

# A Formalization of the Theorem of Existence of First-Order Most General Unifiers\*

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This work presents a formalization of the theorem of existence of most general unifiers in first-order signatures in the higher-order proof assistant PVS. The distinguishing feature of this formalization is that it remains close to the textbook proofs that are based on proving the correctness of the well-known Robinson's first-order unification algorithm. The formalization was applied inside a PVS development for term rewriting systems that provides a complete formalization of the Knuth-Bendix Critical Pair theorem, among other relevant theorems of the theory of rewriting. In addition, the formalization methodology has been proved of practical use in order to verify the correctness of unification algorithms in the style of the original Robinson's unification algorithm.

## 1 Introduction

A formalization in the proof assistant PVS of the theorem of existence of most general unifiers (mgu's) in first-order theories is presented. There are several applications of this theorem on computational logic, which range from the correctness of first-order resolution [19], the correctness of the Knuth-Bendix completion algorithm [15] to the correctness of principal type algorithms [13] and their implementations in programming and specification languages. This well-known result is stated as follows:

**Theorem 1 (Existence of mgu's)** *Let  $s$  and  $t$  be terms. Then, if  $s$  and  $t$  are unifiable then there exists an mgu of  $s$  and  $t$ .*

The analytic proof of this theorem is constructive and the first proof was introduced by Robinson himself in [19]. In Robinson's seminal paper, the unification algorithm either gives as output a most general unifier for each unifiable pair of terms, or fails when there are no unifiers. Essentially, the proof of correctness of this algorithm consists in, firstly, proving that the algorithm always terminates and, secondly, proving that, when it terminates and returns an mgu it implies the existence theorem.

Several variants of this first-order unification algorithm appear in well-known textbooks on computational and mathematical logic, semantics of programming languages, rewriting theory, type theory etc. (e.g., [17, 9, 6, 3, 2, 14]). Since the presented formalization follows the classical proof schema, only a sketch of this proof will be given here.

The development of the PVS *theory unification* was motivated by the formalization of a PVS library for term rewriting systems [11] in which the theorem of existence of mgu's is essential in order to obtain complete formalizations of relevant results such as the well-known Knuth-Bendix(-Huet) Critical Pair

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theorem [12]. In addition to this application of the formalization of the theorem of existence of mgu's, in [1] it was reported a general verification methodology of first-order unification algorithms, illustrated through the formalization of the correctness of a greedy version of Robinson's unification algorithm, that follows the lines of the formalization of the theorem of existence of mgu's presented in this paper, in order to check *termination* and *soundness* of the algorithm. Essentially, in that work it is illustrated how the verification of *completeness* of a unification algorithm depends on the particular way in that the algorithm deals with the detection of non unifiable inputs. But also, in the exercise of formalization of correctness of efficient unifications algorithms, it is of main relevance the specific data types and refined strategies used to efficiently detect and solve differences appearing among the terms being unified.

In Sec. 2, the necessary analytic concepts (terms, subterms, positions and substitutions) together with their corresponding specifications in PVS are given. The formalization of the theorem of existence of mgu's is presented in Sec. 3. Also in Sec. 3 it is illustrated how specific unification algorithms *à la* Robinson are verified using this methodology. In the sequel related work and conclusions are presented. The PVS files of the formalization of the theorem of existence of mgu's and verification of Robinson's style unification algorithms are available as part of the theory for term rewriting systems (trs) in the NASA LaRC PVS libraries <http://shemesh.larc.nasa.gov/fm/ftp/larc/PVS-library/pvslib.html>.

## 2 Specification of terms, positions, subterms and substitutions

Although it is supposed familiarity with unification and its standard notations (e.g. as in [2, 3]), analytical concepts will be presented together with their associated specifications in PVS.

Consider a signature  $\Sigma$  in which function symbols and their associated arities are given as well as an enumerable set  $V$  of variables.

**Definition 1 (Well-formed terms)** *The set of well-formed terms, denoted by  $T(\Sigma, V)$ , over the signature  $\Sigma$  and the set  $V$  of variables is recursively defined as: i)  $x \in V$  is a well-formed term and ii) for each  $n$ -ary function symbol  $f \in \Sigma$  and well-formed terms  $t_1, \dots, t_n$ ,  $f(t_1, \dots, t_n)$  is a well-formed term.*

Note that constants are 0-ary well-formed terms.

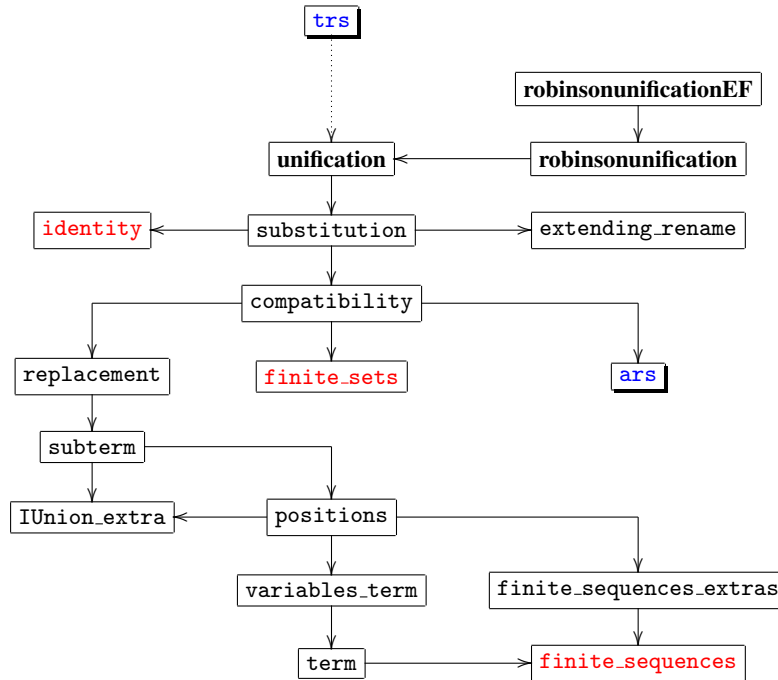
In the sequel, for brevity “terms” instead of “well-formed terms” will be used.

The hierarchy of the *theory unification* is presented in Fig. 1. This is part of the *theory trs* for term rewriting systems presented in [11], which includes also the *subtheory ars* for abstract reduction systems [10]. The most relevant notions related with unification are inside the *subtheories* *positions*, *subterm* and *substitution*. The PVS notions used for specifying these basic concepts are taken from the prelude *theories* for *finite\_sequences* and *finite\_sets*. Finite sequences are used to specify well-formed terms which are built from variables and function symbols with their associated arities. This is done by application of the PVS DATATYPE mechanism which is used to define recursive types.

```
term[variable: TYPE+, symbol: TYPE+, arity: [symbol -> nat]] : DATATYPE
BEGIN vars(v:variable): vars?
      app(f:symbol, args:{args:finite_sequence[term] | args'length=arity(f)}): app?
END term
```

Notice that the fact that a term is well-formed, that is, that function symbols are applied to the right number of arguments is guaranteed by typing the arguments of each function symbol  $f$  as a finite sequence of length  $\text{arity}(f)$ .

Finite sets and sequences are also used to specify sets of subterms and sets of term positions, as is shown below.

Figure 1: Hierarchy of unification inside the *theory trs*

## 2.1 The *subtheories* positions and subterm

As usual, positions of a term are defined as finite sequences of positive naturals, which simplifies the definitions of subterms and occurrences. A dot “.” is used for the operation of concatenation of two naturals  $m$  and  $n$ ,  $m \cdot n$ , and for the concatenation of the elements in sets of naturals; that is  $N \cdot M := \{n \cdot m \mid n \in N, m \in M\}$ . For simplicity  $n \cdot M$  denotes  $\{n\} \cdot M$ .

**Definition 2 (Positions, subterms, occurrences)** *The set of positions of a term  $t$  in  $T(\Sigma, V)$ , denoted as  $Pos(t)$ , is defined inductively as i)  $Pos(x) := \{\varepsilon\}$  and ii)  $Pos(f(t_1, \dots, t_n)) := \{\varepsilon\} \cup \bigcup_{i=1}^n i \cdot Pos(t_i)$ , where  $\varepsilon$  denotes the empty sequence that represents the root position of the term  $t$ . The subterm at a given position  $\pi \in Pos(t)$  of a term  $t$  is defined inductively as i)  $t|_\varepsilon := t$  and ii)  $f(t_1, \dots, t_n)|_{i \cdot \pi} := t_i|_\pi$ .*

*The set of subterms of a term  $t$  is the set  $\{t|_\pi \mid \pi \in Pos(t)\}$ .*

*Whenever  $s = t|_\pi$ , it is said that there is an occurrence of the subterm  $s$  of  $t$  at position  $\pi$ . The set of positions of occurrences of a term  $s$  in  $t$  is given by the set  $\{\pi \mid t|_\pi = s\}$ .*

The (finite) set of positions `positionsOF` of a term  $t$  is recursively specified on its structure as below, where `only_empty_seq` is a set containing an empty finite sequence only, that is the set containing the root position only.

```

positionsOF(t: term): RECURSIVE positions =
  (CASES t OF
    vars(t): only_empty_seq,
    app(f, st): IF length(st) = 0 THEN only_empty_seq
                ELSE union(only_empty_seq,
                          IUnion((LAMBDA (i: upto?(length(st))):
                                catenate(i, positionsOF(st(i-1))))))
                ENDIF
  ENDCASES)
MEASURE t BY <<
  
```

where the operator `IUnion` builds the union of all sets of positions of the arguments of a functional term `app(f, st)` in which `f` is the name of the function and `st` is the sequence of arguments, that is a sequence of length equal to the arity of `f`. The positions of the  $i^{\text{th}}$  argument are prefixed by `i` in order to build the sequence of positions inside this argument relative to the whole term.

Several necessary results on terms, subterms and positions are formalized by induction on the structure of terms following the lines of this abstract datatype specification. For instance, properties, such as the one that states that the set of positions of a term is finite and that terms with the same heading symbol (applications) have the same number of arguments, presented below, are proved by structural induction on the abstract datatype for terms.

```
positions_of_terms_finite : LEMMA is_finite(positionsOF(t))
```

```
equal_symbol_equal_length_arg : LEMMA
  FORALL (s, t: term, fs, ft: symbol,
    ss:{args: finite_sequence[term] | args'length = arity(fs)},
    st:{argt: finite_sequence[term] | argt'length = arity(ft)}) :
  (s = app(fs, ss) AND t = app(ft,st) AND fs = ft) => ss'length = st'length
```

For  $p \in \text{Pos}(t)$ , in the *subtheory* subterm, the subterm of `t` at position `p` also is specified in a recursive way (now on the length of `p`), as follows:

```
subtermOF(t: term, (p: positions?(t))): RECURSIVE term =
  IF length(p) = 0 THEN t ELSE LET st = args(t), i = first(p), q = rest(p) IN
    subtermOF(st(i-1), q) ENDIF
MEASURE length(p)
```

where `first` and `rest` are constructors that return, respectively, the first element and the rest of a finite sequence, and `positions?(t)` is the (dependent) type of all positions in `t`, which is specified as follows:

```
positions?(t: term): TYPE = {p: position | positionsOF(t)(p)}
```

Several necessary results on terms, subterms and positions are formalized by induction on the structure of terms following the lines of these definitions. For instance, properties such as the one that states that the set of variables occurring in a term is finite (lemma `vars_of_term_finite` in the *subtheory* subterm). Other results are formalized by induction on the length of (sequences representing) positions; for instance the ones below stating the equality  $t|_{p.q} = (t|_p)|_q$  and that whenever  $p$  is a position of  $t$  and  $q$  a position of  $t|_p$ ,  $p.q$  is a position of  $t$ , are proved by structural induction on terms.

```
pos_subterm: LEMMA FORALL (p, q: position, t: term):
  positionsOF(t)(p o q) => subtermOF(t, p o q) = subtermOF(subtermOF(t, p), q)
```

```
pos_o_term: LEMMA FORALL (p, q: position, t: term):
  positionsOF(t)(p) & positionsOF(subtermOF(t, p))(q) => positionsOF(t)(p o q)
```

## 2.2 The *subtheory* substitution

By using the definition of position, the notion of replacement of a subterm of a term is stated easily.

**Definition 3 (Replacement of subterms)** Consider  $t \in T(\Sigma, V)$  and  $\pi \in \text{Pos}(t)$ . The term resulting from replacing the subterm at position  $\pi$  of  $t$  by the term  $s$  is denoted by  $t[\pi \leftarrow s]$ .

Alternatively, the notation  $t[s]_\pi$  is also frequently used in the literature.

**Definition 4 (Substitution)** A substitution  $\sigma$  is defined as a function from  $V$  to  $T(\Sigma, V)$ , such that the domain of  $\sigma$ , defined as the set of variables  $\{x \mid x \in V, x\sigma \neq x\}$  and denoted by  $Dom(\sigma)$ , is finite.

**Definition 5 (Homomorphic extension of a substitution)** The homomorphic extension of a substitution  $\sigma$ , denoted as  $\hat{\sigma}$ , is inductively defined over the set  $T(\Sigma, V)$  as i)  $x\hat{\sigma} := x\sigma$  and ii)  $f(t_1, \dots, t_n)\hat{\sigma} := f(t_1\hat{\sigma}, \dots, t_n\hat{\sigma})$ .

Given the notion of homomorphic extension, it is possible to define substitution composition.

**Definition 6 (Composition of substitutions)** Consider two substitutions  $\sigma$  and  $\tau$ , their composition  $\sigma \circ \tau$  is defined as the substitution  $\sigma \circ \tau$  such that  $Dom(\sigma \circ \tau) = Dom(\sigma) \cup Dom(\tau)$  and for each variable  $x$  in this domain,  $x(\sigma \circ \tau) := (x\tau)\hat{\sigma}$ .

The *subtheory* substitution specifies the algebra of substitutions. In this *subtheory* the type of substitutions is built as functions from variables to terms  $sig : [V \rightarrow term]$ , whose domain is finite:  $Sub?(sig) : bool = is\_finite(Dom(sig))$  and  $Sub : TYPE = (Sub?)$ . Also, the notions of domain, range, and the variable range are specified, closer to the usual theory of substitution as presented in well-known textbooks (e.g., [2]). These notions are specified as follows:

$Dom(sig) : set[(V)] = \{x : (V) \mid sig(x) \neq x\}$

$Ran(sig) : set[term] = \{y : term \mid EXISTS (x : (V)) : member(x, Dom(sig)) \ \& \ y = sig(x)\}$

$VRan(sig) : set[(V)] = IUnion(LAMBDA (x \mid Dom(sig)(x)) : Vars(sig(x)))$

where  $(V)$  denotes the type of all terms that are variables and  $Vars(t)$  denotes the set of all variables occurring in a term  $t$ .

Also, in the *subtheory* substitution the homomorphic extension  $ext(sig)$  of a substitution  $sig$  is specified inductively over the structure of terms:

```
ext(sigma)(t): RECURSIVE term =
  CASES t OF vars(t): sigma(t),
  app(f, st):
    IF length(st) = 0 THEN t ELSE LET sst = (# length := st'length,
      seq := (LAMBDA (n: below[st'length]): ext(sigma)(st(n)))#) IN app(f, sst) ENDIF
  ENDCASES
MEASURE t BY <<
```

The composition of two substitutions, denoted by  $comp$ , is specified as

$comp(sigma, tau)(x : (V)) : term = ext(sigma)(tau(x))$

In standard rewriting notation, the homomorphic extension of a substitution  $\sigma$  from its domain of variables to the domain of terms is denoted by  $\hat{\sigma}$ , but to simplify notation, usually textbooks do not distinguish between a substitution  $\sigma$  and its extension  $\hat{\sigma}$ . In the formalization this distinction should be maintained carefully. For instance observe the following lemma and its formalization.

**Lemma 2** Let  $s$  be term,  $p$  a position of  $s$  and  $\sigma$  a substitution. Then  $(s\hat{\sigma})|_p = (s|_p)\hat{\sigma}$ .

```
subterm_ext_commute: LEMMA FORALL (p: position, s: term, sigma: Sub):
  positionsOF(s)(p) => subtermOF(ext(sigma)(s), p) = ext(sigma)(subtermOF(s, p))
```

Several important results useful for the development of *subtheory unification* were formalized in the *subtheory* substitution, e.g., the property that states that the application of a homomorphic extension of a substitution preserves the original set of positions of the instantiated term, formalized as:

```
ext_preserv_pos: LEMMA FORALL (p: position, s: term, sigma: Sub):
  positionsOF(s)(p) => positionsOF(ext(sigma)(s))(p)
```

The lemma below formalizes the set of positions of the instantiation of a term by a substitution.

```
positions_of_ext: LEMMA positionsOF(ext(sigma)(t)) =
  union({p | positionsOF(t)(p) & (NOT vars?(subtermOF(t, p)))},
    {q | EXISTS p1, p2: q = p1 o p2 AND positionsOF(t)(p1) AND
      vars?(subtermOF(t, p1)) AND positionsOF(ext(sigma)(subtermOF(t, p1)))(p2)})
```

Additional formalized lemmas, presented below, state that all variables in the domain but not in the range of a substitution  $\sigma$  disappear in all  $\sigma$  instantiated terms and that non-variable subterms, i.e. function symbols, remain untouched after any possible instantiation.

```
vars_subst_not_in: LEMMA FORALL t, sigma, x:
  Dom(sigma)(x) AND (FORALL r: Ran(sigma)(r) => NOT member(x, Vars(r)))
  => NOT member(x, Vars(ext(sigma)(t)))

ext_preserve_symbol : LEMMA FORALL(s:term, sig:Sub, p:position | positionsOF(s)(p)):
  app?(subtermOF(s, p)) => f(subtermOF(s, p)) = f(subtermOF(ext(sig)(s), p))
```

### 3 Formalization of first-order unification

The formalization of the existence of first-order mgu's is presented and then it is explained how the formalization technology was applied to verify a specific unification algorithm. Again, definitions and their corresponding specifications are included. The *theory unification* consists of 57 lemmas from which 30 are *type proof obligations* (TCCs) that are lemmas automatically generated by the prover during the type checking. The specification file has 273 lines and its size is 9.8 KB and of the proof file has 11540 lines and 657 KB.

Two terms  $s$  and  $t$  are said to be unifiable whenever there exists a substitution  $\sigma$  such that  $s\hat{\sigma} = t\hat{\sigma}$ .

**Definition 7 (Unifiers)** *The set of unifiers of two terms  $s$  and  $t$  is defined as  $U(s,t) := \{\sigma \mid s\hat{\sigma} = t\hat{\sigma}\}$ .*

**Definition 8 (More general substitutions)** *Given two substitutions  $\sigma$  and  $\tau$ ,  $\sigma$  is said to be more general than  $\tau$  whenever, there exists a substitution  $\gamma$  such that  $\gamma \circ \sigma = \tau$ . This is denoted as  $\sigma \leq \tau$ .*

**Definition 9 (Most General Unifier)** *Given two terms  $s$  and  $t$  such that  $U(s,t) \neq \emptyset$ . A substitution  $\sigma$  such that for each  $\tau \in U(s,t)$ ,  $\sigma \leq \tau$ , is said to be a most general unifier of  $s$  and  $t$ . For short it is said that  $\sigma$  is an mgu of  $s$  and  $t$ .*

Now, it is possible to state the theorem of existence of mgu's.

**Theorem 3 (Existence of mgu's)** *Let  $s$  and  $t$  be terms built over a signature  $T(\Sigma, V)$ . Then,  $U(s,t) \neq \emptyset$  implies that there exists an mgu of  $s$  and  $t$ .*

The analytic proof of this theorem is constructive and the first introduced proof was presented by Robinson himself in [19]. In Robinson's paper, a unification algorithm was introduced, which either gives as output a most general unifier for each unifiable pair of terms or fails when there are no unifiers. The proof of correctness of this algorithm, which consists in proving that the algorithm always terminates and that when it terminates it gives an mgu implies the existence theorem. Several variants of this first-order unification algorithm appear in well-known textbooks on computational and mathematical logic, semantics of programming languages, rewriting theory, etc. (e.g., [17, 9, 6, 3, 2, 14]). Since the presented formalization follows the classical proof schema, no analytic presentation of this proof is given here.

Basic notions on unification are specified straightforwardly in the language of PVS. For instance the notion of most general substitution is given as

```
<=(theta, sigma): bool = EXISTS tau: sigma = comp(tau, theta)
```

From this specification, one proves that the relation  $\leq$  is a pre-order (i.e., reflexivity and transitivity).

The notions of unifier, unifiable, the set of unifiers of two terms and a most general unifier of two terms are specified as

```
unifier(sigma)(s,t): bool = ext(sigma)(s) = ext(sigma)(t)
unifiable(s,t): bool = EXISTS sigma: unifier(sigma)(s,t)
U(s,t): set[Sub] = {sigma: Sub | unifier(sigma)(s,t)}
mgu(theta)(s,t): bool =
  member(theta, U(s,t)) & FORALL sigma: member(sigma, U(s,t)) => theta <= sigma
```

Several auxiliary lemmas related with the previous notions were also formalized as the ones presented below: `unifier_o` formalizes the facts that, whenever  $\sigma \in U(s\hat{\theta}, t\hat{\theta})$ ,  $\sigma \circ \theta \in U(s, t)$ ; `mgu_o`, that whenever  $\rho \geq \sigma$ ,  $\rho \circ \theta \geq \sigma \circ \theta$ ; `unifier_and_sub`, that instantiations of unifiers are unifiers; `idemp_mgu_iff_all_unifier` that idempotence property of mgu's, and; the lemma that formalizes the fact that corresponding subterms of unifiable terms are unifiable, `unifiable_terms_unifiable_args`.

```
unifier_o: LEMMA
  member(sig, U(ext(theta)(s), ext(theta)(t))) => member(comp(sig, theta), U(s, t))
mgu_o: LEMMA sig <= rho => comp(sig, theta) <= comp(rho, theta)
unifier_and_subs: LEMMA
  member(theta, U(s, t)) => (FORALL (sig: Sub): member(comp(sig, theta), U(s, t)))
idemp_mgu_iff_all_unifier: LEMMA FORALL (theta: Sub | member(theta, U(s, t))):
  mgu(theta)(s, t) & idempotent_sub?(theta) <=>
  (FORALL (sig: Sub | member(sig, U(s, t))): sig = comp(sig, theta))
unifiable_terms_unifiable_args: LEMMA
FORALL (s: term, t: term, p: position | positionsOF(s)(p) & positionsOF(t)(p)):
  member(sig, U(s, t)) => member(sig, U(subtermOF(s, p), subtermOF(t, p)))
```

The unification algorithm receives two unifiable terms as arguments and is specified as the function `unification_algorithm`, presented below. This function together with the two auxiliary functions `sub_of_frst_diff` and `resolving_diff`, to be explained in the remaining of this section, conform the kernel of the unification specified mechanism.

```
unification_algorithm(s: term, (t: term | unifiable(s, t))): RECURSIVE Sub =
IF s = t THEN identity ELSE LET sig = sub_of_frst_diff(s, t) IN
  comp( unification_algorithm((ext(sig))(s), (ext(sig))(t))), sig) ENDIF
MEASURE Card(union(Vars(s), Vars(t)))
```

In this specification, the function `sub_of_frst_diff(s, t)`, presented below, gives as result a substitution that resolves the first difference (left-most, outer-most in the structure of the terms) between the terms  $s$  and  $t$ , that are unifiable and different terms. In order to generate this substitution, the subterms that generate the difference must occur in the same position of  $s$  and  $t$ , one of these terms must be a variable and the other, a term without occurrences of this variable. The `unification_algorithm` recursive function has a pair of unifiable terms as domain type, given by the parameters  $s$  and  $t$ , and in the interesting case, after encountering the resolving substitution  $\sigma$  for the first difference, it returns the composition of the result of the recursive call with the arguments  $s\hat{\sigma}$  and  $t\hat{\sigma}$  and  $\sigma$ .

The functions `resolving_diff` and `sub_of_frst_diff`, presented below, have the same type of parameters, and the former returns the first (left-most, outer-most) position of conflict between the unifiable and different terms  $s$  and  $t$ , as previously explained, while the latter returns the substitution that solves the conflict at the position generated by the function `resolving_diff`.

```

resolving_diff(s: term, (t: term | unifiable(s,t) & s /= t ) ): RECURSIVE position =
  (CASES s OF
    vars(s): empty_seq,
    app(f, st): IF length(st) = 0 THEN empty_seq
                ELSE (CASES t OF
                  vars(t): empty_seq,
                  app(fp, stp): LET k: below[length(stp)] =
                                min({kk: below[length(stp)] |
                                    subtermOF(s,#(kk+1)) /= subtermOF(t,#(kk+1))}) IN
                                add_first(k+1, resolving_diff(subtermOF(s,#(k+1)), subtermOF(t,#(k+1))))
                  ENDCASES)   ENDIF ENDCASES)
  MEASURE s BY <<

```

```

sub_of_frst_diff(s: term , (t: term | unifiable(s,t) & s /= t )): Sub =
  LET k: position = resolving_diff(s,t) IN
  LET sp = subtermOF(s,k) , tp = subtermOF(t,k) IN
  IF vars?(sp) THEN (LAMBDA (x: (V)): IF x = sp THEN tp ELSE x ENDIF)
  ELSE (LAMBDA (x: (V)): IF x = tp THEN sp ELSE x ENDIF) ENDIF

```

### 3.1 Termination

Notice that the measure of the function `unification_algorithm` is the cardinality of the union of the sets of variables occurring in the term parameters  $s$  and  $t$ . From this measure, the PVS type-checker generates an interesting type proof obligation concerning the property of decreasingness of this measure, that guarantees the termination of the algorithm for all pairs of unifiable terms.

```

unification_algorithm_TCC6: OBLIGATION FORALL (s, (t | unifiable(s, t))):
NOT s = t => (FORALL (sig: Sub): sig = sub_of_frst_diff(s, t) =>
  Card(union(Vars(ext(sig)(s)), Vars(ext(sig)(t)))) < Card(union(Vars(s), Vars(t))))

```

Although this key TCC is automatically generated, it is not automatically proved by PVS. In order to prove this TCC, one should first prove the following auxiliary lemma:

```

vars_ext_sub_of_frst_diff_decrease: LEMMA
FORALL (s: term, t: term | unifiable(s, t) & s /= t):
  LET sig = sub_of_frst_diff(s, t) IN
  Card(union( Vars(ext(sig)(s)), Vars(ext(sig)(t)))) < Card(union( Vars(s), Vars(t)))

```

To prove the previous lemma, one requires the following additional lemma:

```

union_vars_ext_sub_of_frst_diff : LEMMA
FORALL (s : term, t : term | unifiable(s, t) & s /= t) :
  LET sig = sub_of_frst_diff(s, t) IN union(Vars(ext(sig)(s)), Vars(ext(sig)(t))) =
    difference(union( Vars(s), Vars(t)), Dom(sig))

```

The proof of the previous lemma requires that the substitution  $\sigma$ , that resolves the first conflict between the given terms, maps a variable into a term without occurrences of this variable. From this fact, it is possible to guarantee that the mapped variable disappears from the instantiated terms  $s\hat{\sigma}$  and  $t\hat{\sigma}$ , and hence the decreasing property holds. This is formalized as the lemma:

```

sub_of_frst_diff_remove_x : LEMMA FORALL (s:term, t:term | unifiable(s, t) & s /= t):
  LET sig = sub_of_frst_diff(s, t) IN Dom(sig)(x) =>
    (NOT member(x, Vars(ext(sig)(s)))) AND (NOT member(x, Vars(ext(sig)(t))))

```



Two other lemmas, one for  $s$  and the other for  $t$ , formalize the fact that the variables in the  $\sigma$  instantiated terms are contained in the set of variables occurring in the original terms being unified.

```
vars_sub_of_frst_diff_s_is_subset_union : LEMMA
  FORALL (s : term, t : term | unifiable(s, t) & s /= t):
    LET sig = sub_of_frst_diff(s, t) IN
      subset?(Vars(ext(sig)(s)), union( Vars(s), Vars(t)))
```

Applying the previous lemmas, it is formalized the fact that the cardinality of the set of variables occurring in the terms being unified decreases after resolving each conflict between the terms.

In the remaining of this section the formalization of lemma `union_vars_ext_sub_of_frst_diff`, the lemma presented above, will be explained. After a first step of skolemization and simplifications, the following sequent is obtained.

```
{-1} sub_of_frst_diff(s, t) = sig
|-----
{1} union(Vars(ext(sig)(s)), Vars(ext(sig)(t)))(x) IFF
    difference(union(Vars(s), Vars(t)), Dom(sig))(x)
```

Note that there is a variable  $x$ , resulting from an application of the PVS proof command “decompose-equality” that simplifies the equality between sets in the consequent formula into a biconditional, where the following assertion is established:  $x$  is a member of  $Vars(s\hat{\sigma}) \cup Vars(t\hat{\sigma})$  if, and only if,  $x$  is a member of  $Vars(s) \cup Vars(t) \setminus Dom(\sigma)$ . At this point, a propositional simplification is applied and the proof is divided in two branches, presented below, one for each direction of the biconditional:

- $x \in Vars(s\hat{\sigma}) \cup Vars(t\hat{\sigma})$  implies  $x \in Vars(s) \cup Vars(t) \setminus Dom(\sigma)$ .

After expanding the definitions of `difference` and `union`, the following sequent is obtained:

```
{-1} Vars(ext(sig)(s))(x) OR Vars(ext(sig)(t))(x)
[-2] sub_of_frst_diff(s, t) = sig
|-----
{1} (Vars(s)(x) OR Vars(t)(x)) AND NOT Dom(sig)(x)
```

Then, after propositional simplification, the proof divides into four branches:

1. In this case,  $x \in Vars(s\hat{\sigma})$  and one should verify that either  $x \in Vars(s)$  or  $x \in Vars(t)$ , which is done by application of lemma `vars_sub_of_frst_diff_s_is_subset_union`.
  2. In this case,  $x \in Vars(s\hat{\sigma})$  and one should verify that  $x \notin Dom(\sigma)$ , which is done by application of lemma `sub_of_frst_diff_remove_x`.
  - 3, 4. These cases are similar to the previous two cases for the term  $t$ .
- $x \in Vars(s) \cup Vars(t) \setminus Dom(\sigma)$  implies  $x \in Vars(s\hat{\sigma}) \cup Vars(t\hat{\sigma})$ .

In this branch, after propositional simplification, one should verify that  $x \in Vars(s)$  implies  $x \in Vars(s\hat{\sigma})$  or,  $x \in Vars(t)$  implies  $x \in Vars(t\hat{\sigma})$ . This is true because if  $x \notin Dom(\sigma)$ , then for a position  $\pi \in Pos(s)$  such that  $s|_{\pi} = x$ , one has  $(s|_{\pi})\hat{\sigma} = (s\hat{\sigma})|_{\pi} = x$ .

## 3.2 Soundness

After establishing the termination of the specified function `unification_algorithm`, its correctness is formalized and applied in order to prove the Theorem 1 of existence of mgu’s that is specified as:

unification: LEMMA unifiable(s,t) => EXISTS theta: mgu(theta)(s,t)

This lemma is proved applying the two lemmas below. The first one states that the substitution given by the function `unification_algorithm` is, in fact, a unifier and the second one that it is an mgu.

unification\_algorithm\_gives\_unifier: LEMMA  
unifiable(s,t) => member(unification\_algorithm(s, t), U(s, t))

unification\_algorithm\_gives\_mg\_subs: LEMMA  
member(rho, U(s, t)) => unification\_algorithm(s, t) <= rho

The formalization of the lemma `unification_algorithm_gives_unifier` is done by induction on the cardinality of the set of variables occurring in `s` and `t`. For proving this lemma three auxiliary lemmas are necessary:

- the lemma `vars_ext_sub_of_frst_diff_decrease` described in the previous subsection, which guarantees that the set of variables decreases;
- `ext_sub_of_frst_diff_unifiable`: LEMMA  
FORALL (s: term, t: term | unifiable(s, t) & s /= t):  
LET sig = sub\_of\_frst\_diff(s, t) IN unifiable(ext(sig)(s), (ext(sig)(t)))  
which states that the instantiations of two different and unifiable terms  $s\hat{\sigma}$  and  $t\hat{\sigma}$  with the substitution  $\sigma$  that resolves the first conflict between these terms, are still unifiable; and
- the lemma `unifier_o`, presented at the beginning of this section, which states that for any unifier  $\theta$  of  $s\hat{\sigma}$  and  $t\hat{\sigma}$ ,  $\theta \circ \sigma$  is a unifier of `s` and `t`.

The formalization of the lemma `unification_algorithm_gives_mg_subs` is done by induction on the cardinality of the set of variables occurring in `s` and `t` too. For proving this lemma two auxiliary lemmas are applied: the lemma `vars_ext_sub_of_frst_diff_decrease` and the lemma presented below, which states that for each unifier  $\rho$  of `s` and `t`, two different and unifiable terms, and given  $\sigma$  the substitution that resolves the first difference between these terms, there exist  $\theta$  such that  $\theta \circ \sigma = \rho$ .

sub\_of\_frst\_diff\_unifier\_o: LEMMA FORALL (s:term, t:term | unifiable(s, t) & s /= t):  
member(rho, U(s, t)) =>  
LET sig = sub\_of\_frst\_diff(s, t) IN EXISTS theta: rho = comp(theta, sig)

In the remaining of this section the formalization of `sub_of_frst_diff_unifier_o` will be explained.

It should be proved that  $\theta \circ \sigma$  and  $\rho$  map each variable `x` in their domain, that should be the same set of variables, into the same terms. The formalization starts by a skolemization and then, in order to provide a name, `p`, for the position in which the first difference between terms `s` and `t` is detected, an application of the PVS proof command “name” is done. In this way the additional premise `resolving_diff(s, t) = p` is included.

```
{-1} resolving_diff(s, t) = p    [-2] sub_of_frst_diff(s, t) = sig
[-3] member(rho, U(s, t))
    |-----
[1] EXISTS theta: rho = comp(theta, sig)
```

The proof strategy is to instantiate the existential formula in the consequent with  $\rho$  itself, having in mind that if  $\rho \in U(s, t)$  then  $\rho \in U(s|_q, t|_q)$ , for any valid position `q` of `s` and `t`, and in particular, for the position of the first detected difference `p`. It is known that at position `p`, either  $s|_p$  or  $t|_p$  should be a variable; so the strategy is to analyze both possible cases. The sequent below is obtained in the case in which  $s|_p$  is a variable. In this sequent `x` is an arbitrary variable.

```

{-1} vars?(subtermOF(s, p))      [-2] ext(rho)(subtermOF(s, p)) =
      ext(rho)(subtermOF(t, p))  [-3] resolving_diff(s, t) = p
[-4] sub_of_frst_diff(s, t) = sig [-5] ext(rho)(s) = ext(rho)(t)
      |-----
[1]  rho(x) = ext(rho)(sig(x))

```

The variable  $x$  in the consequent of this sequent appears after an application of the PVS proof command “decompose-equality” that simplifies equality between substitutions into equality of the application of the substitutions to any variable:  $\rho \circ \sigma = \rho$ , whenever for any  $x$   $(x\sigma)\hat{\rho} = x\rho$ .

The proof is obtained by case analysis: when  $x = s|_p$  and when  $x \neq s|_p$ ,

- In the former case, the formula  $x = \text{subtermOF}(s, p)$  is added to the antecedents.

Note that  $(s|_p)\hat{\sigma} = t|_p$ , that is  $\text{ext}(\text{sig})(\text{subtermOF}(s, p)) = \text{subtermOF}(t, p)$ , by definition of `sub_of_frst_diff`, and  $(s|_p)\hat{\rho} = (t|_p)\hat{\rho}$ . Then, one can conclude that  $(s|_p)\hat{\rho} = ((s|_p)\hat{\sigma})\hat{\rho}$ . But, in this case,  $x = s|_p$ ; thus, one can complete this branch of the proof expanding the definition of `sub_of_frst_diff` with an application of the proof command “expand” and making simplifications with the commands “replace” and “assert”.

- In the latter case, the sequent to be considered is presented below. Notice that the negated equality that characterizes this case is positively presented as a consequent of the sequent.

```

[-1] vars?(subtermOF(s, p))      [-2] ext(rho)(subtermOF(s, p)) =
      ext(rho)(subtermOF(t, p))  [-3] resolving_diff(s, t) = p
[-4] sub_of_frst_diff(s, t) = sig [-5] ext(rho)(s) = ext(rho)(t)
      |-----
{1}  x = subtermOF(s, p)          [2]  rho(x) = ext(rho)(sig(x))

```

In this case, note that  $x$  does not belong to the domain of substitution  $\sigma$ , because the domain of  $\sigma$  is the singleton  $\{s|_p\}$ . Then  $x\sigma = x$ . Therefore the equality  $x\rho = (x\sigma)\hat{\rho}$  is true, which is sufficient to complete this branch of the proof.

At this point, two cases remain to be considered: the case where  $t|_p$  is a variable, that is formalized in a way entirely analogous to the previous case, and the case where neither  $s|_p$  nor  $t|_p$  are variables.

In the latter case, again one should apply that at a conflicting position of two unifiable terms it is impossible that none of the subterms is a variable. This result was already formalized as a lemma called `resolving_diff_vars`. Then using this lemma and instantiating appropriately one obtains the sequent:

```

{-1} p = resolving_diff(s, t) => vars?(subtermOF(s, p)) OR vars?(subtermOF(t, p))
[-2] resolving_diff(s, t) = p
      |-----
[1]  vars?(subtermOF(t, p))      [2]  vars?(subtermOF(s, p))

```

In this sequent the contradiction is already established, and can be captured with a simple application of the PVS proof command “assert”. The proof of the main lemma used in this branch of the proof, `resolving_diff_vars`, previously mentioned, follows by induction on the structure of the term  $s$  as explained below.

If  $s$  is a variable, the position  $p$  should be the root position `empty_seq` and at this position, the term  $s|_\varepsilon$  is a variable. If  $s$  is an application, the proof follows by expanding the definition of `resolving_diff` and considering the three possible cases, namely:

1.  $s$  is a constant. Then the position of the first difference should be  $\varepsilon$  and  $t$  should be a variable, since the terms are unifiable.

2.  $s$  is a non constant application and  $t$  is a variable. Similar to the previous case.
3.  $s$  is a non constant application and  $t$  is an application. The position  $p$  cannot be the root position. The sequent corresponding to this case is presented below.

```

{-1} p = add_first(k, resolving_diff(subtermOF(s, #(k)), subtermOF(t, #(k))))
[-2] FORALL (x: below[args(s)'length]):
      FORALL (t: term | unifiable(args(s)'seq(x), t) & args(s)'seq(x) /= t,
              p: position | positionsOF(args(s)'seq(x))(p) & positionsOF(t)(p)):
        p = resolving_diff(args(s)'seq(x), t) =>
          vars?(subtermOF(args(s)'seq(x), p)) OR vars?(subtermOF(t, p))
|-----
[1]  vars?(t)                [2]  length(args(s)) = 0
[3]  vars?(subtermOF(s, p))  [4]  vars?(subtermOF(t, p))

```

In this sequent the induction hypothesis, that is the antecedent formula [-2], should be instantiated with  $k - 1$ , in order to capture the subterm of  $s|_k$ , i.e., the  $(k - 1)$ -th element of the sequence of arguments of the root symbol of  $s$ ,  $\text{args}(s)'seq(k - 1)$ . Then, the position  $p$  equals the concatenation of  $k$  with the first difference between terms  $s|_k$  and  $t|_k$ , here denoted as  $p = k \circ q$ . By induction hypothesis either  $(s|_k)|_q$  or  $(t|_k)|_q$  is a variable. But  $(s|_k)|_q = s|_{k \circ q}$  and  $(t|_k)|_q = t|_{k \circ q}$ , which concludes the proof.

### 3.3 Verification of unification algorithms

This methodology of proof of the existence of mgu's can be applied in order to formalize the completeness of unification algorithms *à la* Robinson, as presented in detail in [1] for a greedy unification algorithm. This is illustrated in the *theory* **robinsonunification** also available inside **trs** as well as in a more recent efficient specification **robinsonunificationEF** (see the **trs** hierarchy in Fig. 1).

The main functions in the *theory* **robinsonunification** are: `first_diff`, `link_of_frst_diff` and `robinson_unification_algorithm` whose roles are analogous respectively to the ones of the functions `resolving_diff`, `sub_of_frst_diff` and `unification_algorithm`. These functions are specified in such a way that whenever unsolvable differences are detected (by the function `first_diff`) the substitution “fail” is returned. This substitution is built explicitly as the substitution with the singleton domain  $\{xx\}$  and image  $ff(xx)$ , where  $xx$  and  $ff$  are, respectively, a constant and a unary function. In this way, the substitution `fail` is discriminated from any other possible unifier which is built by the function `robinson_unification_algorithm` for all pair of terms.

The function `link_of_frst_diff`, presented below, either builds the resolving link substitution for the first difference whose position is detected by `first_diff` or returns `fail`. According to these two options, the function `robinson_unification_algorithm`, also presented below, either builds the mgu or returns `fail`.

```

link_of_frst_diff(s : term , (t : term | s /= t )) : Sub =
  LET k : position = first_diff(s,t) IN
    LET sp = subtermOF(s,k) , tp = subtermOF(t,k) IN
      IF vars?(sp)
      THEN IF NOT member(sp, Vars(tp))
            THEN (LAMBDA (x : (V)) : IF x = sp THEN tp ELSE x ENDIF)
            ELSE fail ENDIF
      ELSE IF vars?(tp) THEN
            IF NOT member(tp, Vars(sp))

```

```

      THEN (LAMBDA (x : (V)) : IF x = tp THEN sp ELSE x ENDIF)
      ELSE fail ENDIF
    ELSE fail ENDIF  ENDIF

```

```

robinson_unification_algorithm(s, t : term) : RECURSIVE Sub =
  IF s = t THEN identity
  ELSE LET sig = link_of_frst_diff(s,t) IN
    IF sig = fail THEN fail
    ELSE LET sigma = robinson_unification_algorithm(ext(sig)(s) , ext(sig)(t)) IN
      IF sigma = fail THEN fail ELSE comp(sigma, sig) ENDIF
    ENDIF  ENDIF
  MEASURE Card(union(Vars(s), Vars(t)))

```

The *theory* **robinsonunification** consists of 47 lemmas from which 24 are TCCs. The specification file has 249 lines and its size is 8.6 KB, and the whole proof file has 12091 lines and 739 KB and was described in detail in [1].

The *subtheory* **robinsonunificationEF** includes an “efficient” version of the unification algorithm in which after resolving each conflicting position between two terms the next conflict is searched starting from the position of conflict previously resolved instead from the root position of the instantiated terms as it is done in the *theories* **unification** and **robinsonunification**. The main functions found in this improved version of the algorithm are `next_position` and `robinson_unification_algorithm_aux`.

The function `next_position` takes as arguments two terms and a valid position  $\pi$  of both terms, and returns the next conflicting position. Once all differences between the terms occurring in previous positions to  $\pi$  (left-most, outer-most) and at position  $\pi$  itself have been resolved, the next conflict should occur in a position to the right, and therefore there is no need to scan again the instantiated terms starting from the root position.

The function `robinson_unification_algorithm_aux` also takes as arguments two terms and a position of these terms, and returns a substitution, but now in the process of unification the next conflict position is fetched from the first position of conflict, using the function `next_position`.

```

next_position(s, t : term,
             p : position | positionsOF(s)(p) AND positionsOF(t)(p)):
RECURSIVE position =
  IF p = empty_seq THEN empty_seq
  ELSE LET pi0 = delete(p,length(p) - 1) IN
    IF f(subtermOF(s,pi0)) /= f(subtermOF(t,pi0)) THEN pi0
    ELSE LET pi = add_last(delete(p, length(p) - 1), last(p) + 1) IN
      IF positionsOF(s)(pi) THEN
        IF subtermOF(s, pi) /= subtermOF(t, pi) THEN pi
        ELSE next_position(s,t, pi) ENDIF
      ELSE IF pi0 /= empty_seq THEN next_position(s, t, pi0)
        ELSE empty_seq ENDIF
      ENDIF  ENDIF  ENDIF
  MEASURE IF p = empty_seq THEN lex2(0,0)
    ELSE lex2(length(p),
              arity(f(subtermOF(s, delete(p,length(p) - 1)))) - last(p))
  ENDIF

```

```

robinson_unification_algorithm_aux(s, t : term, p : position |
  positionsOF(s)(p) AND positionsOF(t)(p)) : RECURSIVE Sub =
  IF subtermOF(s,p) = subtermOF(t,p) THEN

```

```

LET pi = next_position(s, t, p) IN
  IF pi = empty_seq THEN identity
  ELSE robinson_unification_algorithm_aux(s,t,pi)
  ENDIF
ELSE LET sig = link_of_frst_diff(subtermOF(s,p),subtermOF(t,p)) IN
  IF sig = fail THEN fail
  ELSE LET pi = next_position(ext(sig)(s), ext(sig)(t),
    p o first_diff(subtermOF(s,p),subtermOF(t,p))) IN
    IF pi = empty_seq THEN sig
    ELSE LET sigma = robinson_unification_algorithm_aux(
      ext(sig)(s), ext(sig)(t), pi) IN
      IF sigma = fail THEN fail ELSE comp(sigma, sig) ENDIF
    ENDIF ENDIF ENDIF
MEASURE lex2(Card(union(Vars(s), Vars(t))), Card(right_pos(s,p)))

```

Formalization of correctness of this specification requires several additional effort and, in particular, specialized inductive proof that are based on the more elaborated measures necessities for the previous two functions.

## 4 Related work

Correctness of unification algorithms has been the center of several formalizations in a variety of theorem provers. Starting from a formalization in LCF [18], other formal proofs have been given, for example, in Isabelle/HOL, Coq [20, 4, 16], ALF [5] and ACL2 [21].

The earlier LCF formalization of the unification algorithm was given by Paulson [18]. Paulson's approach was followed by Konrad Slind in the theory `Unify` formalized in Isabelle/HOL from which an improved version called `Unification` is available now. Unlike other approaches, in Slind's formalization as in the presented here idempotence of the computed unifiers is unnecessary to prove neither termination nor correctness of the specified unification algorithm. In contrast with our textbook style termination proof, which is based on the fact that the number of different variables occurring in the terms being unified decreases after each step of the unification algorithm (Section 3.1), the termination proof of the theory `Unify` is based on separated proofs of *non-nested* and *nested* termination conditions and the unification algorithm is specified taking as basis a specification of terms built by a binary combinator operator (`Comb`).

Recent Coq formalizations of unification algorithms were presented in [4] and [16]. The formalization in [4] is part of a library called `CoLoR`, and the most significant difference is that here substitutions are specified as finite maps from unrestricted variables into general terms, whereas in `CoLoR` they are specified as functions from type variables to a generalized term structure. In [16], Kothari and Caldwell presented a specification of a unification algorithm for equalities in the language of simple types. This kind of unification has direct applications in type inference algorithms. This unification algorithm is proved correct by showing that it satisfies four axioms: that the computed mgu is a unifier; that it is in fact a most general unifier; that its domain is restricted to the set of free variables in the input equational problem and that the theorem of existence of mgu's holds. In a later work, the same authors showed that three additional axioms, being one of them idempotence of mgu's, are also satisfied. Since simple types are built in a language of symbols for basic types and a unique binary operator symbol, ( $\rightarrow$ ), the current approach can be directly applied to the restricted language of simple types treated in [16]. An additional fact that makes the current formalization closer to the usual theory of unification as presented in well-known textbooks (e.g., [17, 2]), is the decision to specify terms as a data type built from variables and

the operator `app` that builds terms as an application of a function symbol (of a given arity) to a sequence of terms with the right length. In this way, substitutions were specified as a function from variables to terms and the construction of the homomorphic extension results straightforward.

Earlier related work in Coq includes [20], where an algorithm similar to Robinson’s one was extracted from a formalization that uses a generalized notion of terms, that uses binary constructors in the style of Manna and Waldinger, whose translation to the usual notation is not straightforward. More recently, in [7], a certified resolution algorithm for the propositional calculus is extracted from a Coq specification that requires unification of propositional expressions.

In [5] a formalization of a first-order unification algorithm is given. The main difference with the current formalization is that here one defines the application of a substitution to a term only by recursion on the term, and there the author defines the application of a substitution to a term in two ways: by recursion on the term (parallel application) and by recursion on the substitution (sequential application). Thus, for a given substitution and a given term, the application of the substitution to the term might result in different terms, depending on whether one follows the definition of the parallel application or the sequential application. However, both applications give the same result for idempotent substitutions. In other words, unlike the current approach, idempotence of the computed unifiers is necessary to prove the correctness of the specified unification algorithm.

In [21] a formalization of the correctness of an implementation of an  $O(n^2)$  run-time unification algorithm in ACL2 is presented. The specification is based on Corbin and Bidoit’s development [8] as presented in [2] in which terms are represented as directed acyclic graphs (DAGs). The merit of this formalization is that by taking care of an specific data structure such as DAGs for representing terms, the correctness proof results much more elaborated than the current one. But in the current paper, the focus is to have a natural mechanical proof of the existence of mgu’s, that is the strictly necessary in a formalization of the correctness of the Critical Pair Knuth-Bendix theorem. Although the representation of terms is sophisticated (via DAGs), the referred formalization diverges from textbooks proofs of correctness of the unification algorithm in which it is first-order restricted. In fact, instead representing second-order objects such as substitutions as functions from the domain of variables to the range of terms, they are specified as first-order association lists. In our approach, taking the decision to specify substitutions as functions allows us to apply all the theory of functions available in the higher-order proof assistant PVS, which makes our formalization very close to the ones available in textbooks.

As mentioned in the introduction, as part of the PVS *theory trs* presented in [11] there are formalizations of non-trivial results on rewriting, such as the well-known Knuth-Bendix Critical Pair Theorem, that requires the theorem of existence of mgu’s. The style of formalization of existence of mgu’s can be followed in order to verify the soundness and completeness of unification algorithms à la Robinson, as illustrated in [1] for a greedy algorithm. The proof methodology used to prove termination and soundness in the formalization of the theorem of existence of mgu’s is adapted in order to verify the correctness of unification algorithms as described in [1].

## 5 Conclusions and Future Work

A formalization developed in the language of the proof assistant PVS of the theorem of existence of mgu’s was presented. This formalization is close to textbooks proofs and was applied to present a complete formalization of the well-know Knuth-Bendix Critical Pair theorem. The methodology of proof can be directly applied in order to certify the correctness of first-order unification algorithms à la Robinson.

As future work, it is of great interest the extraction of certified unification algorithms alone or in several contexts of its possible applications such as the ones of first order resolution and of type inference.

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