# 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  $\alpha$ -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**  $\alpha$ -conversion; Binding operations; Efficiency; Unification

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# 1 Introduction and background

The rules that identify terms, such as  $\alpha$ ,  $\beta$ , and  $\eta$  in the  $\lambda$ -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  $\alpha$ -rule, has inspired extensions of logic programming languages, like  $\alpha$ Prolog [Chenev and Urban, 2004] and  $\alpha$ Kanren [Byrd and Friedman, 2007], as well as theorem provers, like nominal Isabelle [Urban and Tasson, 2005] and  $\alpha$ LeanTAP [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

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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 (atom) 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  $\alpha$ -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. De Bruijn numbers enable 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  $\alpha$ -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 the convenience when implementing  $\alpha$ -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  $\alpha$ -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  $\alpha$ -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  $\Phi$ , where the scope is an ordered list of names for the binders in the enclosing context.

When the term of a closure is a name, the closure itself represents a de Bruijn number. For example, consider the term  $\lambda x.\lambda y.x$ . The de Bruijn number of the name x is 1 and the closure-representation of this number is  $\langle x; (yx) \rangle$ . We can retrieve the number-representation by finding the position of the first appearance of the name in the scope. In this case, the position of x in the scope (yx) 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, which extends the scope by adding a name to the front of the scope; idx—name, which returns the name of a given index starting from the front of the scope; and name—idx, which returns the location of the first appearance of a given name counting from the front of the scope. As we are building the scope in reversed order, if repeated names appear, the first appearance in a scope shadows the others.

#### Figure 1 Terms

$$t, l, r$$
 ::=  $a$  name  
 $\begin{vmatrix} \lambda a.t \\ l \end{vmatrix}$  abstractions

Figure 2 Free and bound

$$\frac{a \notin \Phi}{\Phi \vdash \operatorname{Fr} a} \operatorname{FREE}$$

$$\begin{split} &(\mathtt{name} \!\!\to\! \mathtt{idx}\, \Phi\, a) = i \\ &(\underbrace{\mathtt{idx} \!\!\to\! \mathtt{name}\, \Phi\, i) = a}_{\Phi\;\vdash\; \mathtt{Bd}\;\; a\;\; i} \;\; \mathtt{Bound} \end{split}$$

Figure 3 ≈-rules

$$\begin{array}{l} a_1 = a_2 \\ \underline{\Phi_1 \vdash \mathtt{Fr} \ a_1 \quad \Phi_2 \vdash \mathtt{Fr} \ a_2} \\ \overline{\langle a_1; \Phi_1 \rangle} \approx \langle a_2; \Phi_2 \rangle \end{array} \ \mathrm{SAME-FREE} \end{array}$$

$$\begin{aligned} i_1 &= i_2 \\ \frac{\Phi_1 \vdash \text{Bd } a_1 \ i_1 \quad \Phi_2 \vdash \text{Bd } a_2 \ i_2}{\langle a_1; \Phi_1 \rangle \approx \langle a_2; \Phi_2 \rangle} \ \text{Same-Bound} \end{aligned}$$

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 a name, a, does not appear in the scope,  $\Phi$ , we say, "a is free with respect to  $\Phi$ ," written as  $\Phi \vdash \operatorname{Fr} a$ ; when a's first appearance in  $\Phi$  is the position i, we say, "a is bound at i with respect to  $\Phi$ ," written as  $\Phi \vdash \operatorname{Bd} a i$ . The BOUND rule has two premises to be algorithmic in both directions, that is, given a name we can find its index and given an index we can find its name, if no shadowings occur. Figure 3 defines the rules to decide whether two names are  $\alpha$ -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 a name, that is, finding the unifier of two terms that share the same structure but differ in names and variables. A unifier consists of two parts:  $\sigma$  and  $\delta$ .

- ▶ **Definition 2.** A substitution  $\sigma$  is a partial finite function from variables,  $X_i$ , to terms,  $t_i$ . For readability, we write  $\sigma$  as a set,  $\{X_1/t_1,...,X_j/t_j\}$  and we write  $\{X/t\} \cup \sigma$  for extending  $\sigma$  with X/t. For the simplified problems, we restrict t to a name.
- ▶ **Definition 3.** A closure equation is a pair of two closures that are  $\alpha$ -equivalent.  $\Delta$  is a set of closure-equations. We write  $\Delta$  as  $\{(\langle t_1; \Phi_1 \rangle \langle t_1'; \Phi_1' \rangle), ..., (\langle t_i; \Phi_1 \rangle \langle t_i'; \Phi_1' \rangle)\}$

Figure 4 Unification terms and problems

and we write  $\{(\langle t; \Phi \rangle \langle t'; \Phi' \rangle)\} \cup \Delta$  for extending  $\Delta$  with  $(\langle t; \Phi \rangle \langle t'; \Phi' \rangle)$ . We write  $\delta$  as a special form of  $\Delta$ : for each equation in  $\delta$ , 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: namename, name-var, and var-var. As defined in Figure 4, we refer to a name-name or name-var equation as an  $e_{\nu}$  and refer to a var-var equation as an  $e_{\delta}$ . Given two lists,  $p_{\nu}$  and  $p_{\delta}$ , of these equations, we first run the  $\nu$ -machine, defined in Figure 5, on  $p_{\nu}$ to generate a substitution. The  $\delta$ -machine, defined in Figure 6, then computes the final unifier on three inputs: the substitution resulted from the  $\nu$ -machine,  $\delta$ , 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 $\nu$ -machine

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

$$\frac{\sigma_0 \vdash \epsilon \Rightarrow_{\nu} \sigma_0}{\sigma_0 \vdash p \Rightarrow_{\nu} \sigma_1} \xrightarrow{\sigma_1} \frac{\langle a_1; \Phi_1 \rangle \approx \langle a_2; \Phi_2 \rangle}{\sigma_0 \vdash \langle a_1; \Phi_1 \rangle = \langle a_2; \Phi_2 \rangle, p \Rightarrow_{\nu} \sigma_1} \xrightarrow{\text{NAME-NAME}}$$

$$\begin{split} & \frac{\langle a_1; \Phi_1 \rangle \approx \langle a_2; \Phi_2 \rangle}{\{X_2/a_2\} \cup \sigma_0 \vdash p \Rightarrow_{\nu} \sigma_1} \\ & \frac{\{X_2/a_2\} \cup \sigma_0 \vdash p \Rightarrow_{\nu} \sigma_1}{\sigma_0 \vdash \langle a_1; \Phi_1 \rangle = \langle a_2; \Phi_2 \rangle, \, p \Rightarrow_{\nu} \sigma_1} \end{split} \text{ NAME-VAR}$$

▶ **Lemma 4.** For all finite input, the  $\nu$ -machine and the  $\delta$ -machine terminate; for all input, the  $\nu$ -machine and the  $\delta$ -machine succeed 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 names, can we re-shape the two terms to create a proper input to the two machines?

### **Figure 6** $\delta$ -machine and the pull operation

$$\sigma; p_{\delta} \vdash xs \Rightarrow_{\delta} \sigma; p_{\delta} 
\sigma; xs \vdash p_{\delta} \Rightarrow_{\text{pull}} \sigma; xs$$

$$EMPTY-XS$$

$$\overline{\sigma; \delta \vdash \epsilon \Rightarrow_{\delta} \sigma; \epsilon} \quad \text{EMPTY-D}$$

$$\sigma_{0}; xs_{0} \vdash \delta_{0}(X) \Rightarrow_{\text{pull}} \sigma'_{0}; xs_{1} 
\sigma'_{0}; \delta_{0} \setminus \delta_{0}(X) \vdash xs_{1} \Rightarrow_{\delta} \sigma_{1}; \delta_{1} 
\overline{\sigma_{0}}; \delta_{0} \vdash X, xs_{0} \Rightarrow_{\delta} \sigma_{1}; \delta_{1}$$
Pull
$$\overline{\sigma; xs \vdash \emptyset \Rightarrow_{\text{pull}} \sigma; xs} \quad \text{EMPTY}$$

$$\langle a_{1}; \Phi_{1} \rangle \approx \langle a_{2}; \Phi_{2} \rangle 
\sigma_{0}(Y_{1}) = a_{1} \quad \sigma_{0}(Y_{2}) = a_{2} 
\sigma_{0}; xs_{0} \vdash p \Rightarrow_{\text{pull}} \sigma_{1}; xs_{1}$$

$$\overline{\sigma_{0}}; xs_{0} \vdash \langle Y_{1}; \Phi_{1} \rangle = \langle Y_{2}; \Phi_{2} \rangle, p \Rightarrow_{\text{pull}} \sigma_{1}; xs_{1}$$
NAME-NAME
$$\langle a_{1}; \Phi_{1} \rangle \approx \langle a_{2}; \Phi_{2} \rangle 
\sigma_{0}(Y_{1}) = a_{1} \quad Y_{2} \notin dom(\sigma_{0})$$

$$\frac{\{Y_{2}/a_{2}\} \cup \sigma_{0}; (Y_{2}, xs_{0}) \vdash p \Rightarrow_{\text{pull}} \sigma_{1}; xs_{1}}{\sigma_{0}; xs_{0} \vdash \langle Y_{1}; \Phi_{1} \rangle = \langle Y_{2}; \Phi_{2} \rangle, p \Rightarrow_{\text{pull}} \sigma_{1}; xs_{1}}$$
NAME-VAR

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Here we use the idea of Martelli-Montanari, in particular, finding the shared shape of two terms by computing the common parts and frontiers over a multi-equation. Martelli and Montanari [1982] define the common part of two terms to be a term obtained by superimposing, and the frontier as the substitution that captures the differences between each term and the common part. For example, given distinct names a, b, and c, distinct vars c and c, and two terms c and c and c and c and the frontier is the substitution c and c and the frontier is the substitution c and c are on the left-hand side, and the non-variable-closures are on the right-hand side.

The  $\rho$ -machine, defined in Figure 7, reduces an arbitrary nominal unification problem to  $p_{\nu}$ ,  $p_{\delta}$ , and a substitution where the co-domain is unrestricted. Unlike the Martelli-Montanari algorithm, the  $\rho$ -machine finds the maximum common part instead of the minimum. Thus, in the VAR-APP and VAR-ABS rules, we need to create new names and new variables to extend the shape of a variable with its counterpart.

#### **Figure 7** $\rho$ -machine

$$(p_{\nu}, p_{\delta}, \sigma) \vdash multieqn^* \Rightarrow_{\rho} (p_{\nu}, p_{\delta}, \sigma) \\ (p_{\nu}, p_{\delta}, \sigma) \vdash multieqn \Rightarrow_{\text{step}} (p_{\nu}, p_{\delta}, \sigma)$$

$$\overline{(p_{0}, \delta_{0}, \sigma_{0}) \vdash \emptyset} \Rightarrow_{\rho} (p_{0}, \delta_{0}, \sigma_{0}) \quad \text{EMPTY}$$

$$(p_{0}, \delta_{0}, \sigma_{0}) \vdash \emptyset \Rightarrow_{\rho} (p_{0}, \delta_{0}, \sigma_{0}) \quad \text{EMPTY}$$

$$(p_{0}, \delta_{0}, \sigma_{0}) \vdash U \Rightarrow_{\text{step}} (p'_{0}, \delta'_{0}, \sigma'_{0}) \quad \underline{(p'_{0}, \delta'_{0}, \sigma'_{0}) \vdash (U, U^{*})} \Rightarrow_{\rho} (p_{1}, \delta_{1}, \sigma_{1}) \quad \text{STEP}$$

$$p_{1} = (\langle a_{1}; \Phi_{1} \rangle \langle a_{2}; \Phi_{2} \rangle) \cup p_{0} \quad \text{NAME-NAME}$$

$$p_{1} = (\langle a_{1}; \Phi_{1} \rangle \langle X_{2}; \Phi_{2} \rangle) \cup p_{0} \quad \text{NAME-VAR}$$

$$\frac{p_{1} = (\langle a_{1}; \Phi_{1} \rangle \langle X_{2}; \Phi_{2} \rangle) \cup p_{0}}{(p_{0}, \delta_{0}, \sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle X_{2}; \Phi_{2} \rangle) \cup p_{0}} \quad \text{NAME-VAR}$$

$$\frac{\delta_{1} = (\langle X_{1}; \Phi_{1} \rangle \langle X_{2}; \Phi_{2} \rangle) \cup \delta_{0}}{(p_{0}, \delta_{0}, \sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle X_{2}; \Phi_{2} \rangle) \cup \delta_{0}} \quad \text{VAR-VAR}$$

$$\frac{\delta_{1} = (\langle X_{1}; \Phi_{1} \rangle \langle X_{2}; \Phi_{2} \rangle) \cup \delta_{0}}{(p_{0}, \delta_{0}, \sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle X_{2}; \Phi_{2} \rangle) \cup \delta_{0}} \quad \text{VAR-VAR}$$

$$\frac{(p_{0}, \delta_{0}, \sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle X_{2}; \Phi_{2} \rangle) \cup \delta_{0}}{(p_{0}, \delta_{0}, \sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle X_{2}; \Phi_{2} \rangle) \cup \delta_{0}} \quad \text{VAR-VAR}$$

$$\frac{(p_{0}, \delta_{0}, \sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle A_{2}; \Phi_{2} \rangle) \cup \delta_{0}}{(p_{0}, \delta_{0}, \sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle A_{2}; \Phi_{2} \rangle) \cup \delta_{0}} \quad \text{APP-APP}$$

$$\frac{(p_{0}, \delta_{0}, \sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle a_{2}; \Phi_{2} \rangle) \cup \delta_{0}}{(p_{0}, \delta_{0}, \sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle a_{2}; \Phi_{2} \rangle) \cup \delta_{0}} \quad \text{ABS-ABS}}$$

$$\frac{(p_{0}, \delta_{0}, sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle a_{2}; \Phi_{2} \rangle) \cup \delta_{0}}{(p_{0}, \delta_{0}, \sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle a_{2}; \Phi_{2} \rangle) \cup \delta_{0}} \quad \text{ABS-ABS}}$$

$$\frac{(p_{0}, \delta_{0}, \delta_{0}; \Phi_{1}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle a_{2}; \Phi_{2} \rangle) \cup \delta_{0}}{(p_{0}, \delta_{0}, \sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle a_{2}; \Phi_{2} \rangle) \cup \delta_{0}} \quad \text{ABS-ABS}}$$

$$\frac{(p_{0}, \delta_{0}, \delta_{0}; \Phi_{1}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle a_{2}; \Phi_{2} \rangle) \cup \delta_{0}}{(p_{0}, \delta_{0}, \sigma_{0}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle a_{2}; \Phi_{2} \rangle) \cup \delta_{0}} \quad \text{ABS-ABS}}$$

$$\frac{(p_{0}, \delta_{0}, \delta_{0}; \Phi_{1}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle a_{2}; \Phi_{2} \rangle) \cup \delta_{0}}{(p_{0}, \delta_{0}; \Phi_{1}) \vdash (\langle a_{1}; \Phi_{1} \rangle \langle a_{2}; \Phi_{2} \rangle$$

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# 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 a counter and two persistent hashtables, also known as HAMT [Bagwell, 2001]. 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. A persistent hashtable, in practice, has constant time for update and lookup, although the worst case scenario could be O(log(n)). Thus, ext,  $idx\rightarrow name$ , and  $name\rightarrow idx$  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  $\rho$ -machine.

We implement  $\delta$  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  $\nu$ -machine and the  $\delta$ -machine are both worst case  $O(n \times log(n))$ , where n is the sum of name 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  $\rho$ -machine is similar except that two new factors are involved: the update operation of HAMT and the generation of names and variables. We consider the former one to have O(log(n)) complexity, and we implement name and variable creation with state monads in constant time. Thus reducing an arbitrary unification problem to the input of the  $\nu$  and  $\delta$  machines becomes  $O(n \times log(n) \times G(n))$ .

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