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Unification for Quantified Formulae

by

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Abstract. Unification for a first order language is a method that attempts to make terms of the language ~ via appropriate substitutions - syntactically identical. The method can be applied directly to quantifier-free formulae and, in this paper, will be extended in a natural and straightforward way to quanfifiedfornudae. The main issue is the treatment of bound variables. Our method is based on a canonical renaming of the bound variables occurring in the input formulae, so that every binding is associated in a special way with a distinct variable. Then, unification works as usual by treating logical connectives like functors and bound variables like constants. Our work is meant to help limit the search of theorem proving algorithms, in particular of those that search directly for natural deduction proofs.

0. Introduction. Modern automated theorem proving started with work in the late fifties and early sixties that is broadly represented in the volume Automation of Reasoning [SW83]. However, the underlying logical techniques went frequently back to pioneering work in the late twenties and early thirties. That work, in particular Herbrand's and Gentzen's, was motivated by foundational concerns connected with Hilbert's Program. Such concerns were replaced by one crucial problem related to the efficient use of Herbrand's fundamental theorem, namely the choice of terms for the instantiation of quantifiers and the identification of contradictory pairs of literals. Herbrand [H71, p. 148] introduced *unification* already for that very purpose, and Robinson [R65] incorporated unification via his *resolution rule* directly into a machine-oriented deductive system. The central question of the unification problem for a first order language L is this: Given terms t and t' of L, is there a substitution or term-assignment c such that sub(a,t) and sub(a,t^t) are syntactically identical? (Here A,x.sub(a,x) is the unique extension of a to all terms.) A substitution that allows such an identification is called a *unifier* for t and t\ Robinson presented a particular unification algorithm and established that, if the algorithm yields a unifier at all, then it is a *most general unifier* (or mgu).

Unification is not only crucial for resolution, but in fact for any refutation method — whether based on the *sequent calculus, semantic tableaux,* or *mating,* to name just some possibilities (compare [GMW79], [F90], [A81].) We use unification for automated proof search, i.e. in algorithms that search directly for natural deduction proofs in classical first order logic (see [SS89], [SS92], [K93]). The basic tenet is that *searching* for a proof of a *proposition* from given *assumptions* should not necessarily resort to the atomic level. Thus, we have to solve the unification problem simultaneously for terms and quantified formulae, or for *q-terms;* if we denote by "quantified terms" the general category of syntactic expressions including terms as well as formulae. As the main technical device for our solution we introduce the three place *C-substitution operation* subc and formulate the generalized problem for q-terms e and e¹ as follows:

• Is there a substitution a such that subc(a,id,e) = subc(o,id,e')?

That means, informally, does σ make e and e' identical modulo renaming of bound variables? -- The spirit of our solution (though developed independently) is in line with Snyder's general strategy in [S91, p. 4]: by examining what it should mean for two expressions to be "the same" after a unifying substitution, the appropriate extensions or modifications of the (Herbrand-style) unification method suggest themselves naturally. Our solution is clearly not tied to the particular motivation from automated proof search, but can be used in theorem proving algorithms based on refutation methods or, for that matter, in quite different contexts, where unification is a useful tool; see [KK89]. Finally, the simplicity of our approach should be compared to the complexity of the proposal made by Staples and Robinson in [SR88] and [SR90].

1. C-substitution. The *first order* languages L we use consist of the following symbols: universal and existential quantifiers: \forall , respectively \exists ; variables x_n , $n \in N$; sentential connectives including \neg , \land , \lor , \rightarrow ; for each $n \in N$, countably many n-place relation symbols and n-ary function symbols. Terms t, t', ... and formulae A, A', ... are inductively defined as usual, but taken to be in prefix notation; *q-terms* e, e', ... are either terms or formulae. It can be shown that q-terms have a unique presentation $ue_1 \dots e_n$, where u is a variable (with n=0), a logical connective, a relation or function symbol of the appropriate (number of) arguments. Thus, we can give recursive definitions and inductive arguments for q-terms considering three cases: e is a variable, e is of the form $@e_1 \dots e_n$ (where @ is a sentential connective, a relation or function symbol), or e is of the form Qx_ne' (where Q is either the universal or existential quantifier). The following expressions are examples of qterms: the atomic formula Pt₁ ... t_n, the conditional $\rightarrow \land AA' \lor AA'$, and the quantified statement Qx_nA. The set of free variables of a q-term e is denoted by FV(e).

A term-assignment σ is a function from the set V of all variables to the set of terms, such that the set of variables x_n for which $\sigma(x_n) \neq x_n$ is finite; this finite subset of V is called the support of σ , briefly sup(σ). The term-assignment with empty support is obviously the *identity function* id on V. The set of variables FV(σ) of a term-assignment σ is the set of variables occurring in the terms $\sigma(x_n)$ for $x_n \in \sup(\sigma)$. A term-assignment for variables can be uniquely extended to a substitution operation on all terms. We will use σ to indicate a term-assignment or its uniquely associated extension; indeed, following common usage, we will call term-assignments also substitutions. Given substitutions σ and η , their composition $\sigma\eta$ is defined by $\sigma\eta(x_n)=\sigma(\eta(x_n))$ for all variables x_n . A substitution σ is called *idempotent* iff $\sigma\sigma = \sigma$. To extend substitutions not only to terms, but to q-terms, we use modified termassignments $\sigma^{t_{x_n}}$; the latter have value $\sigma(x_m)$ for variables different from x_n , and they have value t for x_n . The *replacement operation* rep(σ ,e) is defined by:

- 1. rep $(\sigma, \mathbf{x}_n) = \sigma(\mathbf{x}_n);$
- 2. rep $(\sigma,@e_1 \dots e_n) = @rep(\sigma,e_1) \dots rep(\sigma,e_n);$
- 3. rep $(\sigma, Qx_n e) = Qx_n \operatorname{rep}(\sigma_{x_n}^{x_n}, e)$.

This operation replaces all free occurrences of a variable in a q-term e by its σ -value, but leaves bound occurrences untouched. From a logical point of view, however, rep is an incorrect "substitution operation" for q-terms e involving quantifiers: it allows the replacement of free variables in the scope of a quantifier by terms that contain the quantified variable. We have two well-known choices: either we require terms $\sigma(x_n)$ to be free for x_n in e, or we rename bound variables in such a way that this requirement is always satisfied. We take the second alternative and define the *substitution operation* sub(σ ,e) with *minimal and canonical renaming* of bound variables. Let $\sigma|_e$ be " σ restricted to e" so that $\sigma|_e(x_n) = \sigma(x_n)$, if $x_n \in FV(e)$, and $\sigma|_e(x_n)=x_n$ otherwise. sub(σ ,e) is defined as follows:

1. $sub(\sigma, x_n) = \sigma(x_n);$

2.
$$\operatorname{sub}(\sigma, @e_1 \dots e_n) = (\operatorname{sub}(\sigma, e_1) \dots \operatorname{sub}(\sigma, e_n);$$

3.
$$\operatorname{sub}(\sigma, Qx_n e) = \begin{cases} Qx_n \operatorname{sub}(\sigma^{x_n}_{x_n}, e) & \text{if } x_n \notin FV(\sigma|_e) \text{ or } x_n \notin FV(e) \\ Qx_m \operatorname{sub}(\sigma^{x_m}_{x_n}, e) & \text{otherwise} \end{cases}$$

where x_m is the first variable that does not belong to $FV(\sigma|e) \cup FV(e)$.

Considering id for σ we have the operation sub(id,e) that renames the bound variables of e. Finally, the *C*-substitution operation sub_C(σ,τ,e) performs a substitution and generates a canonical renaming relative to a context given by a set C of variables.

1. $\operatorname{sub}_{\mathbb{C}}(\sigma,\tau,x_n) = \begin{cases} \tau(x_n) & \text{if } x_n \in \operatorname{sup}(\tau) \\ \\ \sigma(x_n) & \text{otherwise} \end{cases}$

2. $\operatorname{sub}_{C}(\sigma,\tau,@e_1 \dots e_n) = (@\operatorname{sub}_{C}(\sigma,\tau,e_1) \dots \operatorname{sub}_{C}(\sigma,\tau,e_n))$

3. $sub_C(\sigma,\tau,Qx_ne) = Qx_msub_C(\sigma,\tau^{x_m}x_n,e)$, where x_m is the first variable whose subscript is greater than the subscripts of all variables in $C \cup FV(e) \cup FV(\sigma) \cup FV(\tau)$. subc(id,id,e) yields a canonical renaming of bound variables in e relative to the context C. That this renaming has the desired logical effect is shown by the next lemma.

Lemma 1.1. Let e be a q-term and a, x substitutions, and assume that C is a finite set of variables such that (i) sup(a)uFV(e)uFV(a) is included in C and (ii) the subscripts of variables in FV(x) are all greater than those of elements in C; then we have:

subc(a,x,e)=rep(a,subc(id,x,e)).

Proof. The proof proceeds by induction on q-terms e; the case that e is a variable follows directly from the definitions, the case that e is of the form @ei ... e_n from induction hypothesis. The case that $e=Qx_nei$ is the critical one; here we have by definition

 $(l)subc(a,x,Qx_nei)=Qx_msubc(a,x^{Xm}x_n,ei),$

where x_m is the first variable with subscript greater than the subscripts of variables in CuFV(x); by induction hypothesis we have:

(2) $Qx_msubc(a, x^{Xm}x_n, ei) = Qx_mrep(a, sub_c(id, x^{Xm}x_n, ei)).$

As x_m is not in sup(a), $c=a^{Xm}x_m$ and thus by definition of rep:

$$(3)Qx_mrep(a,sub_c(id,x^{Xm}x_n,ei))=rep(a,Qx_msub_c(id,x^{Xm}x_{11},ei)).$$

By choice of m and definition of subc:

$$(4)rep(a,Qx_msub_c(id,x^{Xm}x_n,ei)) = rep(a,subc(id,x,Qx_nei)).$$

The claim follows from (l)-(4). Q.E.D.

The lemma insures that subc behaves on a q-term e as replacement does on the canonically renamed q-terms e*=subc(id,id,e), because subc(o,id,e)=rep(a,e*). — The operation subc will be used for the unification of q-terms e and e¹, where the context C is provided by the set $FV(e)uFV(e^{f})$. Indeed, we call e and e^f *unifiable* if and only if there is a term-assignment o with subc(a,id,e)=subc(a,id,e') and C=FV(e)uFV(e'); the substitution a is called a unifier for e and e¹.¹ In section 3 we present a unification algorithm for q-terms, whose output determines a unifier a for e and e¹ if a is more general than any other unifier TI for those q-terms; i.e., for some substitution x, we have $r \models To$. But first we should convince ourselves that subc(a,x,e) is an operation providing an appropriate identity criterion for the ''unifiability of q-terms'' by considering a few (typical) examples.

¹ The role of the second argument is similar to that of the "binding states" in [SR88] and [SR90]: the substitution x keeps track of information on bound variables.

To re-emphasize, we want to find a unification algorithm mainly for automated proof search and use unification extensively, in order to be able to fill the gap between goal and premises without necessarily resorting to the atomic level. Let us make this point clearer with an example. Suppose we want to derive the goal $G=\vee\forall x_nPx_nfgx_mguRx_nx_m$ (where the free variables in G are taken to be existentially quantified) from a set of propositions S containing $A=\vee\forall x_nPx_nfx_jgx_mRgux_m$ (where the free variables of A are taken to be universally quantified). We would like to recognize the provability of G from S *in one step* without decomposing G and A, since a substitution σ exists, namely { $\langle x_j, gx_m \rangle$, $\langle x_m, u \rangle$, $\langle x_n, gu \rangle$ }, such that sub_C(σ ,id,G)=sub_C(σ ,id,A). Notice, that the values of λx .sub_C(σ ,id,x) for A and G are syntactically identical expressions; i.e., we consider formulae to be unifiable, if the application of sub_C for a suitable term-assignment yields syntactic identities! That corresponds perfectly to the ordinary understanding of bound variables as refelected graphically in Bourbaki's way of indicating bindings. Based on this understanding, the following examples show when a unification algorithm for q-terms should succeed and when, instead, it should fail:

- 1. Qx_nPx_n and Qx_mPx_m should unify.
- 2. Qx_nPx_n and Qx_mPa should not unify.
- 3. Qx_nPx_m and Qx_mPx_n should unify, but not with Qx_kPx_k .
- 4. $Qx_nQx_nPx_nx_n$ and $Qx_nQx_mPx_nx_m$ should not unify.
- 5. $Qx_nQx_mPx_nx_m$ and $Qx_mQx_nPx_nx_m$ should not unify.

Note that in the last case unification should fail even though the two formulas are logically equivalent, as our approach to quantificational unification is not modulo quantification theory. It will be interesting to explore the efficiency of proof search procedures, when invoking unification algorithms with built-in logical identities (like the one in 5).

2. An equational calculus. The work in this section is preliminary to that in section 3, where we present Martelli and Montanari's unification algorithm [MM 82] extended to q-terms. In rough outline the algorithm proceeds as follows. Given e and e', it constructs sets of equations, starting from the equation between the renamed q-terms $sub_C(id,id,e)$ and $sub_C(id,id,e')$ with C=FV(e) \cup FV(e') and then transforming sets according to the rules formulated below, until it fails or until it cannot apply any transformation rule. In the latter case the output will be a system of equations that determines a unifier.

We introduce four transformations on systems of equations. Note that the distinction between bound and free variables (of the input formulae) can be made by looking at their subscripts, since the q-terms we are considering have been renamed. Bound variables are of the form x_n with $n \ge k$, where k is the successor of the largest number used as a subscript of a free variable occurring in the input q-terms; while *free* variables are of the form x_n with n < k. (As above, $e_i = e_j$ expresses that the q-terms e_i and e_j are syntactically identical, whereas $e_i = e_j$ denotes an element of a system E of equations.)

(1) Exchange.

 $\{e \approx x_n\} \cup E \implies \{x_n \approx e\} \cup E$, if e is not a variable.

(2) Equation Elimination.

 $\{\mathbf{x}_n \approx \mathbf{x}_n\} \cup \mathbf{E} \implies \mathbf{E}.$

(3) Q-Term Reductions.

 $\{ @e_1 \dots e_n \approx @e'_1 \dots e'_n \} \cup E \implies \{ e_1 \approx e'_1, \dots, e_n \approx e'_n \} \cup E;^2$

 $\{Qx_ne_1 \approx Qx_ne_2\} \cup E \implies \{e_1 \approx e_2\} \cup E.$

(4) Variable Elimination.

 $\{x_n \approx t\} \cup E \implies \{x_n \approx t\} \cup \{\langle x_n, t \rangle\} E^3$, provided n<k and x_n does not occur in t; furthermore, t must not contain any variable x_m with m $\geq k$.

We want to show that the application of these transformation rules to the singleton $E=\{sub_C(id,id,e) \approx sub_C(id,id,e')\}\$ leads to a system of equations that determines a unifier for e and e' (if e and e' are indeed unifiable). If we can find a term-assignment σ such that $rep(\sigma,sub_C(id,id,e))=rep(\sigma,sub_C(id,id,e'))$, then we are done, as by Lemma 1.1 the latter equation holds if and only if $sub_C(\sigma,id,e)=sub_C(\sigma,id,e')$, i.e., e and e' are unifiable. -- We call a set of equations E^* derived from E iff it has been obtained from E by successive applications of the rules (1) through (4). Finally, σ is called a solution for E iff $rep(\sigma,e_j)=rep(\sigma,e_k)$ for every equation $e_j\approx e_k$ in E; E and E' are equivalent iff E and E' have the same set of solutions. Now we can formulate and prove the following theorem.

Theorem 2.1. Any system E^* of equations derived from an equation E between canonically renamed q-terms is equivalent to E.

Proof (by induction on the number of rule applications). Exchange and equation elimination preserve obviously equivalence to E. Let us consider the remaining rules.

² Note that in case n=0, the set of new equations is clearly empty.

³ This indicates replacement of t for x_n throughout E.

Assume E* has been obtained from a derived set of equations E by a q-term reduction; this transformation replaces equations of the form $@e_t ... e_n \ll @e'_1 ... e'_n$ in E¹ by equations $e^e^$, ..., $e_n \ll e'_n$ and those of the form $Qx_n ei \ll Qx_n e2$ by $ei \ll e2$. But any solution a for E^f is a solution for E* and vice versa, as $rep(a,ei)=rep(a,e^{f_i})$ for all i iff $rep(a,@e! ... e_n)=iev(o,@e| ... e'_n)$, respectively $rep(a,Qx_nei)=rep(a,Qx_ne_2)$, recalling the proof of Lemma 1.1. Therefore, E* and E¹ are equivalent; but by induction hypothesis E¹ is equivalent to E, thus E* is equivalent to E.

Assume now that E* has been obtained from E'=E''u{x_n«t} by variable elimination, where x_n is a free variable (i.e., n<k) and does not occur in t; furthermore, t must not contain any variable x_m with m>k. This transformation replaces x_n by t in all equations of E'' and yields E* by joining { x_n «t} to { $<x_n,t$ »E''. Solutions for E^f are clearly also solutions for E*. So let a be a solution for E*; as E* contains the equation x_n «t, a is a solution for it and also for all equations in E'' not containing x_n , as the latter equations occur unchanged in E*. For equations u«v of E^{ff} containing x_n , E* will have corresponding equations u'«v' with { $<x_n,t>$ }(u)=u^f and { $<x_n,t>$ (v)=v^f. But then rep(a,u)=rep(a,u') and rep(a,v)=rep(a,v^f). Thus, every solution for E* is also a solution for E^f (and thus E* is, as above, equivalent to E). Q.E.D.

A system E^* of equations is in *solved form* iff the following two conditions are satisfied: (a) every equation is of the form $x_n \ll t$, where n is less than k and the subscripts j of all variables occurring in t are less than k and different from n; (b) if x_n is the left member of some equation, then it does not occur in any other equation of E^* . The equations of such an E^* obviously determine a term-assignment a by setting $a(x_n)=x_n$, if x_n does not occur on the left-hand side of any equation in E^* , and $a(x_n)=t$, if $x_n\ll t$ is in E^* . If E^* is in solved form (derived from $E=\{subc(id,id,e)\ll subc(id,id,e')\}$ for q-terms e and e^1) the a just defined is actually an idempotent mgu for the input q-terms. After all, a is a solution for E^* and, by Theorem 2.1, of E; thus a is a unifier for e and e_1 Because of condition (b) for systems of equations in solved form, a must be idempotent and, because of (a), an mgu. So we have:

Theorem 2.2. Let E^* be derived from $E=\{subc(id,id,e) \otimes subc(id,id,e^f)\}$ for arbitrary q-terms e and e^f ; if E^* is in solved form, then it determines a solution a that is an idempotent mgu for e and $e \setminus$

Having established that a derived set E* of equations in solved form determines a unifier, we formulate now an algorithm that decides the unifiability of two q-terms and provides an

idempotent mgu in case the decision is positive. Indeed, the algorithm U will transform the initial equation between the canonically renamed q-terms systematically into a system of equations in solved form, if the q-terms are unifiable; if they are not unifiable, the algorithm will end with "failure".

3. **The unification algorithm U.** The algorithm U constructs a sequence of systems of equations starting from {subc(id,id,e) « subc(id,id,e')} by applying the following operations:

1. select an equation of the form $t \ll x_n$ and apply *exchange*;

2. select an equation $x_n \ll t$,

a. if $t = x_n$, apply equation elimination;

b. if t * x_n

- i. if x_n is a bound variable, i.e., $n \ge k$, then *fail*;
- ii. if x_n or a bound variable occurs in t, then/a//;
- iii. if x_n occurs in some other equation, apply *variable elimination*;
- 3. select an equation of the form $e \ll e$
 - a. If the root symbols (function, predicate, connective or quantifier symbols⁴) or their arities are different, then/a//;
 - b. otherwise, apply term reduction;
- 4. If none of the previous operations can be applied, then stop.

An *example* will highlight the crucial features of U. Consider q-terms $e=\forall x_5Pchx_5x_3$ and e'=VxgPx5hxgX5. A canonical renaming of all bound variables leads to q-terms e*=Vx9Pchx9X3 and e'*=Vx9Px5hx9X5 and the initial set of equations{e*«e'*}. U applies *term reduction* to get {Pchx9X3~Px5hx9X5>. Both terms start with the same predicate symbol P, so U applies term reduction again to obtain {c«X5, hx9X3«hx9X5> and uses *exchange* to rewrite the first equation as xs~c. *Variable elimination with* xs«c applied to {hx9X3«hx9X5, X5«c} and subsequent term reduction for hx9X3«hx9C yields the set {X9=X9, X3«c, X5«c}. U drops the first equation from the set by *equation elimination* to obtain E*={X3=c, X5«c}. No other rule can be applied, so U will stop with the set of equations E*. Note that E* is in solved form.

⁴ We consider a quantifier symbol Q together with the first occurrence of the variable x_n bound by Q, i.e., Qx_n .

Theorem 3.1 (Termination and correctness of **U**). Let E be the system of equations $\{sub_C(id,id,e) \approx sub_C(id,id,e')\}$ for arbitrary q-terms e and e'; **U** applied to E always terminates: if **U** terminates with failure, then e and e' are not unifiable; otherwise, **U** terminates with step 4 and presents a system E^{*} of equations in solved form that is equivalent to E.

Proof. U applies rules of the equational calculus, unless **U** meets one of the exit conditions. If **U** exits through one of the failure points 2.b.i, 2.b.ii, or 3.a, then **U** terminates and the terms e and e' are obviously not unifiable. Otherwise only steps 1., 2.a, 2.b.iii, or 3.b are applied. We claim that in this case E is eventually transformed into a system E^* , such that none of these steps is applicable, and **U** terminates on account of 4. As E^* is derived from E, E^* and E are equivalent by Theorem 2.1. And because of the termination condition, E^* must be in solved form. That establishes the correctness of **U** also in this case -- if **U** indeed terminates.

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To establish termination of **U** under the stated circumstances, it suffices to show that any sequence of steps 1., 2.a, 2.b.iii, or 3.b must be finite, when started with an application to E. For that purpose we associate with any set E' of equations a triple of natural numbers $cp(E')=\langle n_1,n_2,n_3\rangle$, where n_1 is the number of free variables with more than one occurrence, n_2 is the number of occurrences of function symbols, relation symbols, and of logical connectives (i.e., quantifiers as well as sentential connectives), and n_3 is the number of equations that are either of the form $x_n \approx x_n$ or of the form $t=x_n$ with x_n a free variable and t a non-variable term.

The lexicographic ordering > of triples of natural numbers is a well-ordering; thus, the finiteness claim has been established, as soon as we have shown that any single application of steps 1., 2.a, 2.b.iii, or 3.b to an equation E' leads to an equation E'' with cp(E')> cp(E''). Recall that $\langle n_1, n_2, n_3 \rangle \rangle \langle n'_1, n'_2, n'_3 \rangle$ holds if at least one $n_i \rangle n'_i$, for $1 \le i \le 3$, and all $n_j=n'_j$ for $0 \le j < i \le 3$. Now consider the various possible steps applicable to E':

step 1. of **U**, exchange, reduces only the number n_3 of equations of the form $t \approx x_n$, leaving all the other factors unchanged, so cp(E')>cp(E'');

step 2.a of **U**, equation elimination, reduces the number n_3 of equations of the form $x_n \approx x_n$, may reduce n_1 , but does not effect n_2 , thus we have in any case cp(E')>cp(E'');

2.b.iii of \mathbf{u} , variable elimination, reduces n_1 and may increase n_2 , but even if n_2 is increased, we have that cp(E')>cp(E'');

3.b of \mathbf{U} , term reduction, reduces n_2 and may increase n_3 , but even if n_3 is increased, we have that cp(E')>cp(E''). Q.E.D.

4. Final remarks. First, Martelli and Montanari's algorithm has been modified only to treat bound variables. It seems to be clear that other algorithms, e.g. from [PW78], can be modified in a similar way; our way of proceeding provides a case study. The complexity of the original algorithm is not essentially increased. Indeed, even the addition of canonical renaming does not change the overall complexity, as that procedure is only linear in the input.

Second, our goal was to limit the search for theorem provers, in particular for those used in automated proof search. From that, the need of an algorithm for the unification of quantified terms arose. Our proposal to use a canonical renaming seems to be a very natural way of treating bound variables in this context. Indeed, after renaming, our unification algorithm behaves as a usual unification algorithm for terms, treating quantifiers as functors and bound variables as special constants.

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