each case is simple enough: we call combine' if there are two left subtrees or two right subtrees, combine'_l if there is only a left subtree, combine'_r if there is only a right subtree. Likewise, reasoning about these 49 cases is relatively easy, using Coq's tactic language for automation. But writing all the cases in the first place is a pain!

Even so, *proofs* about the 49-case combine' function can be concise. Consider this theorem, about the interaction of combine' with get':

```
Lemma gcombine': ∀m1 m2 i,
        get i (combine' m1 m2) = f (get' i m1) (get' i m2).
Proof.
    induction m1; destruct m2; intros; simpl; rewrite gNode;
    destruct i; simpl; auto using gcombine'_l, gcombine'_r.
Qed.
```

Tactics make it easy to chain induction on m1, case analysis (destruct) on m2, simplification, rewriting, and case analysis on i, all in two lines of Ltac scripting.

5 Defining functions with case analysis, in Coq

Our 49-case combine' function has a regular structure that is motivated by the way that canonical tries relate to original tries. We briefly digress to show how to define such functions—that do a large (but regularly structured) case analysis—concisely in Coq. We show two approaches: tactical function definition, and *views*.

5.1 Tactical function definition.

Here is a definition combine'_by_tac that produces the same function as the 49-case combine' described above:

```
Fixpoint combine'_by_tac (m1: tree' A) (m2: tree' B) {struct m1} : tree C.
Proof.
  destruct m1 as [ r1 | x1 | x1 r1 | l1 | l1 r1 | l1 x1 | l1 x1 r1 ];
  destruct m2 as [ r2 | x2 | x2 r2 | l2 | l2 r2 | l2 x2 | l2 x2 r2 ];
  (apply Node;
   [ solve [ exact (combine'_by_tac l1 l2)
           | exact (combine'_l l1)
           | exact (combine'_r l2)
           | exact Empty]
   | solve [ exact (f (Some x1) (Some x2))
           | exact (f None (Some x2))
           | exact (f (Some x1) None)
           | exact None]
   | solve [ exact (combine'_by_tac r1 r2)
           | exact (combine'_l r1)
           | exact (combine'_r r2)
           | exact Empty ]
   ]).
Defined.
```

This definition is in the same context that binds parameters A,B,C,f as the definition above of combine'. The first line describes a *goal:* define a recursive function of a particular type by structural induction on m1. The "Proof" is a case analysis described in Coq's tactic language: the destruct builds a pattern-**match** into the "proof" (in this case, into the "program"). So we start with two nested 7-case matches, that is, a 49-case double pattern match. Each one of those has a right-hand-side that's an application of the Node pseudo constructor, so we say apply Node in the tactic language. Since Node is a 3-argument function, we have three subgoals remaining, separated by the punctuation [| |]. In each case, we try four different things (the exact tactics), in the order given. The first of the four that type-checks is the one that will be chosen for use in defining the function.

The reader may not be confident that this defines the right function! Indeed, the author of the tactic may not be confident. One can gain confidence by this theorem, which shows that the new implementation is $\beta\delta$-convertible with the hand-written 49-case version:

```
Lemma combine'_by_tac_eq: combine'_by_tac = combine'.
Proof. reflexivity. Qed.
```

However, the purpose of this tactic is to *avoid* having to write the 49-case version by hand. So a more useful theorem to prove correctness of the tactical implementation (or any implementation) is that combine' interacts properly with get'. And indeed, the same gcombine' lemma-statement (as shown in §4) *and exactly the same tactical proof* works to prove that theorem for combine'_by_tac as for the direct implementation of combine'.

5.2 Views

Instead of definition-by-tactic, another way to avoid explosion in the number of cases is to work with canonical binary tries using a *view* consisting of two cases only: either an empty leaf or a node consisting of a left subtree, an optional value, and a right subtree. In other words, the view is isomorphic to the concrete representation of the original binary tries from section 2. One half of this view—the one that lets us construct values of type tree A—consists of the Empty constructor and the Node function mentioned above:

```
Empty : ∀A, tree A
Node : ∀A, tree A → option A → tree A → option A
```

The other half of the view—the one that lets us inspect and recurse over values of type tree A—is provided by elimination and induction principles. Here is a simple, nonrecursive case analysis with two cases:

```
Definition tree_case {A B} (empty: B)
                           (node: tree A → option A → tree A → B)
                           (m: tree A) : B :=
  match m with
    | Empty ⇒ empty
    | Nodes (Node001 r) ⇒ node Empty None (Nodes r)
    | Nodes (Node010 x) ⇒ node Empty (Some x) Empty
    | Nodes (Node011 x r) ⇒ node Empty (Some x) (Nodes r)
    | Nodes (Node100 l) ⇒ node (Nodes l) None Empty
    | Nodes (Node101 l r) ⇒ node (Nodes l) None (Nodes r)
    | Nodes (Node110 l x) ⇒ node (Nodes l) (Some x) Empty
    | Nodes (Node111 l x r) ⇒ node (Nodes l) (Some x) (Nodes r)
    end.
```

We expect this case analysis principle to satisfy the two equations

```
tree_case empty node Empty = empty
tree_case empty node (Node l o r) = node l o r
```

The second equation is not true in general: in the case where l and r are Empty and o is None, Node l o r is Empty and the tree_case analysis returns empty, whereas our second equation requires it to return node Empty None Empty. To support the equation, we can require that node Empty None Empty = empty, showing that the two cases of the analysis agree in this special case. Alternatively, we can rule out the special case by adding the precondition not_trivially_empty l o r to the second equation. The not_trivially_empty predicate is defined as

```
Definition not_trivially_empty {A} (l: tree A) (o: option A) (r: tree A) :=
  match l, o, r with
  | Empty, None, Empty ⇒ False
  | _, _, _ ⇒ True
  end.
```

The custom induction principle that we define later in this section provides us with the not_trivially_empty l o r guarantee in the Node l o r case. Hence we can always apply the tree_case equations when reasoning with this induction principle.

A minor variant of tree_case implements a recursion principle. We still have two cases, empty and node, but the node case also receives the results of recursing over the left and right subtrees.

```
tree_rec: ∀{A B} (empty: B)
                 (node: tree A → B → option A → tree A → B → B),
                 tree A → B.
```

Along the same lines, we can also define a general, dependently typed induction principle, usable both for computations and for proofs. Its type is similar to that of the Coq-generated induction principle for the two-constructor tree type of section 2, except that the node case also receives a proof of the not_trivially_empty guarantee:

```
tree_ind: ∀{A: Type} (B: A → Type)
                (empty: B Empty)
                (node: ∀l, B l → ∀o r, B r → not_trivially_empty l o r → B (Node l o r)),
                (m: tree A), B m.
```

One use for this induction principle is to simplify proofs about hand-written functions over type tree. For example, to prove properties of the set function defined above, we can first show the following equations:

```
        set xH v Empty = Node Empty (Some v) Empty
     set (xO q) v Empty = Node (set q v Empty) None Empty
      set (xI q) v Empty = Node Empty None (set q v Empty)
    set xH v (Node l o r) = Node l (Some v) r
set (xO q) v (Node l o r) = Node (set q v l) o r
 set (xI q) v (Node l o r) = Node l o (set q v r)
```

which follow by a trivial case analysis on l, o and r. Then, we can prove properties such as get i (set i v m) = Some v by an outer structural induction over i and an inner induction over m that uses the tree_ind custom induction principle. This reduces the number of cases to consider to $3 \times 2 = 6$ cases.

Custom case analysis and induction principles can also be used to define functions over trees. For instance, the infamous combine function can be defined quite concisely by:

```
tree_rec combine_r
         (fun l1 rec_l1 o1 r1 rec_r1 m2 ⇒
           tree_case
             (combine_l (Node l1 o1 r1))
             (fun l2 o2 r2 ⇒ Node (rec_l1 l2) (f o1 o2) (rec_r1 r2))
             m2)
```

This definition is much more compact than the hand-written, 49-case definition. However, the tree_rec and tree_case functions add significant run-time overhead. We can recover most of the efficiency of the hand-written version by partial evaluation within Coq: as shown above for map_filter', we can use Eval cbv to force Coq to expand the tree_rec and tree_case functions, then simplify. Even then, a minor inefficiency remains: the second argument to combine is tested for emptiness at each recursive step over the first argument, instead of being tested once and for all in the hand-written or tactic-based implementations. A custom double induction principle, operating over two trees at once, can remove this last inefficiency.

To conclude this discussion: the canonical representation of binary tries greatly increases the number of cases in function definitions and in proofs. This increase can be challenging for functions operating on two or more tries at the same time, but can be managed either by writing tactics that define these functions, or by defining appropriate case analysis and induction principles that reduce the number of cases, then using Coq's built-in evaluation facilities to remove the execution overhead caused by these principles. In our experience, the former approach based on views make it easy to define correct functions on the first try, while the tactics-based approach requires more trial and error. However, tactics are able to produce function definitions that have exactly the required shape for optimal performance; this is not always the case with partial evaluation of definitions that use views, which provides less control on the exact shape of the final definition.

6 Other approaches to extensionality

The canonical, first-order representation we have just presented in section 4 is not the only way to achieve extensionality: another way is to use dependent types, as we now demonstrate. The reader may choose to skip this section, because it turns out that none of these other approaches performs as well, in a wide enough range of applications, as the canonical representation.

6.1 Subset types

The simple tries from section 2 are not extensional because they might contain subtrees Node Leaf None Leaf, which contain no elements but structurally differ from Leaf. The extensionality property holds if we restrict ourselves to trees that satisfy the following invariant wf, "well-formed: the tree contains no empty nodes Node Leaf None Leaf."

```
Definition not_trivially_empty {A} (l: tree A) (o: option A) (r: tree A) :=
  match l, o, r with
  | Leaf, None, Leaf ⇒ False
  | _, _, _ ⇒ True
  end.

Inductive wf {A}: tree A → Prop :=
  | wf_Leaf: wf Leaf
  | wf_Node: ∀l o r, wf l → wf r → not_trivially_empty l o r → wf (Node l o r).
```

It is not difficult to show that if wf m_1 and wf m_2 hold, and if m_1 and m_2 are equivalent (for any i, get i m_1 = get i m_2), then m_1 and m_2 are structurally equal.

To maintain the invariant through all operations over trees, we define the type of tries m that satisfy wf m as a Coq subset type, also called sigma-type:

```
Definition t (A: Type) : Type := { m: tree A | wf m }.
```

Values of this type are dependent pairs of a tree m and a proof of wf m. This approach is used in the Std++ library [12]. Earlier, it was used by Filliâtre and Letouzey in their implementations of finite sets and finite maps by AVL trees [9], to maintain the invariant that all trees considered are binary search trees.

A strength of this approach is that it reuses the previous implementation of tries (definitions of operations and proofs of properties), simply wrapping them up with proofs of the wf invariant.

```
Fixpoint set_raw {A : Type} (i : positive) (v : A) (m : tree A) : tree A :=
  match m with ... end.

Lemma set_wf: ∀{A: Type} i (v: A) {m: tree A}, wf m → wf (set_raw i v m).
Proof. ... Qed.

Definition set {A: Type} (i: positive) (v: A) (m: t A) : t A :=
  exist _ (set_raw i v (proj1_sig m)) (set_wf i v (proj2_sig m)).
```

The "subset type" approach executes efficiently after extraction: propositions and proofs are erased during extraction, hence the type t is identical to tree in the extracted OCaml code, and there is no overhead compared with the original implementation of tries.

However, execution within Coq is inefficient because the proof of wf m grows linearly *in the number of operations performed over m*. In effect, the proof part of a value of type t A contains the history of all operations applied to produce this value.

Consider for instance the result of setting the key xH to values $v_1, \ldots, v_n$ successively. The value part is the small tree Node Leaf (Some v_n) Leaf, but the proof part is set_wf xH v_n (... (set_wf xH v_1 wf_Leaf) ...), a term of size $O(n)$. Assuming the proof of lemma set_wf is opaque, this proof term does not reduce and takes $O(n)$ space and $O(n)$ time when normalization is requested.

We experimented with alternate, "transparent" definitions of set_wf and related lemmas that would reduce to small proof terms during normalization, but failed to find definitions that would be efficient both in space and in normalization time.

In logics (such as HOL and Isabelle/HOL) that use the LCF approach [10] to the representation of proofs—i.e., that do not represent proof terms at all—these "subset types" are likely to be quite efficient. But Coq represents proof trees explicitly. If only the proof terms of these sigma types could be erased in computation within Coq, as they are erased in extraction, then the subset-type implementation might perform very well inside Coq. An early implementation of Agda followed this approach of erasing irrelevant terms in the internal syntax, following the model-theoretic study by Abel, Coquand and Pagano [1]. It was later found to cause problems with higher-order unification and abandoned.[5] More recently, Pujet and Tabareau [19] have worked out another type theory of this kind of organic computational proof-irrelevance. If it were implemented in the Coq kernel, then many kinds of data structures could be made extensional using sigma types.

6.2 A poor man's inductive-inductive definition

Rather than maintaining the wf invariant as a separate proof term, as in section 6.1, we could try to make it part of the main tree data structure, along the following lines:

```
Inductive tree (A : Type) :=
  | Leaf : tree A
  | Node : ∀(l: tree A) (o: option A) (r: tree A),   not_trivially_empty l o r → tree A.
```

The Node constructor carries not only an optional value and left and right subtrees, but also a proof that the node is not trivially empty. We would expect this representation to compute within Coq more efficiently than the subset type representation, since proofs of not_trivially_empty are small, and only those proofs relevant to the nodes of the tree are kept.

The definition above is incorrect, of course, since the not_trivially_empty predicate mentions the Leaf constructor of the type tree that we are defining. We need to define the predicate and the tree simultaneously, along the following lines:

```
Inductive tree (A : Type) :=
  | Leaf : tree A
  | Node : ∀(l: tree A) (o: option A) (r: tree A),   not_trivially_empty l o r → tree A.

with not_trivially_empty {A: Type}: tree A → option A → tree A → Prop :=
  | not_trivially_empty_intro: ∀l o r,
            ~(l = Leaf ∧ o = None ∧ r = Leaf) → not_trivially_empty l o r.
```

This is called an *inductive-inductive definition*: the type tree is defined mutually recursively with the type family not_trivially_empty that is indexed over type tree.

Such inductive-inductive types are supported in Agda but not in Coq. However, our use of induction-induction is so simple that we can work around this limitation of Coq. We index

[5] Andreas Abel, personal communications, Aug-Sept 2022. Examples of problematic unifications can be found at https://github.com/agda/agda/issues/483

the type of trees with an additional parameter of type kind, with the kind Empty standing for the constructor Leaf, and the kind Nonempty standing for the constructor Node:

```
Inductive kind : Type := Empty | Nonempty.

Definition not_trivially_empty {A: Type} (kl: kind) (o: option A) (kr: kind) :=
  ~(kl = Empty ∧ o = None ∧ kr = Empty).

Inductive tree (A : Type) : kind → Type :=
  | Leaf : tree A Empty
  | Node : ∀(kl kr: kind) (l: tree A kl) (o: option A) (r: tree A kr),
                    not_trivially_empty kl o kr → tree A Nonempty.
```

This breaks the circularity in the definition of not_trivially_empty and turns tree into a regular inductive type. Finally, a well-formed tree is defined as a dependent pair of a kind and a tree of that kind:

```
Inductive t (A: Type) : Type :=
  | Tree : ∀(k: kind), tree A k → t A.
```

With some elbow grease, we can adapt the definitions of operations over trees, first at type tree A k, then at type t A after abstracting over the kind k. For example, the set operation looks as follows:

```
Fixpoint set' {A: Type} (k: kind) (i: positive) (v: A) (m: tree A k) : tree A Nonempty := ...

Definition set {A: Type} (i: positive) (v: A) (m: t A) : t A :=
  let '(Tree k m) := m in Tree Nonempty (set' k i v m).
```

Concerning efficiency of evaluation, canonical binary tries seem to have the same asymptotic time and space complexity as the original, nonextensional implementation from section 2, both after extraction and within Coq—see Table 1. However, the Node constructor is bigger by a constant factor: in Coq, it additionally carries two kinds (kl and kr) and a proof of not_trivially_empty; after extraction to OCaml, it still carries the two kinds kl and kr, even if they do not participate in the computations. Consequently, the constant factors for space and time complexity are noticeably higher than in the original implementation.

7 Benchmarks

7.1 Performance of binary trie implementations

We now evaluate the performance of the various binary trie implementations mentioned in this paper, on synthetic benchmarks, both for execution within Coq or after extraction to OCaml. The implementations and the benchmark harness can be found in the companion development [14]. Here are the implementations:

Original: The original, nonextensional implementation described in section 2:

```
Inductive tree (A : Type) := Leaf : tree A | Node : tree A → option A → tree A → tree A.
```

Canonical: The canonical binary tries of section 4, based on space-efficient representation:

```
Inductive tree' (A: Type) : Type :=
  | Node001: tree' A → tree' A
  | Node010: A → tree' A
  | Node011: A → tree' A → tree' A
  | Node100: tree' A → tree' A
```

```
  | Node101: tree' A → tree' A → tree' A
  | Node110: tree' A → A → tree' A
  | Node111: tree' A → A → tree' A → tree' A.
Inductive tree (A: Type) : Type :=
  | Empty : tree A
  | Nodes: tree' A → tree A.
```

Node01: A nonextensional implementation that avoids storing option values in nodes, using two constructors Node0 (node carrying no value) and Node1 (node carrying a value) instead:

```
Inductive tree (A : Type) :=
  | Leaf : tree A
  | Node0 : tree A → tree A → tree A.
  | Node1 : tree A → A → tree A → tree A.
```

This is a middle point between the Original and the Canonical implementations, both in terms of space efficiency and in terms of complexity of implementation.

Sigma: An extensional implementation built on top of the Original implementation using a subset type to guarantee well-formedness of trees, as in section 6.1:

```
Inductive tree (A : Type) := Leaf : tree A | Node : tree A → option A → tree A → tree A.
Definition t (A: Type) : Type := { m: tree A | wf m }.
```

GADT: An extensional implementation based on an indexed type, also known as a GADT (generalized algebraic data type), as described in section 6.2:

```
Inductive tree (A : Type) : kind → Type :=
  | Leaf : tree A Empty
  | Node : ∀(kl kr: kind) (l: tree A kl) (o: option A) (r: tree A kr),
                 not_trivially_empty kl o kr → tree A Nonempty.
Inductive t (A: Type) : Type :=
  | Tree : ∀(k: kind), tree A k → t A.
```

Patricia: A nonextensional implementation based on the Patricia binary trees from *Functional Algorithms, Verified!*, [18, §12.3]. Each node contains a prefix (a list of bits, represented as a positive integer) that must be matched before reaching the node, thus compressing skinny branches.

```
Inductive tree (A : Type) : Type :=
  | Leaf : tree A
  | Node : positive → tree A → option A → tree A → tree A.
```

AVL: The implementation of finite maps by Filliâtre and Letouzey [9], using AVL balanced binary search trees. It is much more versatile than our binary tries, as it supports keys of any type equipped with a decidable total ordering, not just positive numbers. We include this implementation in the comparison because it is the most efficient finite map data structure provided by the Coq standard library.

Red-Black: Another generic implementation of finite maps, using red-black balanced binary search trees, developed by Letouzey [17]. It supports keys of any type equipped with a decidable total ordering, like the AVL implementation, but performs better in general.

We compare the performance of these implementations using three benchmarks:

Dense: The keys 1 to 2048 are successively inserted in a trie, then every key is looked up. This produces a dense, perfectly balanced binary trie. This is representative of how binary tries are used in the back-end of the CompCert compiler to represent control-flow graphs, in particular.

Sparse: As in the Dense test, we insert then look up a number of keys. The keys correspond to words randomly chosen from an English dictionary, then converted to positive numbers by viewing the words as strings of bits, with 8 bits per character and an ASCII encoding. We have 5064 words with length ranging from 1 to 18 characters (average 8 characters). This test produces sparse, poorly balanced tries with long, nearly empty branches. It is representative of some uses of binary tries in the VST infrastructure, where keys are encodings of program identifiers. The static analyses of the CompCert back-end also use sparse tries intensively.

Repeated: We insert the same seven keys (1 to 7) a million times in a trie. The purpose of this test is to check that the trie remains small (7 nodes) and does not grow at each insertion. It is representative of the use of binary tries as environments in a reference interpreter: there are few variables in the program being interpreted, but they are assigned many times.

For execution within Coq, we use `vm_compute` as our primary evaluation mechanism. It implements call-by-value through compilation to a virtual machine. For comparison, we also give some numbers obtained with the `cbv` and `lazy` mechanisms. These are interpreters that follow either call-by-value (`cbv`) or call-by-need (`lazy`). These mechanisms are much slower than `vm_compute`, hence we report results for the Sparse benchmark only. We also extract the benchmarks to OCaml and compile them to native code using the `ocamlopt` compiler. For OCaml executions, we report execution times, amount of memory allocated (in bytes), and memory size of the data structure being built (in bytes). For executions within Coq, we were unable to measure memory usage and only report execution times. The experimental results are listed in table 1.

We see that the Canonical implementation significantly improves on the Original implementation for the Sparse test: Coq execution times decrease by 22%, OCaml execution times by 33%, and memory allocations and in-memory data size are halved. For the Dense and Repeated tests, memory allocation is reduced by about 12%, and data size is halved, but execution times increase a bit.

The Node01 implementation stands halfway between the Original and the Canonical implementations in terms of OCaml execution times and memory consumption. Coq execution times show no improvement compared with the Original implementation. Combined with the lack of extensionality, these results show that Node01 is not an interesting alternative to Canonical.

The Sigma implementation performs exactly like the Original implementation after extraction to OCaml. This is unsurprising: the subset type is erased during extraction, resulting in very similar OCaml code for the Sigma and Original implementations. As expected, execution inside Coq is slowed down by the construction and propagation of proof terms for the well-formedness invariant: modestly so (5% to 37% depending on the Coq evaluation mechanism used) for the Sparse and Dense tests, but dramatically so (a 5-times increase) for the Repeated test.

The GADT implementation avoids the dramatic degradations of the Sigma implementation, but runs 17% to 100% slower than the Original implementation, both within Coq and after extraction to OCaml. The extra arguments to the Node constructor increase memory usage by 50%.

The Patricia implementation is quite efficient on sparse maps, beating all the other implementations after extraction to OCaml, and second only to the Canonical implementation for evaluation within Coq. On dense maps, performance is worse than the Original and

	Original	Node01	Canonical	Sigma	GADT	Patricia	AVL	Red-Black
	Coq execution, `vm_compute`, Sparse test							
Time in s	1.78e-02							
Relative time	100%	99%	78%	105%	155%	87%	1080%	778%
	Coq execution, `vm_compute`, Dense test							
Time in s	1.10e-03							
Relative time	100%	97%	100%	123%	152%	196%	2804%	960%
	Coq execution, `vm_compute`, Repeated test							
Time in s	5.20e-01							
Relative time	100%	97%	122%	506%	207%	238%	2577%	710%
	Coq execution, `cbv`, Dense test							
Time in s	1.97e-02							
Relative time	100%	95%	100%	137%	219%	224%	3881%	1070%
	Coq execution, `lazy`, Dense test							
Time in s	3.56e-03							
Relative time	100%	79%	94%	109%	118%	127%	11426%	4904%
	Extraction to OCaml, Sparse test							
Time in s	1.09e-02							
Relative time	100%	92%	69%	101%	127%	49%	371%	339%
Allocated bytes	1.07e+07							
Relative alloc	100%	76%	56%	100%	151%	118%	97%	34%
Data size	6.11e+06							
Relative size	100%	75%	50%	100%	149%	22%	45%	44%
	Extraction to OCaml, Dense test							
Time in s	1.96e-04							
Relative time	100%	102%	119%	101%	115%	198%	1724%	1102%
Allocated bytes	6.88e+05							
Relative alloc	100%	87%	87%	100%	156%	298%	568%	241%
Data size	9.83e+04							
Relative size	100%	67%	50%	100%	133%	117%	160%	133%
	Extraction to OCaml, Repeated test							
Time in s	3.67e-02							
Relative time	100%	122%	155%	100%	146%	231%	1847%	409%
Allocated bytes	6.56e+08							
Relative alloc	100%	83%	90%	100%	168%	245%	271%	175%

Table 1 Performance figures for 6 implementations of binary trees and for two reference implementations based on AVL or Red-Black balanced trees. The implementations and the benchmark tests are described in the main text, section 7.1. The tests were executed on a single core of an AMD Ryzen 7 3700X processor running Ubuntu Linux 20.4, using Coq version 8.15.1 and OCaml version 4.14.0 in "no naked pointers" mode. All tests were repeated enough times so that the measured running time is between 1 and 10 seconds. Timing variations between multiple measurements are below 5%. For the Repeated tests, the size of the data structure is not reported, as it is very small.

Canonical implementations, owing to more complex algorithms, such as the need to compute the common prefix between two lists of bits represented as positive integers.

The AVL and Red-Black implementations perform poorly compared to the binary trie implementations: between 3 and 114 times slower than the Original implementation. These are generic implementations of maps that, unlike the binary trie implementations, do not take advantage of the specific structure of keys as positive numbers. Instead, these implementations spends much time in rebalancing and in comparing positive keys, a comparison that is quite slow since positive numbers are isomorphic to lists of bits. The Red-Black implementation is always more efficient than the AVL implementation, by a factor of up to 4.

	AVL	Red-Black	Char-Trie	Canonical
	Coq execution, `vm_compute`			
Time in s	1.86e-01			
Relative time	100%	31%	195%	14%
	Extraction to OCaml			
Time in s	7.02e-03			
Relative time	100%	35%	62%	154%
Allocated bytes	1.04e+07			
Relative alloc	100%	35%	84%	159%
Data size	8.55e+05			
Relative size	100%	90%	170%	331%

Table 2 Performance figures for 4 implementations of the dictionary data structure. The implementations and the benchmark tests are described in the main text, section 7.2. The measurements use same the methodology and hardware and software configuration as in Table 1.

7.2 Comparison with other dictionary data structures

CompCert and VST occasionally use binary tries as dictionaries, that is, finite maps indexed by character strings instead of by positive numbers. This is achieved by a simple encoding of strings as bit sequences represented as positive numbers. It is interesting to compare the performance of these dictionaries derived from binary tries with the performance of other implementations of dictionaries. Table 2 shows some measurements for the following 4 dictionary implementations:

Canonical : This is the better of the binary trie implementations used in section 7.1, composed with string to positive conversions. In other words, the `get` and `set` operations take strings as keys, convert them to positive numbers on the fly, and invoke the `get` and `set` operations of the Canonical binary trie implementations.

AVL: The AVL balanced binary search trees from Coq's standard library, using strings as keys.

Red-Black: The Red-Black balanced binary search trees by Letouzey, using strings as keys.

Char-Trie: A trie data structure that branches on characters, instead of on single bits like the binary tries. More precisely, each node of the trie carries a sparse, sorted association list mapping the next character to the corresponding sub-trie.

The benchmark used in table 2 is similar to the Sparse benchmark from section 7.1: 5064 words randomly chosen from an English dictionary are inserted in the data structure, then looked up.

For executions within Coq, the implementation based on canonical binary tries is 2 to 14 times faster than the AVL, Red-Black and Char-Trie implementations, despite the overhead of converting strings to positive numbers at each operation. This can be explained by the way Coq represents strings: a string is isomorphic to a list of characters, each character being isomorphic to a 8-tuple of Booleans. This makes comparisons between characters and comparisons between strings rather expensive. The AVL and Red-Black implementations perform many string comparisons, and the Char-Trie implementation performs many character comparisons.

After extraction to OCaml, Coq's characters are mapped to OCaml's characters, which are small machine integers that can be compared very efficiently. Strings remain as lists of small integers. Consequently, the AVL, Red-Black and Char-Trie implementations run significantly faster than the binary trie-based implementation, up to 4 times faster for Red-

	Lines of code	Time for 3.9	Time 3.10 change	Memory usage for 3.9	Memory usage 3.10 change
Compilation					
Raytracer	2879	0.42s	+2.4%	33 MiB	0.0%
Spass	82111	17.9s	+1.0%	96 MiB	-32.3%
Unit1	19755	108.7s	-4.3%	2.1 GiB	-5.9%
Unit2	36709	73.9s	-7.8%	1.5 GiB	-8.6%
Unit3	118952	208.4s	-7.5%	5.4 GiB	-17.1%
Interpretation					
Fib	19	12.8s	+2.2%	2.2 GiB	-7.0%
Qsort	50	53.0s	+1.4%	2.8 GiB	-9.1%

Table 3 Impact of the change to canonical binary tries on CompCert compilation and interpretation times and memory usage. We used CompCert versions 3.9 and 3.10, built with Coq version 8.13.2 and OCaml version 4.12. Measurements were taken on a single core of an AMD Ryzen 7 3700X processor running Ubuntu Linux 20.4.

Black. The performance of the dictionaries based on binary tries remains acceptable, given the simplicity of the implementation, and could be improved by "fusing" the string-to-positive conversion and the recursive tree traversals, avoiding the construction of positive numbers.

8 Integration in CompCert

The canonical binary tries described in this paper were integrated in version 3.10 of the CompCert verified C compiler, replacing the original, non-extensional tries that had been used since the beginning of CompCert. The implementation follows exactly the approach described in this paper and its companion Coq development, but provides more operations, such as mapping or folding a function over a trie, converting a trie to a list of (key, value) pairs, and comparing two tries. Moreover, a variant of the combine operation that improves in-memory sharing between its result and its two arguments is provided to reduce the memory usage of dataflow analyses.

The implementation of CompCert makes heavy use of binary tries to represent several kinds of finite maps. Control-flow graphs are represented as functional arrays implemented by dense binary tries. Most dataflow analyses use finite maps from pseudoregisters to an abstract domain. These maps are represented by sparse binary tries, omitting the pseudoregisters that are associated with $\top$. Finally, CompCert also provides a reference interpreter that animates its formal C semantics. During interpretation, memory states are represented by two levels of binary tries, as mappings from block identifier and block offset to byte contents [4, chap. 32].

We measured compilation and interpretation times and memory usage for a handful of C programs, comparing CompCert 3.9, the last version that uses the original implementation of binary tries, with CompCert 3.10, the first version that uses the canonical binary tries. (There are other changes between 3.9 and 3.10, but they appear to have no measurable impact on compilation and interpretation times.) The results are summarized in table 3.

For the compilation tests, we have five programs: Raytracer and Spass, which are hand-written, and Unit1, Unit2, and Unit3, which are automatically-generated unit tests with a peculiarity: all the tests are put in a single function, resulting in huge functions that cause high compilation times and memory usage. For the interpretation tests, we use two tiny C programs: the Fibonacci function and the Quicksort algorithm.

As table 3 shows, the switch to canonical binary tries decreases memory usage of compilation and interpretation by up to 30%. This was to be expected, given that binary tries are used a lot and the canonical kind has a more compact in-memory representation. Compilation and interpretation times increase slightly, by up to 2.4%, except for the "one huge function" unit tests, where compilation times decrease noticeably, by up to 7.8%.

For finer analysis, we profiled two of the compilations using the Linux `perf` tool, focusing on the functions that account for more than 0.5% of the total compilation time. For the Spass test, binary tries operations account for 14% of the CompCert 3.9 compilation time, and slow down by about 20% when moving to 3.10. (This is consistent with the 20% slowdown on dense maps after extraction to OCaml reported in table 1.) However, memory management (allocation and GC) account for 25% of the CompCert 3.9 time, and speed up by 6% in 3.10, owing to the reduced memory usage. The two effects almost cancel each other, resulting in a small slowdown overall. For the Unit3 test, binary tries operations account for 26% of the 3.9 compilation time, and take about the same time in 3.10, while memory management accounts for 44% of the 3.9 compilation time, and decrease by 12% in 3.10 owing to the reduced memory usage. The result is a clear decrease in compilation times.

9 Efficiency improvements in VST

The Verified Software Toolchain (VST) [2] comprises a program logic (Verifiable C) for the C programming language, proved sound in Coq with respect to the operational semantics of CompCert Clight, and a proof automation system (VST-Floyd) [8] to assist users in applying the program logic to their program. Like CompCert, VST heavily uses PTrees for many purposes: mapping function-names to function-bodies, function-names to their specifications, global variable names to their types, local variable names to their types, local variable names to their symbolic contents, and so on.

Unlike CompCert, which runs in extracted OCaml, VST runs inside Coq's Gallina logic, because it must manipulate proof goals and proof terms, and even the PTrees must map names to values that contain fragments of Coq terms and proofs. Therefore, unlike in extracted OCaml where propositions and proofs-of-propositions have been erased, computations inside VST are unerased. This means that the sigma-type representation would be much less efficient in VST than it would be in CompCert.[6]

A recent enhancement to VST is *Verified Software Units*, which allows modular verification of modular C programs [5]. The VSU system uses PTrees even more heavily, in reasoning about linkage of programs, of specifications, and of proofs. Furthermore, in the VSU system it is often necessary to compare two PTrees for equivalence, which is much faster to do in a data structure with extensionality.

Furthermore, VST theorem statements (and intermediate proof goals) often contain concrete PTrees, mapping C program identifiers to various program specifications and AST terms. A more compact representation of these PTrees would reduce the proof-checking burden on the Coq kernel.

So it would not be surprising if a faster, more memory-efficient, extensional representation of PTrees would significantly improve performance of the VST interactive verifier. And

[6] In table 1, performance of PTrees in VST could be predicted in row "Coq execution, vm_compute, Sparse test," column Sigma versus columns Original and Canonical; whereas PTree performance in CompCert could be predicted in row "Extraction to OCaml, Sparse test", same columns.

indeed, we are not suprised. VST/VSU verifications run 10% faster *overall* with Canonical Binary Tries.

Measurement method. We compared VST 2.8 (with original PTrees) and VST 2.9 (with canonical PTrees). In release 2.9 there were no other changes that would significantly impact performance. We benchmarked the "pile" benchmark [6, Fig. 1] as adapted to VSUs[7] We measured performance of all the *verifications* (verif_∗.v); we omitted specification files, which are not generally time-consuming and did not show significant improvement. Checking those Coq proofs[8] totaled 105 seconds with original PTrees and 95.5 seconds with canonical PTrees[9], an improvement of 10%.

10 Conclusion

Our quest for finite maps that enjoy the extensionality property led us to a new data structure, *canonical binary tries,* that performs very well in many contexts: extracted to OCaml and compiled to native code, or represented in Coq proofs. In OCaml code, canonical binary trees reduce memory usage significantly and improve execution times somewhat compared with simple binary tries. When keys are character strings, other implementations such as balanced binary trees are faster, but they require primitive integers, whose associated implementations would then have to be trusted (or proved).

In functional programs written in Coq, canonical binary tries are also significantly faster than simple binary tries. But when (concrete) tries must appear in Coq theorem statements and in Coq proofs, canonical tries offer additional benefits: proof-checking efficiency (smaller theorem statements, smaller proofs) and theorem simplicity (the ability to reason by Leibnitz equality instead of equivalence relations).

At first, we were worried about the increase in the number of cases for function definitions and for proofs, compared with the original binary tries where there are only two cases to consider. We demonstrated two approaches to synthesizing large case analyses instead of writing them by hand: one is based on Coq's tactic language and lets us fluidly combine synthesis-time case analysis, run-time case analysis, and synthesis-time symbolic analysis; the other is based on custom constructors and induction principles that lets us view the new data structure as the original, two-case data structure, combined with partial evaluation within Coq to eliminate the run-time overhead of the view. More generally, Coq offers powerful metaprogramming facilities that have great potential to facilitate not just the verification but also the implementation of complex data structures.

Besides binary tries, are there other useful data structures that admit canonical representations? And are these canonical representations always more memory-efficient than other representations? We have no general answers to these questions, but we can offer two other examples of canonical representations.

The first example is the clever representations of binary numbers used in Coq (the type positive of positive integers mentioned in section 2) and in HOL, where natural numbers can be represented by the constant ZERO and two constructors BIT1 and BIT2, with BIT1(p)

[7] This Coq verification is at https://github.com/PrincetonUniversity/VST/releases/tag/v2.9.1 in subdirectory progs/VSUpile.

[8] verif_stdlib, verif_pile, verif_onepile, verif_apile, verif_triang, verif_core, verif_main

[9] Measurements were performed on a Lenovo t440p laptop with Intel Core i7-4810MQ @ 2.8GHz with 32GB memory, using Coq 8.14/8.15.1 in 32-bit mode with virtual-memory limit of 1GB. The Clight abstract-syntax-tree files were produced by clightgen in its default canonical—idents mode.

denoting $2p+1$ and $\mathsf{BIT2}(p)$ denoting $2p+2$. These representations are canonical, unlike the obvious representation as lists of bits, and use less memory space, since the constructors xO, xI, BIT1, BIT2 have one argument only, instead of the two arguments of the "cons" list constructor.

For a less familiar example, consider sets of positive numbers. The usual representation of sets as lists is neither canonical nor extensional: the set $\{1,2\}$ has several representations, $[1,2]$ or $[2,1]$ or $[1,1,2,1,2]$. We can recover extensionality by using a subset type { l : list positive | sorted l }, where the sorted predicate ensures that the list is increasing and without repetitions. However, a canonical representation exists, as the list of (positive) differences from one set element to the next greater element. For instance, the set $\{1,4,9,11\}$ is uniquely represented by the list $[1,4-1,9-4,11-9]$, that is, $[1,3,5,2]$. This encoding is not only canonical, but also slighty more memory efficient than the usual sorted list representation, as the numbers stored in the list of differences are smaller than those stored in the sorted list.

Can we play similar tricks for more complex data structures? We leave this question for future work.

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