Efficiency of a good but not linear nominal unification algorithm

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Abstract

We present a nominal unification algorithm that runs in $O(n \times log(n) \times G(n))$ time, where G is the functional inverse of Ackermann's function. Nominal unification generates a set of variable assignments, if there exists one, that makes terms involving binding operations α-equivalent. We preserve names while using special representations of de Bruijn numbers to enable efficient name management. We use Martelli-Montanari style multi-equation reduction to generate these name management problems from arbitrary unification terms.

Keywords and phrases α-conversion; Binding operations; Efficiency; Unification

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1 Introduction and background

The rules that identify terms, such as α, β, and η in the λ-calculus [Church, 1941], are critical to building programming languages and formal systems. As users of logic programming languages and theorem provers, we desire such rules to be out-of-the-box in the tool-kit. Two theories have aimed to provide this convenience: higher-order pattern unification of Miller [1989] and nominal unification of Urban et al. [2004]. Higher-order pattern unification, which handles a fragment of $\beta\eta$-rules, is the foundation of Isabelle [Paulson, 1986], λProlog [Nadathur et al., 1988], and Twelf [Pfenning and Schürmann, 1999]. Nominal unification, which focuses on the α-rule, has inspired extensions of logic programming languages, like αProlog [Cheney and Urban, 2004] and αKanren [Byrd and Friedman, 2007], as well as theorem provers, like nominal Isabelle [Urban and Tasson, 2005] and αLeanTAP [Near et al., 2008]. Although these two theories can be reduced to one another [Cheney, 2005, Levy and Villaret, 2012], implementing higher-order pattern unification is more complicated because it has to deal with application and capture-avoiding substitution. On the other hand, implementation of nominal unification, which essentially unifies first-order terms, is more straightforward and easier to formalize. Beyond unification, techniques from the nominal approach, such as swapping and freshness environments, have impacted the areas as diverse as rewriting [Fernández et al., 2004, Fernández and Gabbay, 2005, 2007, Aoto and Kikuchi, 2016], equational theories [Ayala-Rincón et al., 2016], and reasoning about bindings in abstract syntax [Pitts and Gabbay, 2000, Gabbay and Pitts, 2002].

Concerning time complexity, Qian [1996] proves that higher-order pattern unification is decidable in linear time. On the other hand, it has been an open problem whether there exists a nominal unification algorithm that can do better than $O(n^2)$. Levy and Villaret [2012] give a quadratic time reduction from nominal unification to higher-order pattern unification. Meanwhile, algorithmic advances by Paterson and Wegman [1978] and Martelli and

Montanari [1982] for unification have inspired many improvements to the efficiency of nominal unification. Also, ideas like applying swappings lazily and composing swappings eagerly and sharing subterms have been explored. Calvès [2010] describes quadratic algorithms that extend Paterson-Wegman and Martelli-Montanari's algorithms with name handling; Levy and Villaret [2010] describe a quadratic algorithm that reduces unification problems to a sequence of freshness and equality constraints and then solves the constraints.

The inefficiency of these nominal unification algorithms comes from the swapping actions, that is, to decide the α-equivalence of two names, we need to linearly traverse a list whose length grows with respect to the number of binders. One might try to replace these lists with a more efficient lookup structure, such as a hash table, but then composing two swappings would take linear time, and that operation is also rather frequent. Here we present an algorithm that does not use swappings but instead represents names with de Bruijn numbers which enables the use of persistent hash tables, in particular, a Hash Array Mapped Trie (HAMT) [Bagwell, 2001]. HAMTs provide efficient lookup and they use sharing to avoid the linear-time costs that would normally be associated with duplicating a hash table.

We organize this paper as follows. In section 2, we show an alternative representation of de Bruijn numbers that is suitable for unification. In section 3, we describe the abstract machines for name management and unification. In section 4, we discuss the time complexity of this algorithm. The proofs of our claims are in progress and are available at the authors' Github, formalized in Agda.

2 De Bruijn numbers should coexist with names

De Bruijn numbers are a technique for representing syntax with binding structure [de Bruijn, 1972]. A *de Bruijn number* is a natural number that indicates the distance from a name occurrence to its corresponding binder. When all names in an expression are replaced with their corresponding de Bruijn numbers, a direct structural equality check is sufficient to decide α-equivalence. A few programming languages [Norell, 2007] use de Bruijn numbers in their internal representations for machine manipulation during operations such as type checking. The idea of using names for free variables and numbers for bound variables, known as the locally nameless approach [Charguéraud, 2012], is employed for formalizing variable-theories [Aydemir et al., 2006, 2008]. Also, de Bruijn numbers, combined with explicit substitution, have been introduced in higher-order unification [Dowek et al., 2000] to improve the efficiency of unification.

Despite its convenience when implementing α-equivalence, programs written with de Bruijn numbers are notoriously obfuscated for humans to read and understand. What's worse, as pointed out by Berghofer and Urban [2007], translating pencil-and-paper style proofs to versions using de Bruijn numbers is surprisingly involved: such translation may alter the structures of proofs. Consequently, reproducing proofs with explicit names from de Bruijn numbers is difficult or even impossible. Thus, for the sake of both readers and writers of proofs, it is worth providing an interface with names.

If our concern is simply deciding the α-equivalence between expressions, an easy way to use de Bruijn numbers while preserving names is to traverse the expressions, annotate each name with its de Bruijn number, then read-back the expressions without numbers. This approach, however, does not work for unification, because it only contains the mapping *from names to numbers*. In unification modulo α-equivalence, one frequently needs the mapping *from numbers to names* to decide what name to assign to a unification variable.

We represent de Bruijn numbers by *static closures*, hereafter referred to as *closures*.

Closures preserve the mappings in both directions: names to numbers and numbers to names.

▶ **Definition 1.** A *closure* is an ordered pair $\langle t; \Phi \rangle$ of a term t, defined in Figure 1, and a scope Φ, where the scope is an ordered list of names for the binders in the enclosing context. Hereafter, we refer to a name as an *atom*.

When the term of a closure is an atom, the closure itself represents a de Bruijn number. For example, consider the term $\lambda x.\lambda y.x$. The de Bruijn number of the atom x is 1 and the closure-representation of this number is $\langle x; (y\, x) \rangle$. We can retrieve the number-representation by finding the position of the first appearance of the atom in the scope. In this case, the position of x in the list $(y\, x)$ is 1, which is its de Bruijn number. Similarly, the de Bruijn number of y is 0.

Figure 1 Terms

t, l, r	::=	a	atom
	|	$\lambda a.t$	abstractions
	|	$(l\, r)$	applications

Figure 2 Free and bound

$$\frac{a \notin \Phi}{\Phi \vdash \texttt{Fr}\ a}\ \text{FREE}$$

$$\frac{(\texttt{atom}{\rightarrow}\texttt{idx}\ \Phi\ a) = i \quad (\texttt{idx}{\rightarrow}\texttt{atom}\ \Phi\ i) = a}{\Phi \vdash \texttt{Bd}\ a\ i}\ \text{BOUND}$$

Figure 3 $\approx$-rules

$$\frac{\Phi_1 \vdash \texttt{Fr}\ a_1 \quad \Phi_2 \vdash \texttt{Fr}\ a_2 \quad a_1 = a_2}{\langle a_1; \Phi_1 \rangle \approx \langle a_2; \Phi_2 \rangle}\ \text{SAME-FREE}$$

$$\frac{\Phi_1 \vdash \texttt{Bd}\ a_1\ i_1 \quad \Phi_2 \vdash \texttt{Bd}\ a_2\ i_2 \quad i_1 = i_2}{\langle a_1; \Phi_1 \rangle \approx \langle a_2; \Phi_2 \rangle}\ \text{SAME-BOUND}$$

A scope, as a list, supports three operations: `ext-scope`, which extends the scope by adding an atom to the front of the list; `idx`→`atom`, which returns the atom of a given index starting from the front of the list; and `atom`→`idx`, which returns the location of the first appearance of a given atom counting from the front of the list. As we are building the list in reversed order, if repeated atoms appear, the first appearance in a list shadows the others.

Now in Figure 2, we can talk about free and bound variables "constructively," with de Bruijn numbers serving as evidence that variables are well-scoped. When an atom, a, does not appear in the scope, Φ, we say, "a is free with respect to Φ," written as $\Phi \vdash \texttt{Fr}\, a$; when a's first appearance in Φ is the position i, we say, "a is bound at i with respect to Φ," written as $\Phi \vdash \texttt{Bd}\, a\, i$. The BOUND rule has two premises to be algorithmic in both directions, that is, given an atom we can find its index and given an index we can find its atom, if no shadowings occur. Figure 3 defines the rules to decide whether two atoms are α-equivalent w.r.t their scopes, written as $\langle a_1; \Phi_1 \rangle \approx \langle a_2; \Phi_2 \rangle$.

3 Unification

In Figure 4, we introduce unification variables, shortened as var. First, let's consider a simplified unification problem: a variable can only be instantiated by an atom, that is, finding the unifier of two terms that share the same structure but differ in atoms and variables. A unifier consists of two parts: σ and δ.

Figure 4 Unification terms and problems

X, Y			variables
xs, ys	$::=$	ϵ	list of variables
	$\mid$	X, xs	
t, l, r	$::=$	a	atoms
	$\mid$	$\lambda a.t$	abstractions
	$\mid$	$(l\, r)$	applications
	$\mid$	X	
e_ν	$::=$	$(a, \Phi) = (a, \Phi)$	ν-equation
	$\mid$	$(X, \Phi) = (a, \Phi)$	
p_ν	$::=$	ϵ	ν-problems
	$\mid$	e_ν, p_ν	
e_δ	$::=$	$(X, \Phi) = (X, \Phi)$	δ-equation
p_δ	$::=$	ϵ	δ-problems
	$\mid$	e_δ, p_δ	

▶ **Definition 2.** A substitution σ is a partial finite function from variables, X_i, to terms, t_i. For readability, we write σ as a set, $\{X_1/t_1, ..., X_j/t_j\}$ and we write $\{X/t\} \cup \sigma$ for extending σ with X/t. For the simplified problems, we restrict t to an atom.

▶ **Definition 3.** A closure equation is a pair of two closures that are α-equivalent. Δ is a set of closure-equations. We write Δ as $\{(\langle t_1; \Phi_1\rangle \langle t_1'; \Phi_1'\rangle), ..., (\langle t_i; \Phi_1\rangle \langle t_i'; \Phi_1'\rangle)\}$ and we write $\{(\langle t; \Phi\rangle \langle t'; \Phi'\rangle)\} \cup \Delta$ for extending Δ with $(\langle t; \Phi\rangle \langle t'; \Phi'\rangle)$. We write δ as a special form of Δ: for each equation in δ, the terms on both sides are variables. Given a variable X, $\delta(X)$ yields the list of closure-equations where X appears at least once.

The simplified problem is about solving three kinds of closure-equations: atom-atom, atom-var, and var-var. As defined in Figure 4, we refer to an atom-atom or atom-var equation as e_ν and refer to a var-var equation as a e_δ. Given two lists, p_ν and p_δ, of these equations, we first run the ν-machine, defined in Figure 5, on p_ν to generate a substitution. The δ-machine, defined in Figure 6, then computes the final unifier on three inputs: the substitution resulted from the ν-machine, δ, and a list of known variables, initialized by the domain of the substitution. If no transitions apply, the machine fails and the unification problem has no unifier.

Figure 5 ν-machine

$$\boxed{\sigma \vdash p_\nu \Rightarrow_\nu \sigma}$$

$$\frac{}{\sigma_0 \vdash \epsilon \Rightarrow_\nu \sigma_0}\ \textsc{Empty}$$

$$\frac{\sigma_0 \vdash p \Rightarrow_\nu \sigma_1 \quad \langle a_1; \Phi_1\rangle \approx \langle a_2; \Phi_2\rangle}{\sigma_0 \vdash \langle a_1; \Phi_1\rangle = \langle a_2; \Phi_2\rangle, p \Rightarrow_\nu \sigma_1}\ \textsc{Name-Name}$$

$$\frac{\{X_2/a_2\} \cup \sigma_0 \vdash p \Rightarrow_\nu \sigma_1 \quad \langle a_1; \Phi_1\rangle \approx \langle a_2; \Phi_2\rangle}{\sigma_0 \vdash \langle a_1; \Phi_1\rangle = \langle X_2; \Phi_2\rangle, p \Rightarrow_\nu \sigma_1}\ \textsc{Name-Var}$$

▶ **Lemma 4.** *For all finite input, the ν-machine and the δ-machine terminates; for all input, the ν-machine and the δ-machine succeeds with the mgu if and only if there exists one.*

Proof. By structural induction on the transitions of the machines. ◀

Now the question is how to generalize the previous algorithm, that is, given two arbitrary terms, where a variable may be instantiated by any term besides atoms, can we re-shape the two terms to create a proper input to the two machines?

Finding the common structure, obviously, is merely a first-order unification problem. The ρ-machine, defined in Figure 7, adapts the idea of Martelli-Montanari and reduces

Figure 6 δ-machine and the pull operation

$$\boxed{\begin{array}{l}\sigma; p_\delta \vdash xs \Rightarrow_\delta \sigma; p_\delta \\ \sigma; xs \vdash p_\delta \Rightarrow_{\text{pull}} \sigma; xs\end{array}}$$

$$\frac{}{\sigma; \delta \vdash \epsilon \Rightarrow_\delta \sigma; \delta}\ \textsc{Empty-Q}$$

$$\frac{}{\sigma; \epsilon \vdash xs \Rightarrow_\delta \sigma; \epsilon}\ \textsc{Empty-D}$$

$$\frac{\begin{array}{l}\sigma_0'; \delta_0 \setminus \delta_0(X) \vdash xs_1 \Rightarrow_\delta \sigma_1; \delta_1 \\ \sigma_0; xs_0 \vdash \delta_0(X) \Rightarrow_{\text{pull}} \sigma_0'; xs_1\end{array}}{\sigma_0; \delta_0 \vdash X, xs_0 \Rightarrow_\delta \sigma_1; \delta_1}\ \textsc{Step}$$

$$\frac{}{\sigma; q \vdash \emptyset \Rightarrow_{\text{pull}} \sigma; q}\ \textsc{Empty}$$

$$\frac{\begin{array}{l}\sigma_0; xs_0 \vdash p \Rightarrow_{\text{pull}} \sigma_1; xs_1 \\ \langle a_1; \Phi_1\rangle \quad \approx \quad \langle a_2; \Phi_2\rangle \quad \sigma_0(Y_1) = a_1 \quad \sigma_0(Y_2) = a_2\end{array}}{\sigma_0; xs_0 \vdash \langle Y_1; \Phi_1\rangle = \langle Y_2; \Phi_2\rangle, p \Rightarrow_{\text{pull}} \sigma_1; xs_1}\ \textsc{Name-Name}$$

$$\frac{\{Y_2/a_2\} \cup \sigma_0; (Y_2, xs_0) \vdash p \Rightarrow_{\text{pull}} \sigma_1; xs_1 \quad \langle a_1; \Phi_1\rangle \approx \langle a_2; \Phi_2\rangle \quad \sigma_0(Y_1) = a_1 \quad Y_2 \notin dom(\sigma_0)}{\sigma_0; xs_0 \vdash \langle Y_1; \Phi_1\rangle = \langle Y_2; \Phi_2\rangle, p \Rightarrow_{\text{pull}} \sigma_1; xs_1}\ \textsc{Name-Var}$$

an arbitrary nominal unification problem to a set of problem_ν, a set of problem_δ, and a substitution. Here we need to extend the definition of substitution: it is now a partial finite function from variables to terms. Also, in the VAR-APP and VAR-ABS rules, we need to create new atoms and new variables.

4 A note on time complexity

Figure 7 ρ-machine

$$\boxed{\begin{array}{l}(problem_\nu^*, problem_\delta^*, \sigma) \vdash multieqn^* \Rightarrow_\rho (problem_\nu^*, problem_\delta^*, \sigma) \\ (problem_\nu^*, problem_\delta^*, \sigma) \vdash multieqn \Rightarrow_{\text{step}} (problem_\nu^*, problem_\delta^*, \sigma)\end{array}}$$

$$\frac{}{(p_0, \delta_0, \sigma_0) \vdash \emptyset \Rightarrow_\rho (p_0, \delta_0, \sigma_0)}\ \textsc{Empty}$$

$$\frac{\begin{array}{l}(p_0', \delta_0', \sigma_0') \vdash U^* \Rightarrow_\rho (p_1, \delta_1, \sigma_1) \\ (p_0, \delta_0, \sigma_0) \vdash U \Rightarrow_{\text{step}} (p_0', \delta_0', \sigma_0')\end{array}}{(p_0, \delta_0, \sigma_0) \vdash (U, U^*) \Rightarrow_\rho (p_1, \delta_1, \sigma_1)}\ \textsc{Step}$$

$$\frac{p_1 = (\langle a_1; \Phi_1\rangle \langle a_2; \Phi_2\rangle) \cup p_0}{(p_0, \delta_0, \sigma_0) \vdash (\langle a_1; \Phi_1\rangle \langle a_2; \Phi_2\rangle) \Rightarrow_{\text{step}} (p_1, \delta_0, \sigma_0)}\ \textsc{Name-Name}$$

$$\frac{p_1 = (\langle a_1; \Phi_1\rangle \langle X_2; \Phi_2\rangle) \cup p_0}{(p_0, \delta_0, \sigma_0) \vdash (\langle a_1; \Phi_1\rangle \langle X_2; \Phi_2\rangle) \Rightarrow_{\text{step}} (p_1, \delta_0, \sigma_0)}\ \textsc{Name-Var}$$

$$\frac{\delta_1 = (\langle X_1; \Phi_1\rangle \langle X_2; \Phi_2\rangle) \cup \delta_0}{(p_0, \delta_0, \sigma_0) \vdash (\langle a_1; \Phi_1\rangle \langle X_2; \Phi_2\rangle) \Rightarrow_{\text{step}} (p_0, \delta_1, \sigma_0)}\ \textsc{Var-Var}$$

$$\frac{\begin{array}{l}(p_0, \delta_0, \sigma_0) \vdash (\langle l_1; \Phi_1\rangle \langle l_2; \Phi_2\rangle) \Rightarrow_{\text{step}} (p_0', \delta_0', \sigma_0') \\ (p_0', \delta_0', \sigma_0') \vdash (\langle r_1; \Phi_1\rangle \langle r_2; \Phi_2\rangle) \Rightarrow_{\text{step}} (p_1, \delta_1, \sigma_1)\end{array}}{(p_0, \delta_0, \sigma_0) \vdash (\langle (l_1\ r_1); \Phi_1\rangle \langle (l_2\ r_2); \Phi_2\rangle) \Rightarrow_{\text{step}} (p_1, \delta_1, \sigma_1)}\ \textsc{App-App}$$

$$\frac{\begin{array}{l}(p_0, \delta_0, \sigma_0) \vdash (\langle t_1; \Phi_1'\rangle \langle t_2; \Phi_2'\rangle) \Rightarrow_{\text{step}} (p_1, \delta_1, \sigma_1) \\ \Phi_1' \quad = \quad (\texttt{ext-scope}\ \Phi_1\ a_1) \quad \Phi_2' = (\texttt{ext-scope}\ \Phi_2\ a_2)\end{array}}{(p_0, \delta_0, \sigma_0) \vdash (\langle \lambda\, a_1.t_1; \Phi_1\rangle \langle \lambda\, a_2.t_2; \Phi_2\rangle) \Rightarrow_{\text{step}} (p_1, \delta_1, \sigma_1)}\ \textsc{Abs-Abs}$$

In the previous sections, we represent scopes by lists for simplicity, but lists are inefficient for variable lookup. To have better time complexity, we represent a scope with a counter and two persistent hashtables, also known as HAMT [Bagwell, 2001]. One hashtable maps from atoms to numbers, the other maps from numbers to atoms, and the counter is used to track the de Bruijn number. When we extend a scope with an atom, we extend the two hashtables with the corresponding maps and add one to the counter. A persistent hashtable, in practice, has constant time for update and lookup, although the worst case scenario could be $O(log(n))$. Thus, `ext-scope`, `idx→atom`, and `atom→idx` are all logarithmic time. In addition, using persistent structures avoids copying the entire data-

structure when branching, in particular, during the APP-APP rule of the ρ-machine.

We implement δ with a hashtable that maps from a variable to the list that contains its closure-equations. Doing so doubles the space consumption, i.e, the equation $\langle X; \Phi_1 \rangle \approx \langle Y; \Phi_2 \rangle$ exists in both X's entry and Y's entry, but improves the time efficiency.

Given the above optimizations, the ν-machine and the δ-machine are both worst case $O(n \times log(n))$, where n is the sum of atom and variable occurrences. The algorithm of Martelli-Montanari is $O(n \times G(n))$, when representing sets with UNION-FIND [Tarjan, 1975], where n is the number of variable occurrences in the original terms. The ρ-machine is similar except that two new factors are involved: the update operation of HAMT and the generation of atoms and variables. We consider the former one to have $O(log(n))$ complexity, and we implement atom and variable creation with state monads in constant time. Thus reducing an arbitrary unification problem to the input of the ν and δ machines becomes $O(n \times log(n) \times G(n))$.

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