Efficiency of a good but not linear nominal unification algorithm

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Abstract

We present a nominal unification algorithm that runs in $O(n \times G(n))$ 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. Operations on name handling, i.e., deciding the α-equivalence of two names and inferring a name that α-equals to a given one, are in constant time. To reduce an arbitrary unification problem to such name handlings, we preprocess the unification terms with the idea of Martelli-Montanari.

1 Introduction and background

The rules that identify terms, such as α, β, and η in the λ-calculus [14], 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: Miller's higher-order pattern unification [24] and nominal unification [34] introduced by Urban, Pitts, and Gabbay. Higher-order pattern unification, which handles a fragment of $\beta\eta$-rules, is the foundation of Isabelle [29], λProlog [25], and Twelf [30]. Nominal unification, which focuses on the α-rule, has inspired extensions of logic programming languages, like αProlog [13] and αKanren [7], as well as theorem provers, like nominal Isabelle [35] and αLeanTAP [26]. Although these two theories have been shown to be equally powerful [12, 22], 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 swappings and freshness environments, have impacted the areas as diverse as rewriting [19, 17, 18, 1], equational theories [2], and reasoning about bindings in abstract syntax [31, 20].

When efficiency is the concern, however, nominal unification is not so practical as higher-order pattern unification. Qian [32] has shown a proof 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 [22] show a translation from nominal unification to higher-order pattern unification in quadratic time while preserving the mgu. Meanwhile, algorithmic advances by Paterson-Wegman [28] and Martelli-Montanari [23] for unification have inspired many improvements to the efficiency of

nominal unification. Also, the ideas like applying swappings lazily and composing swappings eagerly and sharing subterms have been explored. Calves and Fernandez [9, 8, 10] describe quadratic algorithms that extend Paterson-Wegman and Martelli-Montanari's algorithms with name handling; Levy and Villaret [21] describe a new quadratic algorithm that reduces unification problems to a sequence of freshness and equality constraints in linear time and then solves the constraints in quadratic time.

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, with the following contributions.

- **Special representations of de Bruijn numbers** We use *static closures* to represent de Bruijn numbers. Static closures preserve both friendly interfaces for human comprehension and efficient structures for machine manipulation.
- **Better run-time efficiency** The algorithm presented here runs in $O(n \times G(n))$. Since we have constant time name management, the overall time complexity is the same as first-order unification. Previous improvements to nominal unification indicate that it is difficult to improve beyond quadratic [9, 8, 10, 21].
- **Simpler implementation** Unlike traditional nominal unification, we do not use swappings and freshness environments. Using less infrastructure allows an even easier implementation than existing nominal unification algorithms.

We organize this paper as follows. In section 2, we show a 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 related proofs formalized in Agda, available at the authors' Github, is in progress.

2 De Bruijn numbers should coexist with names

De Bruijn numbers [15] are a technique for representing syntax with binding structure. 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 [27] 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 [11], is employed for formalizing variable-theories [3, 4]. Also, de Bruijn numbers, combined with explicit substitution, have been introduced in higher-order unification [16] 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 [6], 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 propose to represent de Bruijn numbers by *static closures*, hereafter referred to as *closures*. Closures preserve the mappings of 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 binders that occur in the enclosing context. Hereafter, we refer to a name as an atom, and we refer to the atom of an abstraction as a binder.

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.

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 $\Phi \vdash \mathtt{Fr}\,a$; when a's first appearance in Φ is the position i, we say, "a is bound at i with respect to Φ," written as $\Phi \vdash \mathtt{Bd}\,a\,i$. 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 shadowing happens. Figure 3 defines the rules to decide whether two atoms are α-equivalent w.r.t theirs scopes, written as $\langle a_1; \Phi_1 \rangle \approx \langle a_2; \Phi_2 \rangle$.

Figure 1 Terms

$$
\begin{array}{rcll}
t, l, r & ::= & a & \text{atom} \\
 & | & \lambda a.t & \text{abstractions} \\
 & | & (l\,r) & \text{applications}
\end{array}
$$

Figure 2 Free and bound

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

$$\frac{(\mathtt{name{\to}idx}\,\Phi\,a) = i \quad (\mathtt{idx{\to}name}\,\Phi\,i) = a}{\Phi \vdash \mathtt{Bd}\,a\,i}\ \text{BOUND}$$

Figure 3 $\approx$-rules

$$\frac{\begin{array}{c}\Phi_1 \vdash \mathtt{Fr}\,a_1 \\ \Phi_2 \vdash \mathtt{Fr}\,a_2 \\ a_1 \ = \ a_2\end{array}}{\langle a_1; \Phi_1 \rangle \approx \langle a_2; \Phi_2 \rangle}\ \text{SAME-FREE}$$

$$\frac{\begin{array}{c}\Phi_1 \vdash \mathtt{Bd}\,a_1\,i_1 \\ \Phi_2 \vdash \mathtt{Bd}\,a_2\,i_2 \\ i_1 \ = \ i_2\end{array}}{\langle a_1; \Phi_1 \rangle \approx \langle a_2; \Phi_2 \rangle}\ \text{SAME-BOUND}$$

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 a name, 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

$$
\begin{array}{lll}
t, l, r & ::= & a & \text{atoms} \\
& | & \lambda a.t & \text{abstractions} \\
& | & (l\,r) & \text{applications} \\
& | & X & \text{variables}
\end{array}
$$

▶ **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 now, we assume the co-domain of a σ only includes atoms.

▶ **Definition 3.** We call a pair of two closures that represent that same de Bruijn number a *closure-equation*. Δ is a partial finite function from variables to closure-equations, where the variable appear in the term position of one side of the equation. We write Δ as $\{(C_1\,C_1'), ..., (C_i\,C_i')\}$ and we write $\{(C\,C')\} \cup \Delta$ for extending Δ with $(C\,C')$. $\Delta(X)$ yields the list of pairs of closures, that X is on one side of.

The simplified problem is about solving three kinds of closure-equations: name-name, name-var, and var-var. Given p^*, a list of name-name and name-var problems and Δ, the var-var problems, we first run the ν-machine, defined in figure 5, on $p*$ to generate a substitution. Then the δ-machine computes the final unifier on three inputs: the substitution from ν, the var-var problems, Δ, and a queue of known variables, which is initialized by the domain of the substitution. We write a transition as $acc[arg]_l \Rightarrow acc'$, where arg is the input, which the machine runs structural recursion on; l is the label of the machine; acc is the input that serves as an accumulator; and acc' is the result. If no transitions apply, the machine fails and the unification problem has no unifier.

▶ **Lemma 4.** *For all finite p^* and Δ, 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

■ **Figure 5** ν-machine

EMPTY $\quad\quad \sigma_0[\emptyset]_\nu \Rightarrow \sigma_0$

NAME-NAME $\quad \sigma_0[((\langle a_1; \Phi_1\rangle\,\langle a_2; \Phi_2\rangle),\ P^*)]_\nu \Rightarrow \sigma_1$
$\quad\quad\quad\quad\quad$ where $\sigma_0[P^*]_\nu \Rightarrow \sigma_1$
$\quad\quad\quad\quad\quad\quad \langle a_1; \Phi_1\rangle \approx \langle a_2; \Phi_2\rangle$

NAME-META $\quad \sigma_0[((\langle a_1; \Phi_1\rangle\,\langle X_2; \Phi_2\rangle),\ P^*)]_\nu \Rightarrow \sigma_1$
$\quad\quad\quad\quad\quad$ where $\sigma_0'[P^*]_\nu \Rightarrow \sigma_1$
$\quad\quad\quad\quad\quad\quad \sigma_0' = \{X_2/a_2\} \cup \sigma_0$
$\quad\quad\quad\quad\quad\quad \langle a_1; \Phi_1\rangle \approx \langle a_2; \Phi_2\rangle$

■ **Figure 6** δ-machine and pull

EMPTY-Q $\quad (\sigma_0, \Delta_0)[\emptyset]_\delta \Rightarrow (\sigma_0, \Delta_0)$

EMPTY-D $\quad (\sigma_0, \emptyset)[q]_\delta \Rightarrow (\sigma_0, \emptyset)$

STEP $\quad\quad (\sigma_0, \Delta_0)[(X, q)]_\delta \Rightarrow (\sigma_1, \Delta_1)$
$\quad\quad\quad\quad$ where $(\sigma_0', \Delta_0')[q']_\delta \Rightarrow (\sigma_1, \Delta_1)$
$\quad\quad\quad\quad\quad (\sigma_0, q)[\Delta_0(X)]_{\text{pull}} \Rightarrow (\sigma_0', q')$
$\quad\quad\quad\quad\quad \Delta_0' = \Delta_0 \setminus \Delta_0(X)$

EMPTY $\quad\quad (\sigma_0, q_0)[\emptyset]_{\text{pull}} \Rightarrow (\sigma_0, q_0)$

NAME-NAME $\quad (\sigma_0, q_0)[((\langle X_1; \Phi_1\rangle\,\langle X_2; \Phi_2\rangle),\ P^*)]_{\text{pull}} \Rightarrow (\sigma_1, q_1)$
$\quad\quad\quad\quad\quad (\sigma_0, q_0)[P^*]_{\text{pull}} \Rightarrow (\sigma_1, q_1)$
$\quad\quad\quad\quad\quad \sigma_0(X_1) = a_1$
$\quad\quad\quad\quad\quad \sigma_0(X_2) = a_2$
$\quad\quad\quad\quad\quad \langle a_1; \Phi_1\rangle \approx \langle a_2; \Phi_2\rangle$

NAME-META $\quad (\sigma_0, q_0)[((\langle X_1; \Phi_1\rangle\,\langle X_2; \Phi_2\rangle),\ P^*)]_{\text{pull}} \Rightarrow (\sigma_1, q_1)$
$\quad\quad\quad\quad\quad (\sigma_0', q_0')[P^*]_{\text{pull}} \Rightarrow (\sigma_1, q_1)$
$\quad\quad\quad\quad\quad \sigma_0' = \{X_2/a_2\} \cup \sigma_0$
$\quad\quad\quad\quad\quad q_0' = (X_2, q_0)$
$\quad\quad\quad\quad\quad \sigma_0(X_1) = a_1$
$\quad\quad\quad\quad\quad X_2 \notin dom(\sigma_0)$
$\quad\quad\quad\quad\quad \langle a_1; \Phi_1\rangle \approx \langle a_2; \Phi_2\rangle$

instantiated by any term besides atoms, can we re-shape the two terms to create a proper input to ν and δ?

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 an arbitrary nominal unification problem to a p^*, a Δ, and a substitution.

4 A note on time complexity

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 two immutable hashtables [5] and a counter. One hashtable maps from names to numbers, the other maps from numbers to names, and the counter is used to track the de Bruijn number. When we extend a scope with a name, we extend the two hashtables with the corresponding maps and add one to the counter. Thus, `ext-scope`, `idx→atom`, and `atom→idx` are amortized constant time. Because there is no need to compose two scopes, we may use hashtables to have constant time name management. In addition, using immutable structures avoids copying the entire datastructure when branching, in particular, the APP-APP rule of the ρ-machine.

Given this optimization, the ν-machine and the δ-machine are both linear w.r.t the size of the problems. The ρ-machine, as shown by Martelli and Montanari, is $O(n \times G(n))$, when representing sets with UNION-FIND [33], where n is the number of variable occurrences in the original terms.

Figure 7 ρ-machine

EMPTY	$(p_0, \Delta_0, \sigma_0)[\emptyset]_\rho \Rightarrow (p_0, \Delta_0, \sigma_0)$
STEP	$(p_0, \Delta_0, \sigma_0)[(U, U^*)]_\rho \Rightarrow (p_1, \Delta_1, \sigma_1)$
	where $(p_0', \Delta_0', \sigma_0')[U*]_\rho \Rightarrow (p_1, \Delta_1, \sigma_1)$
	$\quad (p_0, \Delta_0, \sigma_0)[U]_s \Rightarrow (p_0', \Delta_0', \sigma_0')$
NAME-NAME	$(p_0, \Delta_0, \sigma_0)[(\langle a_1; \Phi_1 \rangle \langle a_2; \Phi_2 \rangle)]_s \Rightarrow (p_0', \Delta_0, \sigma_0)$
	where $p_0' = (\langle a_1; \Phi_1 \rangle \langle a_2; \Phi_2 \rangle) \cup p_0$
NAME-META	$(p_0, \Delta_0, \sigma_0)[(\langle a_1; \Phi_1 \rangle \langle X_2; \Phi_2 \rangle)]_s \Rightarrow (p_0', \Delta_0, \sigma_0)$
	where $p_0' = (\langle a_1; \Phi_1 \rangle \langle X_2; \Phi_2 \rangle) \cup p_0$
META-META	$(p_0, \Delta_0, \sigma_0)[(\langle X_1; \Phi_1 \rangle \langle X_2; \Phi_2 \rangle)]_s \Rightarrow (p_0, \Delta_0', \sigma_0)$
	where $p_0' = (\langle X_1; \Phi_1 \rangle \langle X_2; \Phi_2 \rangle) \cup p_0$
APP-APP	$(p_0, \Delta_0, \sigma_0)[(\langle (l_1\ r_1); \Phi_1 \rangle \langle (l_2\ r_2); \Phi_2 \rangle)]_s \Rightarrow (p_1, \Delta_1, \sigma_1)$
	where $(p_0, \Delta_0, \sigma_0)[(\langle l_1; \Phi_1 \rangle \langle l_2; \Phi_2 \rangle)]_s \Rightarrow (p_0', \Delta_0', \sigma_0')$
	$\quad (p_0', \Delta_0', \sigma_0')[(\langle r_1; \Phi_1 \rangle \langle r_2; \Phi_2 \rangle)]_s \Rightarrow (p_1, \Delta_1, \sigma_1)$
ABS-ABS	$(p_0, \Delta_0, \sigma_0)[(\langle \lambda\, a_1.t_1; \Phi_1 \rangle \langle \lambda\, a_2.t_2; \Phi_2 \rangle)]_s \Rightarrow (p_1, \Delta_1, \sigma_1)$
	where $(p_0, \Delta_0, \sigma_0)[(\langle t_1; \Phi_1' \rangle \langle t_2; \Phi_2' \rangle)]_s \Rightarrow (p_1, \Delta_1, \sigma_1)$
	$\quad \Phi_1' = (\text{ext-scope}\ \Phi_1\ a_1)$
	$\quad \Phi_2' = (\text{ext-scope}\ \Phi_2\ a_2)$
META-APP	$(p_0, \Delta_0, \sigma_0)[(\langle X_1; \Phi_1 \rangle \langle (l_2\ r_2); \Phi_2 \rangle)]_s \Rightarrow (p_1, \Delta_1, \sigma_1)$
	where $(p_0, \Delta_0, \sigma_0')[(\langle X_l; \Phi_1 \rangle \langle l_2; \Phi_2 \rangle)]_s \Rightarrow (p_0', \Delta_0', \sigma_0'')$
	$\quad (p_0', \Delta_0', \sigma_0'')[(\langle X_r; \Phi_1 \rangle \langle r_2; \Phi_2 \rangle)]_s \Rightarrow (p_1, \Delta_1, \sigma_1)$
	$\quad \sigma_0' = \{X_1/(X_l\ X_r)\} \cup \sigma_0$
META-ABS	$(p_0, \Delta_0, \sigma_0)[(\langle X_1; \Phi_1 \rangle \langle \lambda\, a_2.t_2; \Phi_2 \rangle)]_s \Rightarrow (p_1, \Delta_1, \sigma_1)$
	where $(p_0, \Delta_0, \sigma_0')[(\langle X_t; \Phi_1' \rangle \langle t_2; \Phi_2' \rangle)]_s \Rightarrow (p_1, \Delta_1, \sigma_1)$
	$\quad \Phi_1' = (\text{ext-scope}\ \Phi_1\ a_1)$
	$\quad \Phi_2' = (\text{ext-scope}\ \Phi_2\ a_2)$
	$\quad \sigma_0' = \{X_1/\lambda\, a_1.X_t\} \cup \sigma_0$

───── **References** ─────

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