

# Structural Resolution for Logic Programming

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submitted 29 April 2015; accepted 5 June 2015

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## Abstract

We introduce a *Three Tier Tree Calculus* ( $T^3C$ ) that defines in a systematic way three tiers of tree structures underlying proof search in logic programming. We use  $T^3C$  to define a new – structural – version of resolution for logic programming.

**KEYWORDS:** Structural resolution, term trees, rewriting trees, derivation trees.

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## 1 Introduction

As ICLP is celebrating the 200<sup>th</sup> anniversary of George Boole, we are reflecting on the fundamental “laws” underlying derivations in logic programming (LP), and making an attempt to formulate some fundamental principles for first-order proof search, analogous in generality to Boole’s “laws of thought” for propositional logic (Boole 1854).

Any such principles must be able to reflect two important features of first-order proof search in LP: its recursive and non-deterministic nature. For this they must satisfy two criteria: to be able to (a) model infinite structures and (b) reflect the non-determinism of proof search, relating “laws of infinity” with “laws of non-determinism” in LP.

**Example 1.1** *The program  $P_1$  inductively defines the set of natural numbers:*

0.  $\text{nat}(0) \leftarrow$
1.  $\text{nat}(s(X)) \leftarrow \text{nat}(X)$

*To answer the question “Does  $P_1 \vdash \text{nat}(s(X))$  hold?”, we first represent it as the LP query  $? \leftarrow \text{nat}(s(X))$  and then use SLD-resolution to resolve this query with  $P_1$ . The topmost clause selection strategy first resolves  $\text{nat}(s(X))$  with  $P_1$ ’s second clause (Clause 1), and then resolves the resulting term with  $P_1$ ’s first clause (Clause 0). This gives the derivation  $\text{nat}(s(X)) \rightarrow \text{nat}(X) \rightarrow \text{true}$ , which computes the solution  $\{X \mapsto 0\}$  in its last step. So one answer to our question is “Yes, provided  $X$  is 0.”*

Even for this simple inductive program, there will be clause selection strategies (or clause orderings) that will result in infinite SLD-derivations. If Clause 1 is repeatedly resolved against, the infinite computation will compute the first limit ordinal.

The least and greatest Herbrand model semantics (van Emden and Kowalski 1976; Lloyd 1988; van Emden and Abdallah 1985) captured very well the recursive (and corecursive!) nature of LP (thus satisfying our criterion (a)). For example, the least Herbrand model for  $P_1$  is an infinite set of finite terms  $\text{nat}(0)$ ,  $\text{nat}(s(0))$ ,  $\text{nat}(s(s(0)))$ ,  $\dots$ . The greatest complete Herbrand model for program  $P_1$  is the set containing all of the finite terms in the least Herbrand model for  $P_1$  together with the first limit ordinal  $\text{nat}(s(s(\dots)))$ . However, due to its declarative nature, the semantics does not reflect the operational non-deterministic nature of LP, and thus fails our criterion (b).

The operational semantics of LP has seen the introduction of a variety of tree structures reflecting the non-deterministic nature of proof search: *proof trees*, *SLD-derivation trees*, and *and-or-trees*, just to name a few. However, these do not adequately capture the infinite structures arising in LP proof search. It is well-known that SLD-derivations for any program  $P$  are sound and complete with respect to the least Herbrand model for  $P$  (Lloyd 1988), but this soundness and completeness depends crucially on termination of SLD-derivations, and termination is not always available in LP proof search. As a result, logical entailment is only semi-decidable in LP.

In one attempt to match the greatest complete Herbrand semantics for potentially non-terminating programs, an operational counterpart — called *computations at infinity* — was introduced in (Lloyd 1988; van Emden and Abdallah 1985). The operational semantics of a potentially nonterminating logic program  $P$  was then taken to be the set of all infinite ground terms computable by  $P$  at infinity. Computations at infinity better capture the computational behaviour of non-terminating logic programs, but infinite computations do not result in implementations. This observation suggests one more criterion: (c) our operational semantics must be able to provide an observational (constructive) approach to potential infinity and non-determinism of LP proof search, thus incorporating “laws of observability”.

Coinductive logic programming (CoLP) (Gupta et al. 2007; Simon et al. 2007) provides a method for terminating certain infinite SLD-derivations (thus satisfying our criteria (a) and (c)). This is based on the principle of coinduction, which is in turn based on the ability to finitely observe coinductive hypotheses and succeed when coinductive conclusions are reached. CoLP’s search for coinductive hypotheses and conclusions uses a fairly straightforward loop detection mechanism. It requires the programmer to supply annotations classifying every predicate as either inductive or coinductive. Then, for queries marked as coinductive, it observes finite fragments of SLD-derivations, checks them for unifying subgoals, and terminates when loops determined by such subgoals are found.

The loop detection mechanism of CoLP has three major limitations, all arising from the fact that it has relatively weak support for analysis of various proof-search strategies and term structures arising in LP proof search (and thus for our criterion (b)).

(1) It does not work well for cases of mixed induction-coinduction. For example, to coinductively define an infinite stream of Fibonacci numbers, we would need to include inductive clauses defining addition on natural numbers. Coinductive goals will be mixed with inductive subgoals. Closing such computations by simple loop detection is problematic.

(2) There are programs for which computations at infinity *produces* an infinite term, whereas CoLP fails to find unifiable loops.

Consider the following (coinductive) program  $P_2$  that has the single clause

0.  $\text{from}(X, \text{scons}(X, Y)) \leftarrow \text{from}(s(X), Y)$

Given the query  $? \leftarrow \text{from}(0, X)$ , and writing  $[-, -]$  as an abbreviation for the stream constructor  $\text{scons}$ , we have that the infinite term  $t' = \text{from}(0, [0, [s(0), [s(s(0)), \dots]]])$  is computable at infinity by  $P_2$  and is also contained in the greatest Herbrand model for  $P_2$ . However,  $P_2 \vdash \text{from}(0, X)$  cannot be proven using the unification-based loop detection technique of CoLP. Since the terms  $\text{from}(0, \text{scons}(0, X'))$ ,  $\text{from}(s(0), \text{scons}(s(0), X''))$ ,  $\text{from}(s(s(0)), \text{scons}(s(s(0)), X'''))$ , ... arising in the derivation for  $P_2$  and  $? \leftarrow \text{from}(0, X)$  will never unify, CoLP will never terminate.

(3) CoLP fails to reflect the fact that some infinite computations are not productive, i.e., do not produce an infinite term at infinity. The notion of productivity of corecursion is well studied in the semantics of other programming languages (Endrullis et al. 2010; Agda 2015; Coq 2015). For example, no matter how long an SLD-derivation for the following program  $P_3$  runs, it does not *produce* an infinite term, and the resulting computation is thus coinductively meaningless:

0.  $\text{bad}(X) \leftarrow \text{bad}(X)$

Somewhat misleadingly, CoLP's loop detection terminates with success for such programs, thus failing to guarantee coinductive construction of infinite terms (failing criterion (a)).

Is our quest for a theory of LP satisfying criteria (a), (b), and (c) hopeless? We take a step back and recollect that the semantics of first-order logic and recursive schemes offers one classical approach to formulating structural properties of potentially infinite first-order terms. Best summarised in “*Fundamental Properties of Infinite Trees*” (Courcelle 1983), the approach comes down to formulating some structural laws underlying first-order syntax. It starts with definition of a *tree language* as a (possibly infinite) set of sequences of natural numbers satisfying conditions of prefix-closedness and finite branching. Given a first-order signature  $\Sigma$  together with a countable set of variables  $Var$ , a first-order term tree is defined as a map from a tree language  $L$  to the set  $\Sigma \cup Var$ . Size of the domain of the map determines the size of the term tree. The “laws” are then given by imposing several structural properties: (i) in a given term tree, arities imposed by  $\Sigma$  must be reflected by the branching in the underlying tree language; (ii) variables have arity 0 and thus can only occur at leaves of the trees; and (iii) the operation of substitution is given by replacing leaf variables with term trees. A calculus for the operation can be formulated in terms of a suitable unification algorithm. We give formal definitions in Sections 2 and 3.

We extend this elegant theory of infinite trees to give an operational semantics of LP that satisfies criteria (a), (b), and (c). We borrow a few general principles from this theory. Structural properties of trees (given by arity and variable constraints) and operations on trees (substitutions) are defined by means of “structural laws” that hold for finite and infinite trees. This gives us constructive approach to infinity (cf. criteria (a) and (c)). It remains to find the right kind of structures to reflect the non-determinism of proof search in LP.

Given a logic program  $P$  and a term (tree)  $t$ , the first question we may ask is whether  $t$  *matches* any of  $P$ 's clauses. First-order term matching is a restricted form of unifica-

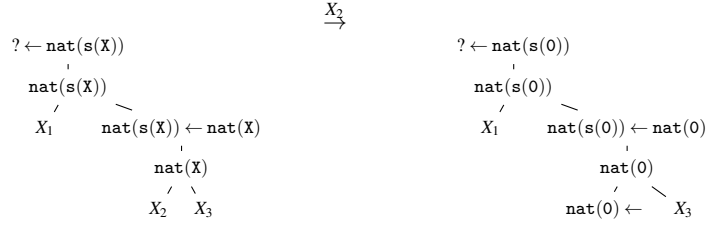


Fig. 1. The rewriting trees for  $P_1$  and  $? \leftarrow \text{nat}(\mathfrak{s}(X))$  and  $? \leftarrow \text{nat}(\mathfrak{s}(0))$ . The trees form a transition relative to the Tier 2 variable  $X_2$  (shown by  $\xrightarrow{X_2}$ ). The second tree is a successful proof for  $? \leftarrow \text{nat}(\mathfrak{s}(X))$ .

tion employed in (first-order) term rewriting systems (TRS) (Terese 2003) and — via pattern-matching — in functional programming. For our  $P$  and  $t$ , we may proceed with term matching steps recursively, mimicking an SLD-derivation in which unification is restricted to term matching. Consider the matching sequences for four different terms and the coinductive program  $P_2$  from above:

$$\begin{array}{cccc}
 \text{from}(0, X) & \text{from}(0, [0, X']) & \text{from}(0, [0, [\mathfrak{s}(0), X'']]) & \text{from}(0, [0, [\mathfrak{s}(0), [\mathfrak{s}(\mathfrak{s}(0)), X''']]]) \\
 \downarrow & \downarrow & \downarrow & \downarrow \\
 \text{from}(\mathfrak{s}(0), X') & \text{from}(\mathfrak{s}(0), [\mathfrak{s}(0), X'']) & \text{from}(\mathfrak{s}(0), [\mathfrak{s}(0), X''']) & \text{from}(\mathfrak{s}(0), [\mathfrak{s}(0), [\mathfrak{s}(\mathfrak{s}(0)), X'''']]) \\
 \downarrow & \downarrow & \downarrow & \downarrow \\
 & \text{from}(\mathfrak{s}(\mathfrak{s}(0)), X'') & \text{from}(\mathfrak{s}(\mathfrak{s}(0)), [\mathfrak{s}(\mathfrak{s}(0)), X''']) & \text{from}(\mathfrak{s}(\mathfrak{s}(0)), X''''') \\
 & & & \downarrow \\
 & & & \text{from}(\mathfrak{s}(\mathfrak{s}(\mathfrak{s}(0))), X''''')
 \end{array}$$

Let us call term matching sequences as above *rewriting trees*, to highlight their relation to TRS. The above sequences can already reveal some of the structural properties of the given logic program. If  $\Sigma_2$  is the signature of the program  $P_2$ , and if we denote all finite term trees that can be formed from this signature as  $\mathbf{Term}(\Sigma_2)$ , then a rewriting tree for  $P_2$  can be defined as a map from a given tree language  $L$  to  $\mathbf{Term}(\Sigma_2)$ . Since rewriting trees are built upon term trees, we may say that term trees give a first tier of tree structures, while the rewriting trees give a second tier of tree structures. To formulate suitable laws for the second tier, we need to refine our notion of rewriting trees.

Given a program  $P$  and a term  $t$ , we may additionally reflect *how many* clauses from  $P$  can be unified with  $t$ , and how many terms those clauses contain in their bodies. We thus introduce a new kind of “or-nodes” to track the matching clauses. If  $P$  has  $n$  clauses,  $t$  may potentially have up to  $n$  alternative matching sequences. When a clause  $i$  does not match a given term tree  $t$ , we may use a *Tier 2 variable* to denote the fact that, although  $t$  does not match clause  $i$  at the moment, a match may be found for some instantiation of  $t$ . Thus, for the program  $P_1$  above and the queries  $? \leftarrow \text{nat}(\mathfrak{s}(X))$  and  $? \leftarrow \text{nat}(\mathfrak{s}(0))$ , we will have the two rewriting trees of Figure 1. We note the alternating or-nodes (given by clauses) and and-nodes (given by terms from clause bodies) and Tier 2 variables.

Two kinds of laws are imposed on structure of rewriting trees:

- arity constraints: the arity of an and-node is the number of clauses in the program, and arity of and or-node is the number of terms in its clause body.
- variable constraints: variable leaves have arity 0, and run over the objects being defined (rewriting trees). Variables are the leaves in which substitution can take place.

In Figure 1, Tier 2 variable  $X_2$  is substituted by a one-node rewriting tree  $\text{nat}(0) \leftarrow$ . Such substitutions constitute the fundamental operation on Tier 2 trees, and give rise to a

calculus for Tier 2 given in terms of so-called rewriting tree transitions. Figure 1 shows a transition from a rewriting tree for  $? \leftarrow \text{nat}(s(X))$  to a rewriting tree for  $? \leftarrow \text{nat}(s(0))$  which corresponds to the SLD-derivation outlined in Example 1.1. Thus, a derivation is a sequence of tree transitions (given by the Tier 2 operation of substitution). We call this method *structural resolution*, or *S-resolution* for short. Its formal relation to TRS and type theory is given in (Fu and Komendantskaya 2015). Section 4 will introduce Tier 2 formally.

We note the remarkably precise analogy between structures and operations of Tier 1 and Tier 2. Rewriting trees can be finite or infinite. For programs  $P_1$  and  $P_2$ , any rewriting tree will be finite, but program  $P_3$  will give rise to infinite rewriting trees. Once again, our structural analysis is fully generic for finite and infinite tree structures at Tier 2, which fits our criterion (a). Rewriting trees perfectly reflect the “non-determinism laws” (criterion (b)), thanks to and-nodes and or-nodes keeping a structural account of all the search options. Finally, our structural analysis perfectly fits criterion (c). For productive programs like  $P_1$  and  $P_2$ , the length of a derivation may be infinite, however, each rewriting tree will necessarily be finite. This ensures observational approach to corecursion and productivity.

We complete the picture by introducing the third tier of trees reflecting different search strategies arising from substitution into different variables of Tier 2. Given the set  $\mathbf{Rew}(P)$  of all finite rewriting trees defined for program  $P$ , a derivation tree is given by a map from a tree language  $L$  to  $\mathbf{Rew}(P)$ . The arity of a given node in a derivation tree (itself given by a rewriting tree) is the number of Tier 2 variables in that rewriting tree. The construction of derivation trees is similar to the construction of SLD-derivation trees (as it accounts for all possible derivation strategies). The trees of Tier 3 are formally defined in Section 5.

The resulting *Three Tier Tree Calculus* ( $T^3C$ ) developed in this paper formalises the fundamental properties of trees arising in LP proof search. Apart from being theoretically pleasing, this new theory can actually deliver very practical results. The finiteness of rewriting trees comprising a possibly infinite derivation gives an important observational property for defining and semi-deciding (observational) productivity for corecursion in LP. This puts LP on par with other languages in terms of observational productivity and coinductive semantics (Endrullis et al. 2010; Agda 2015; Coq 2015). With a notion of productivity in hand for LP, we can ask for results showing inductive and coinductive soundness of derivations given by transitions among rewriting trees. The two pictures above give, respectively, a sound coinductive observation of a proof for  $t' = \text{from}(0, [0, [s(0), [s(s(0)), \dots]]])$  with respect to  $P_2$ , and a sound inductive derivation for  $\text{nat}(s(X))$  with respect to  $P_1$ . Our ongoing and future research based on  $T^3C$  will be further explained in Section 6.

## 2 Background: Tree Languages

Our notation for trees is a variant of that in, e.g., (Lloyd 1988; Courcelle 1983). Let  $\mathbb{N}^*$  denote the set of all finite words (i.e., sequences) over the set  $\mathbb{N}$  of natural numbers. The length of a word  $w \in \mathbb{N}^*$  is denoted by  $|w|$ . The empty word  $\varepsilon$  has length 0. We identify the natural number  $i$  and the word  $i$  of length 1. If  $w$  is a word of length  $l$ , then for each  $i \in \{1, \dots, l\}$ ,  $w_i$  is the  $i^{\text{th}}$  element of  $w$ . We may write  $w = w_1 \dots w_l$  to indicate that  $w$  is a word of length  $l$ . We use letters from the end of the alphabet, such  $u, v$ , and  $w$ , to denote words in  $\mathbb{N}^*$  of any length, and letters from the middle of the alphabet, such as  $i, j$ , and  $k$ , to denote words in  $\mathbb{N}^*$  of length 1 (i.e., individual natural numbers). The concatenation of



Fig. 2. The two figures on the left depict the finite and infinite tree languages  $\{\varepsilon, 0, 00, 01\}$  and  $\{\varepsilon, 0, 1, 10, 11, \dots\}$ . The two figures on the right depict the finite term tree  $\text{stream}(\text{scons}(X, Y))$  and the infinite term tree  $\text{scons}(0, \text{scons}(0, \dots))$ , both over  $\Sigma_1$ .

words  $w$  and  $u$  is denoted  $wu$ . The word  $v$  is a *prefix* of  $w$  if there exists a word  $u$  such that  $w = vu$ , and a *proper prefix* of  $w$  if  $u \neq \varepsilon$ .

**Definition 2.1** A set  $L \subseteq \mathbb{N}^*$  is a (finitely branching) tree language if the following conditions are satisfied:

- For all  $w \in \mathbb{N}^*$  and all  $i, j \in \mathbb{N}$ , if  $wj \in L$  then  $w \in L$  and, for all  $i < j$ ,  $wi \in L$ .
- For all  $w \in L$ , the set of all  $i \in \mathbb{N}$  such that  $wi \in L$  is finite.

A tree language  $L$  is *finite* if it is a finite subset of  $\mathbb{N}^*$ , and *infinite* otherwise. Examples of finite and infinite tree languages are given in Figure 2. We may call a word  $w \in L$  a *node* of  $L$ . If  $w = w_1w_2\dots w_l$ , then a node  $w_1w_2\dots w_k$  for  $k < l$  is an *ancestor* of  $w$ . The node  $w$  is the *parent* of  $wi$ , and nodes  $wi$  for  $i \in \mathbb{N}$  are *children* of  $w$ . A *branch* of a tree language  $L$  is a subset  $L'$  of  $L$  such that, for all  $w, v \in L'$ ,  $w$  is an ancestor of  $v$  or  $v$  is an ancestor of  $w$ . If  $L$  is a tree language and  $w$  is a node of  $L$ , the *subtree of  $L$  at  $w$*  is  $L \setminus w = \{v \mid wv \in L\}$ .

We can now define our three-tier calculus  $T^3C$ .

### 3 Tier 1: Term Trees

In this section, we introduce Tier 1 of  $T^3C$ , highlighting the structural properties of its objects (arity, branching, variables), the operation of first-order substitution, and the relevant calculus given by unification.

#### 3.1 Tier 1 structural properties: Signature as codomain, arity, and variables

The trees of  $T^3C$ 's first tier are term trees over a (first-order) signature. A *signature*  $\Sigma$  is a non-empty set of *function symbols*, each with an associated *arity*. The arity of  $f \in \Sigma$  is denoted  $\text{arity}(f)$ . For example,  $\Sigma_1 = \{\text{stream}, \text{scons}, 0\}$ , with  $\text{arity}(\text{scons}) = 2$ ,  $\text{arity}(\text{stream}) = 1$ , and  $\text{arity}(0) = 0$ , is a signature. To define term trees over  $\Sigma$ , we also need a countably infinite set  $\text{Var}$  of *variables* disjoint from  $\Sigma$ , each with arity 0. We use capital letters from the end of the alphabet, such as  $X, Y$ , and  $Z$ , to denote variables in  $\text{Var}$ .

**Definition 3.1** Let  $L$  be a non-empty tree language and let  $\Sigma$  be a signature. A term tree over  $\Sigma$  is a function  $t : L \rightarrow \Sigma \cup \text{Var}$  such that, for all  $w \in L$ ,  $\text{arity}(t(w)) = |\{i \mid wi \in L\}|$ .

Structural properties of tree languages extend to term trees. For example, a term tree  $t : L \rightarrow \Sigma \cup \text{Var}$  has depth  $\text{depth}(t) = \max\{|w| \mid w \in L\}$ . The subtree of  $t$  at node  $w$  is given by  $t' : (L \setminus w) \rightarrow \Sigma \cup \text{Var}$ , where  $t'(v) = t(wv)$  for each  $v \in L \setminus w$ .

Term trees are finite or infinite according as their domains are finite or infinite. Term trees over  $\Sigma$  may be infinite even if  $\Sigma$  is finite. Figure 2 shows the finite and infinite term trees  $\text{stream}(\text{scons}(X, Y))$  and  $\text{scons}(0, \text{scons}(0, \dots))$  over  $\Sigma_1$ . The set of finite (infinite) term trees over a signature  $\Sigma$  is denoted  $\mathbf{Term}(\Sigma)$  ( $\mathbf{Term}^\infty(\Sigma)$ ). The set of *all* (i.e., finite

and infinite) term trees over  $\Sigma$  is denoted by  $\mathbf{Term}^\omega(\Sigma)$ . Term trees with no occurrences of variables are *ground*. We write  $\mathbf{GTerm}(\Sigma)$  ( $\mathbf{GTerm}^\infty(\Sigma)$ ,  $\mathbf{GTerm}^\omega(\Sigma)$ ) for the set of finite (infinite, *all*) ground term trees over  $\Sigma$ .  $\mathbf{GTerm}(\Sigma)$  is also known as the Herbrand base for  $\Sigma$ , and  $\mathbf{GTerm}^\omega(\Sigma)$  is known as the complete Herbrand base for  $\Sigma$ , in the literature (Lloyd 1988). Both  $\mathbf{GTerm}(\Sigma)$  and  $\mathbf{GTerm}^\omega(\Sigma)$  are used to define the Herbrand model and complete Herbrand model (declarative) semantics of LP (Kowalski 1974; Lloyd 1988). Additionally,  $\mathbf{GTerm}^\omega(\Sigma)$  is used to give an operational semantics to SLD-computations at infinity in (Lloyd 1988; van Emden and Abdallah 1985).

### 3.2 Tier 1 operation: First-order substitution

A *substitution* of term trees over  $\Sigma$  is a total function  $\sigma : \mathit{Var} \rightarrow \mathbf{Term}(\Sigma)$ . We write  $id$  for the identity substitution. If  $\sigma$  has finite support — i.e., if  $|\{X \in \mathit{Var} \mid \sigma(X) \neq X\}| \in \mathbb{N}$  — and if  $\sigma$  maps the variables  $X_i$  to term trees  $t_i$ , respectively, and is the identity on all other variables, then we may write  $\sigma$  as  $\{X_1 \mapsto t_1, \dots, X_n \mapsto t_n\}$ . The set of all substitutions over a signature  $\Sigma$  is  $\mathbf{Subst}(\Sigma)$ . Substitutions are extended from variables to term trees homomorphically: if  $t \in \mathbf{Term}(\Sigma)$  and  $\sigma \in \mathbf{Subst}(\Sigma)$ , then the *application*  $\sigma(t)$  is defined by  $(\sigma(t))(w) = t(w)$  if  $t(w) \notin \mathit{Var}$ , and  $(\sigma(t))(w) = (\sigma(X))(v)$  if  $w = uv$ ,  $t(u) = X$ , and  $X \in \mathit{Var}$ . Composition of substitutions is denoted by juxtaposition, so  $\sigma_2\sigma_1(t)$  is  $\sigma_2(\sigma_1(t))$ . Since composition is associative, we write  $\sigma_3\sigma_2\sigma_1$  rather than  $(\sigma_3\sigma_2)\sigma_1$  or  $\sigma_3(\sigma_2\sigma_1)$ .

### 3.3 Tier 1 calculus: Unification

A substitution  $\sigma$  over  $\Sigma$  is a *unifier* for term trees  $t$  and  $u$  over  $\Sigma$  if  $\sigma(t) = \sigma(u)$ , and a *matcher* for  $t$  against  $u$  if  $\sigma(t) = u$ . A substitution  $\sigma_1$  is *more general* than a substitution  $\sigma_2$ , denoted  $\sigma_1 \leq \sigma_2$ , if there exists a substitution  $\sigma$  such that  $\sigma\sigma_1(X) = \sigma_2(X)$  for every  $X \in \mathit{Var}$ . A substitution  $\sigma$  is a *most general unifier* (*mgu*) for  $t$  and  $u$  if it is a unifier for  $t$  and  $u$ , and is more general than any (other) such unifier. A *most general matcher* (*mgm*) is defined analogously. Both mgms and mgus are unique up to variable renaming.

We write  $t \sim_\sigma u$  if  $\sigma$  is a mgu for  $t$  and  $u$ , and  $t \prec_\sigma u$  if  $\sigma$  is a mgm for  $t$  against  $u$ . Our notation is reasonable: unification is reflexive, symmetric, and transitive, but matching is reflexive and transitive only. Mgms and mgus can be computed using Robinson's seminal unification algorithm (see, e.g., (Lloyd 1988; Pfenning 2007)). Any standard unification algorithm (possibly represented by system of sequent-like rules (Pfenning 2007; Fu and Komendantskaya 2015)) can be seen as the calculus of Tier 1. Additional details about unification and matching can be found in, e.g., (Baader and Snyder 2001).

## 4 Tier 2: Rewriting Trees

In this section, we introduce Tier 2 of  $T^3C$ , highlighting the structural properties of rewriting trees: codomains comprising term trees and clauses, suitable notions of arity, the operation of Tier 2 substitution, and the relevant calculus given by rewriting tree transitions.

### 4.1 Tier 2 structural properties: Terms and clauses as codomain, arity, and variables

In LP, a *clause*  $C$  over a signature  $\Sigma$  is a pair  $(A, [B_0, \dots, B_n])$ , where  $A \in \mathbf{Term}(\Sigma)$  and  $[B_0, \dots, B_n]$  is a list of term trees in  $\mathbf{Term}(\Sigma)$ . Such a clause  $C$  is usually written as  $A \leftarrow B_0, \dots, B_n$ . The *head*  $A$  of  $C$  is denoted  $head(C)$  and the *body*  $B_0, \dots, B_n$  of  $C$  is denoted  $body(C)$ . In  $T^3C$ , a clause over  $\Sigma$  is naturally represented as a total function (also called

$C$ ) from a finite tree language  $L$  of depth 1 to  $\mathbf{Term}(\Sigma)$  such that  $C(\varepsilon) = \mathit{head}(C)$ , and if  $\mathit{body}(C)$  is  $B_0, \dots, B_n$  then, for each  $i \in L$ ,  $C(i) = B_i$ . The set of all clauses over  $\Sigma$  is denoted by  $\mathbf{Clause}(\Sigma)$ . A *goal clause*  $G$  over  $\Sigma$  is a clause  $? \leftarrow B_0, \dots, B_n$  over  $\Sigma \cup \{?\}$ . Here,  $?$  is a specified symbol not occurring in  $\Sigma \cup \mathit{Var}$ , and  $B_0, \dots, B_n$  are term trees in  $\mathbf{Term}(\Sigma)$ . The goal clause  $? \leftarrow$  is called the *empty goal clause* over  $\Sigma$ . We consider every goal clause over  $\Sigma$  to be a clause over  $\Sigma$ . The *arity* of a clause  $A \leftarrow B_0, \dots, B_n$  is  $n + 1$ . The symbol  $\mathit{head}(C)(\varepsilon)$  is the *predicate* of  $C$ .

A *logic program* over  $\Sigma$  is a total function from a set  $\{0, 1, \dots, n\} \subseteq \mathbb{N}$  to the set of non-goal clauses over  $\Sigma$ . The set of all logic programs over  $\Sigma$  is denoted  $\mathbf{LP}(\Sigma)$ . The *arity* of  $P \in \mathbf{LP}(\Sigma)$  is the number  $|\mathit{dom}(P)|$  of clauses in  $P$ .

We extend substitutions from variables to clauses and programs homomorphically. The variables of a clause  $C$  can be renamed with “fresh” variables — i.e., with variables that do not appear elsewhere in the current context — to get a new  $\alpha$ -equivalent clause that can be used interchangeably with  $C$ . We assume variables have been thus *renamed apart* whenever convenient. Renaming apart avoids circular (non-terminating) cases of unification and matching in LP. Under renaming, we can always assume that a mgm or mgu of a clause and a term is *idempotent*, i.e., that  $\sigma\sigma = \sigma$ .

We now define the trees of Tier 2. Rewriting trees allow us to simultaneously track all matching sequences appearing in an LP derivation, and thus to see relationships between them. Since rewriting trees use only matching in their computation steps, they capture theorem proving (i.e., computations holding for *all* compatible term trees). By contrast, the Tier 3 derivation trees defined in Section 5 use full unification, and thus capture problem solving (i.e., computations holding only for *certain* compatible term trees).

We distinguish two kinds of nodes in rewriting trees: *and-nodes* capturing terms coming from clause bodies, and *or-nodes* capturing the idea that every term tree can in principle match several clause heads. We also introduce or-node variables to signify the possibility of unification when matching of a term tree against a program clause fails.

**Definition 4.1** *Let  $V_R$  be a countably infinite set of variables disjoint from  $\mathit{Var}$ . If  $P \in \mathbf{LP}(\Sigma)$ ,  $C \in \mathbf{Clause}(\Sigma)$ , and  $\sigma \in \mathbf{Subst}(\Sigma)$  is idempotent, then  $\mathit{rew}(P, C, \sigma)$  is the function  $T : \mathit{dom}(T) \rightarrow \mathbf{Term}(\Sigma) \cup \mathbf{Clause}(\Sigma) \cup V_R$ , where  $\mathit{dom}(T)$  is a non-empty tree language, satisfying the following conditions:*

1.  $T(\varepsilon) = \sigma(C) \in \mathbf{Clause}(\Sigma)$  and, for all  $i \in \mathit{dom}(C) \setminus \{\varepsilon\}$ ,  $T(i) = \sigma(C(i))$ .
2. For  $w \in \mathit{dom}(T)$  with  $|w|$  even and  $|w| > 0$ ,  $T(w) \in \mathbf{Clause}(\Sigma) \cup V_R$ . Moreover,
  - if  $T(w) \in V_R$ , then  $\{j \mid wj \in \mathit{dom}(T)\} = \emptyset$ , and
  - if  $T(w) = B \in \mathbf{Clause}(\Sigma)$ , then there exists a clause  $P(i)$  and an mgm  $\theta$  for  $P(i)$  against  $\mathit{head}(B)$ . Moreover, for every  $j \in \mathit{dom}(P(i)) \setminus \{\varepsilon\}$ ,  $wj \in \mathit{dom}(T)$  and  $T(wj) = \sigma(\theta(P(i)(j)))$ .
3. For  $w \in \mathit{dom}(T)$  with  $|w|$  odd,  $T(w) \in \mathbf{Term}(\Sigma)$ . Moreover, for every  $i \in \mathit{dom}(P)$ , we have
  - $wi \in \mathit{dom}(T)$ , and
  - $T(wi) = \begin{cases} \sigma(\theta(P(i))) & \text{if } \mathit{head}(P(i)) \prec_{\theta} T(w) \text{ and} \\ \text{a fresh } X \in V_R & \text{otherwise} \end{cases}$
4. No other words are in  $\mathit{dom}(T)$ .

A node  $T(w)$  of  $\mathit{rew}(P, C, \sigma)$  is an *or-node* if  $|w|$  is even and an *and-node* if  $|w|$  is odd. The



node  $T(\varepsilon)$  is the root of  $\text{rew}(P, C, \sigma)$ . If  $P \in \mathbf{LP}(\Sigma)$ , then  $T$  is a rewriting tree for  $P$  if it is either the empty tree or  $\text{rew}(P, C, \sigma)$  for some  $C \in \mathbf{Clause}(\Sigma)$  and  $\sigma \in \mathbf{Subst}(\Sigma)$ .

The arity of a node  $T(w)$  in  $T = \text{rew}(P, C, \sigma)$  is  $\text{arity}(P)$  if  $T(w) \in \mathbf{Term}(\Sigma)$ ,  $\text{arity}(C)$  if  $T(w) \in \mathbf{Clause}(\Sigma)$ , and 0 if  $T(w) \in V_R$ . The role of the parameter  $\sigma$  in the definition of  $\text{rew}$  will become clear when we discuss the notion of substitution for Tier 2. For now, we may think of  $\sigma$  as the identity substitution.

**Example 4.1** The rewriting trees  $\text{rew}(P_1, ? \leftarrow \text{nat}(s(X)), id)$  and  $\text{rew}(P_1, ? \leftarrow \text{nat}(s(0)), id)$  are shown in Figure 1.

A rewriting tree for a program  $P$  is finite or infinite according as its domain is finite or infinite. We write  $\mathbf{Rew}(P)$  for the set of finite rewriting trees for  $P$ ,  $\mathbf{Rew}^\infty(P)$  for the set of infinite rewriting trees for  $P$ , and  $\mathbf{Rew}^{\text{all}}(P)$  for the set of all (finite and infinite) rewriting trees for  $P$ . In (Komendantskaya et al. 2014), a logic program  $P$  is called (observationally) productive, if each rewriting tree constructed for it is in  $\mathbf{Rew}(P)$ . Programs  $P_1$  and  $P_2$  are productive in this sense, whereas program  $P_3$  is not. In future work, we will introduce methods that semi-decide observational productivity.

#### 4.2 Tier 2 operation: Substitution of rewriting trees for Tier 2 variables

With rewriting trees as the objects of Tier 2 and a suitable notion of a Tier 2 variable, we can replay Tier 1 substitution at Tier 2 by defining Tier 2 substitution to be the replacement of Tier 2 variables by rewriting trees. However, in light of the structural dependency of rewriting trees on term trees in Definition 4.1, we must also incorporate first-order substitution into Tier 2 substitution. Exactly how this is done is reflected in the next definition.

**Definition 4.2** Let  $P \in \mathbf{LP}(\Sigma)$ ,  $C \in \mathbf{Clause}(\Sigma)$ ,  $\sigma, \sigma' \in \mathbf{Subst}(\Sigma)$  idempotent, and  $T = \text{rew}(P, C, \sigma)$ . Then the rewriting tree  $\sigma'(T)$  is defined as follows:

- for every  $w \in \text{dom}(T)$  such that  $T(w)$  is an and-node or non-variable or-node,  $(\sigma'(T))(w) = \sigma'(T(w))$ .
- for every  $w_i \in \text{dom}(T)$  such that  $T(w_i) \in V_R$ , if  $\theta$  is an mgm of  $\text{head}(P(i))$  against  $\sigma'(T)(w)$ , then  $(\sigma'(T))(wiv) = \text{rew}(P, \theta(P(i)), \sigma'\sigma)(v)$ . (Note  $v = \varepsilon$  is possible.) If no mgm of  $\text{head}(P(i))$  against  $\sigma'(T)(w)$  exists, then  $(\sigma'(T))(w_i) = T(w_i)$ .

Both items in the above definition are important in order to make sure that, given a rewriting tree  $T$  and a first-order substitution  $\sigma$ ,  $\sigma(T)$  satisfies Definition 4.1.

**Example 4.2** Consider the first rewriting tree  $T$  of Figure 1. Given first-order substitution  $\sigma = \{X \mapsto 0\}$ , the second tree of that Figure gives  $\sigma(T)$ . Note that Tier 2 variable  $X_2$  is substituted by the one-node rewriting tree  $\text{nat}(0) \leftarrow$  as a result. In addition, all occurrences of the first-order variable  $X$  in  $T$  are substituted by 0 in  $\sigma(T)$ .

Drawing from Examples 4.1 and 4.2, we would ideally like to formally connect the definition of a rewriting tree and Tier 2 substitution, and say that, given  $T = \text{rew}(P, C, id)$  and a first-order substitution  $\sigma$ ,  $\sigma(T) = \text{rew}(P, \sigma(C), id)$ . However, this does not hold in general, as was also noticed in (Komendantskaya et al. 2014). Given a clause  $C = (t \leftarrow t_1, \dots, t_n)$ , we say a variable  $X$  is *existential* if it occurs in some  $t_i$  but not in  $t$ . The presence of existential variables shows why the third parameter in definition of  $\text{rew}$  is crucial:

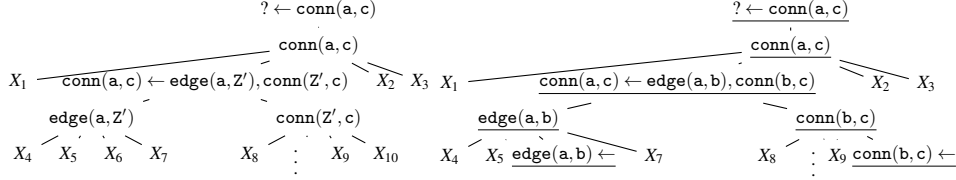


Fig. 3. The infinite rewriting trees  $T$  and  $T'$  for the program  $P_4$  of Example 4.3, the clause  $\text{conn}(a, c)$ , and the substitutions  $id$  and  $\{Z' \mapsto b\}$ , respectively.  $T$  offers no proof that  $P_4$  logically entails  $\text{conn}(a, c)$ , but the underlined steps in  $T'$  comprise precisely such a proof. The figure also illustrates a transition from  $T$  to  $T'$  relative to variable  $X_6$ .

**Example 4.3** *The graph connectivity program  $P_4$  is given by*

0.  $\text{conn}(X, X) \leftarrow$
1.  $\text{conn}(X, Y) \leftarrow \text{edge}(X, Z), \text{conn}(Z, Y)$
2.  $\text{edge}(a, b) \leftarrow$
3.  $\text{conn}(b, c) \leftarrow$

Figure 3 shows rewriting trees  $T = \text{rew}(P_4, C, id)$  and  $T' = \text{rew}(P_4, C, \theta)$ , where  $C = ? \leftarrow \text{conn}(a, c)$ , and  $\theta = \{Z' \mapsto b\}$ . Note that  $\theta(T) = T'$  but  $\text{rew}(P_4, \theta(C), id) \neq T'$ . This happens because Clause 1 contains an existential variable  $Z$  in its body, and construction of  $\text{rew}(P_4, \theta(C), id)$  fails to apply the substitution  $\theta$  down the tree.

Given  $T = \text{rew}(P, C, \sigma)$ , for  $T' = \theta(T) = \text{rew}(P, C, \theta\sigma)$  to hold, we must make sure that the procedure of renaming variables apart used implicitly when computing mgms during the rewriting tree construction is tuned in such a way that existential variables contained in the domain of  $\theta$  are still in correspondence with the existential variables in  $\text{rew}(P, C, \theta\sigma)$ . We achieve this by introducing a new renaming apart convention to supplement Definition 4.1. Given a program  $P$  and a clause  $P(i)$  with distinct existential variables  $Z_1, \dots, Z_n \in \text{Var}$ , we impose an additional condition on the standard *renaming apart* procedure. During the construction of  $T = \text{rew}(P, C, \sigma)$ , when an and-node  $T(w)$  is matched with  $\text{head}(P(i))$  via  $\theta$  in order to form  $T(wi) = \theta(P(i))$ ,  $P(i)$ 's existential variables  $Z_1, \dots, Z_n$  must be renamed apart as follows:

- We partition  $\text{Var}$  into two disjoint sets called  $V_U$  and  $V_E$ . The set  $V_E$  is used to rename existential variables apart, while  $V_U$  is used to (re)name all other variables.
- Moreover, when computing an mgm  $\theta$  for  $T(w)$  and  $(P(i))$ , every existential variable  $Z_k$  from  $Z_1, \dots, Z_n$  is renamed apart from variables of  $T$  using the following indexing convention:  $Z_k \mapsto E_{wi}^k$ , with  $E_{wi}^k \in V_E$ .

When writing  $T(wi) = \theta(P(i))$  we assume that the above renaming convention is already accounted for by  $\theta$ . This ensures that the existential variables will be uniquely determined and synchronized for every two nodes  $T(w)$  and  $T'(w)$  in  $T = \text{rew}(P, C, \sigma)$  and  $T' = \text{rew}(P, C, \theta\sigma)$ . Subject to this renaming convention, the following theorem holds.

**Theorem 4.1** *Let  $P \in \text{LP}(\Sigma)$ ,  $C \in \text{Clause}(\Sigma)$ , and  $\theta, \sigma \in \text{Subst}(\Sigma)$ . Then  $\theta(\text{rew}(P, C, \sigma)) = \text{rew}(P, C, \theta\sigma)$ .*

*Proof.* Let  $T = \text{rew}(P, C, \sigma)$ , and let  $T' = \text{rew}(P, C, \theta\sigma)$ . We need to prove that  $\theta(T) = T'$ .

The proof proceeds by induction on the length of the tree  $T$  and by cases on the types of nodes in  $T$  and  $\theta(T)$ .

– If  $T(w)$  and  $\theta(T(w))$  are non-variable or-nodes (including the case  $T(\varepsilon)$ ), then, by Definition 4.2,  $\theta(T)(w) = \theta(T(w)) = \theta\sigma(C^*)$ , where  $C^*$  is either  $C$  (i.e., it is a root node) or some  $P(i) \in P$ . But, by Definition 4.1,  $T'(w) = \theta\sigma(C^*)$ . (Here, the synchronisation of renamed existential variables is essential, as described.)

– If  $T(w)$  and  $\theta(T(w))$  are and-nodes, then the argument is similar.

– If  $T(wi)$  is a variable or-node, then, by Definition 4.2, two cases are possible:

(1) If no mgm for  $\theta(T(w))$  and  $head(P(i))$  exists, then  $\theta(T)(w) = \theta(T(w))$ . But then no mgm for  $T'(w)$  and  $head(P(i))$  exists either, so  $T'(w) = \theta(T(w))$ .

(2) If the mgm for  $\theta(T(w))$  and  $head(P(i))$  exists, then by Definition 4.2,  $\theta(T)(wi) = \text{rew}(P, \theta'(P(i)), \theta\sigma)(\varepsilon)$ , where  $\theta'$  is the mgm of  $\theta(T(w))$  and  $head(P(i))$ . The rest of the proof proceeds by induction on the depth of  $\text{rew}(P, \theta'(P(i)), \theta\sigma)$ .

Base case. For the root  $\theta(T)(wi) = \text{rew}(P, \theta'(P(i)), \theta\sigma)(\varepsilon)$ , by Definition 4.1 we have that  $\text{rew}(P, \theta'(P(i)), \theta\sigma)(\varepsilon) = (\theta\sigma)(\theta'(P(i)))$ . On the other hand, Definition 4.1 also gives that  $T'(wi) = (\theta\sigma)(\theta''(P(i)))$ , where  $\theta''$  is the mgm of  $T'(w)$  and  $head(P(i))$ . Since  $T'(w) = (\theta(T))(w)$  by the earlier argument for and-nodes,  $\theta'$  and  $\theta''$  are mgms of equal term trees and  $head(P(i))$ , so  $\theta' = \theta''$ . Then  $T'(wi) = (\theta(T))(wi)$ , as desired.

Inductive case. We need only consider the situation when  $T(wivj)$  is undefined, but  $(\theta(T))(wivj)$  is defined. By Definition 4.2,  $\theta(T)(wivj) = \text{rew}(P, \theta'(P(i)), \theta\sigma)(vj)$ . This node can be either an and-node, a variable or-node, or a non-variable or-node. The first two cases are simple; we spell out the latter, more complex case only.

If  $\theta(T)(wivj)$  is a non-variable or-node then, by Definition 4.1, it must be  $(\theta\sigma)(\theta^*P(j))$ , where  $\theta^*$  is the mgm of  $\theta(T)(wiv)$  and  $head(P(j))$ . On the other hand, Definition 4.1 also gives that  $T'(wivj) = (\theta\sigma)(\theta^{**}(P(j)))$ , where  $\theta^{**}$  is the mgm of  $T'(wiv)$  and  $head(P(j))$ . Since  $T'(wiv) = (\theta(T))(wiv)$  by the induction hypothesis,  $\theta^*$  and  $\theta^{**}$  are mgms of equal term trees and  $head(P(j))$ , so  $\theta^* = \theta^{**}$ . Thus  $T'(wivj) = (\theta(T))(wivj)$ , as desired.  $\square$

### 4.3 Tier 2 calculus: Rewriting tree transitions

The operation of Tier 2 substitution is all we need to define transitions among rewriting trees. Let  $P \in \mathbf{LP}(\Sigma)$  and  $t \in \mathbf{Term}(\Sigma)$ . If  $head(P(i)) \sim_\sigma t$ , then  $\sigma$  is the *resolvent* of  $P(i)$  and  $t$ . If no such  $\sigma$  exists then  $P(i)$  and  $t$  have *null resolvent*. A non-null resolvent is an *internal resolvent* if it is an mgm of  $P(i)$  against  $t$ , and it is an *external resolvent* otherwise.

**Definition 4.3** Let  $P \in \mathbf{LP}(\Sigma)$  and  $T = \text{rew}(P, C, \sigma') \in \mathbf{Rew}^\omega(P)$ . If  $X = T(wi) \in V_R$ , then the rewriting tree  $T_X$  is defined as follows. If the external resolvent  $\sigma$  for  $P(i)$  and  $T(w)$  is null, then  $T_X$  is the empty tree. If  $\sigma$  is non-null, then  $T_X = \text{rew}(P, C, \sigma\sigma')$ .

If  $T \in \mathbf{Rew}^\omega(\Sigma)$  and  $X \in V_R$ , then the computation of  $T_X$  from  $T$  is denoted  $\text{Trans}(P, T, X) = T_X$ . If the other parameters are clear we simply write  $T \rightarrow T_X$ . The operation  $T \rightarrow T_X$  is a *tree transition* for  $P$  and  $C$ . A *tree transition* for  $P \in \mathbf{LP}(\Sigma)$  is a tree transition for  $P$  and some  $C \in \mathbf{Clause}(\Sigma)$ . A (finite or infinite) sequence  $T = \text{rew}(P, C, id) \rightarrow T_1 \rightarrow T_2 \rightarrow \dots$  of tree transitions for  $P$  is a *derivation* for  $P$  and  $C$ . Each rewriting tree  $T_i$  in the derivation is given by  $\text{rew}(P, C, \sigma_i \dots \sigma_2 \sigma_1)$ , where  $\sigma_1, \sigma_2 \dots$  is the sequence of external resolvents associated with the derivation. When we want to contrast the above derivations with SLD-derivations, we call them S-derivations, or derivations by *structural resolution*.

**Example 4.4** *Tree transitions for  $P_1$  and  $P_4$  are shown in Figures 1 and 3, respectively.*

It is our current work to prove that S-derivations are sound and complete relative to declarative semantics of LP; see also (Fu and Komendantskaya 2015) for a comparative study of the operational properties of S-derivations and SLD-derivations.

### 5 Tier 3: Derivation Trees

While the rewriting trees of Tier 2 capture transitions between Tier 1 term trees that depend on matching, the derivation trees of Tier 3 capture transitions between Tier 2 rewriting trees that depend on unification. Derivation trees thus allow us to simultaneously track all unification sequences appearing in an LP derivation. The *arity* of a rewriting tree  $T$ , denoted  $arity(T)$ , is the cardinality of the set  $indices(T)$  of indices of variables from  $V_R$  in  $T$ . There is always a bijection  $pos$  from  $indices(T)$  to the (possibly infinite) set  $arity(T)$ .

**Definition 5.1** *If  $P \in \mathbf{LP}(\Sigma)$  and  $C \in \mathbf{Clause}(\Sigma)$ , the derivation tree  $der(P, C)$  is the function  $D : dom(D) \rightarrow \mathbf{Rew}^\omega(P)$  such that  $D(\varepsilon) = \mathbf{rew}(P, C, id)$ , and if  $w \in dom(D)$ ,  $i \in arity(D(w))$ , and  $i = pos(k)$ , then  $wi \in dom(D)$  and  $D(wi)$  is  $\mathbf{Trans}(P, D(w), X_k)$ .*

For  $P \in \mathbf{LP}(\Sigma)$  and  $C \in \mathbf{Clause}(\Sigma)$ , the derivation tree  $der(P, C)$  is unique up to renaming. If  $P \in \mathbf{LP}(\Sigma)$ , then  $D$  is a *derivation tree for  $P$*  if it is  $der(P, C)$  for some  $C \in \mathbf{Clause}(\Sigma)$ . A derivation tree is finite or infinite according as its domain is finite or infinite. Inductive programs like  $P_1$  and coinductive programs like  $P_2$  will have infinite derivation trees, so construction of the full derivation trees for such programs is infeasible. Nevertheless, finite initial fragments of derivation trees may be used to make coinductive observations about various routes for proof search. We are currently exploring this research direction.

### 6 Conclusions and Future Work

This paper gives the first fully formal exposition of the Three Tier Tree Calculus  $T^3C$  for S-resolution, relating “laws of infinity”, “laws of non-determinism”, and “laws of observability” of proof search in LP in a uniform, conceptual way. Implementation of derivations by S-resolution is available (Komendantskaya et al. 2015).

The structural approach to LP put forth in this paper relies on the syntactic structure of programs rather than on their (operational, declarative, or other) semantics. In essence, it presents an LP analogue of the kinds of reasoning that types and pattern matching support in interactive theorem proving (ITP) (Agda 2015; Coq 2015). Further study of this analogy is an interesting direction for future research.

Our next steps will be to formulate a theory of universal and observational productivity of (co)recursion in LP, and to supply  $T^3C$  with semi-decidable algorithms for ensuring program productivity (akin to guardedness checks in ITP). Formally proving that S-resolution is both inductively and coinductively sound is another of our current goals.

Since LP and similar automated proof search methods underlie type inference in ITP and other programming languages, S-resolution also has the potential to impact the design and implementation of typeful programming languages. This is another research direction we are currently pursuing.

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