# LEAN-aided verification of datalog reasoning results

Johannes Tantow

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### 1 Introduction

## 2 Preliminaries

## 2.1 Datalog

Syntactically datalog bears many similarities to first-order logic and may be viewed as a fragment of it, but the semantics are more specialized. In order to define the syntax we will introduce some definitions from first-order logic.

Firstly, we consider in general three countably infinite sets R, that consists of relation symbols, C, that consists of constants, and V, that consists of variables. In order to differentiate between constants and variables we require that  $V \cap C = \emptyset$ . Each relation symbol has an associated arity  $ar: R \to \mathbb{N}$ . As we will only consider finite programs and databases, there will always be at most finitely many relation symbols, constants or variables in usage, but by requiring these sets to be countably infinite we make sure that we always have a sufficient amount

A *term* is either a constant or variable. In contrast to first-order logic or logic programming, we do not allow function symbols in datalog, but there are extensions of datalog that allow using some function symbols like addition or multiplication as terms as well.

An *atom* is of the form  $A(t_1,...,t_{ar(A)})$  where A is a relation symbol and  $t_1,...,t_{ar(A)}$  are terms. The atom variables of  $A(t_1,...,t_{ar(A)})$  are the set of those  $t_i$  which are variables. A *ground atom* is an atom where the atom variables are the empty set, i.e. every term is a constant.

A rule is a expression of the form  $H \leftarrow B_1 \wedge ... \wedge B_n$ , where H and all  $B_i$  are atoms. H is called the head of the rule and  $\{B_1, ..., B_n\}$  is the body of the rule. If H and all  $B_i$  are ground atoms, then we call this rule a ground rule. If the body is empty, we call a rule a fact. A rule is called safe, if every variables in the atom variables of the head is also in the atom variables of some atom in the body.

A program is a finite set of rules. The program is safe, if all its rules are.

A datalog engine calculates the semantics of a datalog program, which we will define shortly. The non-fact rules of program are often general rules that can be used in many contexts, whereas the facts encode a specific context. In order to reuse programs, the facts are often outsourced in database, which we can imagine as a set of ground atoms. In the semantics we assume that these facts are then added back to the program for easier definitions.

Datalog has three major semantics: model-theoretic, proof theoretic and fixed-point based. These three semantics coincide. The semantics of a datalog program  $P = \{r_1, ..., r_k\}$  is a set of ground atoms.

For the model-theoretic semantics we describe the semantics as a specific model of the program. So far P might however contain variables, which have to be mapped to something. Therefore we first transform P into the ground program, ground(P). For this we consider groundings or instantiations, which are functions from V to C. We can apply a grounding g to an atom g to a quire a ground atom by replacing a variable g with g(g). We may write this also as g(g) and can apply grounding to a rule g as well by applying it to every atom in the body and the head, which we denote as g(g). The ground program is then defined as  $ground(P) = \{r' \mid \exists r \in P. \exists g. g(r) = r'\}$ 

A set of ground atoms I (interpretation) is a model of a ground rule r, if whenever the body of r is a subset of I also the head appears inside I. An interpretation is a model of a ground program P if it is all model for all ground rules in P.

We would like to define the model-theoretic semantics of P as the model of ground(P). In general there are however multiple models of ground(P), so that this would not be unambiguous. It might contain ground atoms without a ground rule having this atom as a head. It can however be proven that there always exists a minimal model of ground(P). We define this as the model-theoretic semantics of P

A different view is to look why an atom a is inside the minimal model. It might be because there was a ground rule in ground(P) of which a is the head and for which the body is already in the minimal model. Now we can again ask this for all elements in the body until we reach facts, which have to be true. This can be seen as a proof for a. This proof can be modelled as a rooted tree which nodes are ground atoms. A tree is a valid proof tree for a in P if the following conditions hold.

- 1. The root is a
- 2. For each leaf exists a fact in ground(P)
- 3. For each node n and its predecessors  $m_1, ..., m_k$  exists a rule in ground(P) which the head n and the body  $\{m_1, ..., m_k\}$

The proof-theoretic semantics is then the set of ground atoms for which a valid proof tree in P exists.

The previous two semantics both provide clear definitions, but do not tell us how to arrive at this set. The fixed point semantics offers way to do this. For this we consider the following operator, that takes a set of ground atoms as an input.

```
T_P(I) = \{a \mid \exists r \in ground(P), head(r) = a \land body(r) \subseteq I\}
```

This operator can be proven to be monotonic and therefore a least fixed-point exists by the Knaster-Tarski theorem exists. It can be computed by starting with  $\emptyset$  for I and repeatedly apply  $T_P$  until we find the fixed-point. This semantics is the basis for the practical implementations of datalog engines.

All three semantics can be proven to be equivalent, which we will do later in Lean for the proof-theoretic and model-theoretic semantics.

Additionally, it turns out that every non-safe program can be transformed into a safe program by introducing new relation symbols, such that for all original relation symbols the semantics coincide.

# 3 Datalog in Lean

We introduced Datalog in the previous chapter. Here we show our implementation in Lean that we will use later to show the correctness of our algorithms.

We started defining datalog using sets for constants, variables and relation symbols. In order to have a more compact representation we use the idea of a signature, that stores all these informations.

```
\begin{array}{c} \textbf{structure signature where} \\ \textbf{(constants: Type)} \\ \textbf{(vars: Type)} \\ \textbf{(relationSymbols: Type)} \\ \textbf{(relationArity: relationSymbols} \rightarrow \mathbb{N}) \end{array}
```

We no longer require that the constants and variables are distinct sets as the constructor for terms allows us to identify the type of a term. We will continue to define the other syntactic elements of datalog. The signature unless displayed otherwise will be  $\tau$ .

```
\begin{array}{l} \textbf{inductive term :} \\ | \textbf{ constant : } \tau.\textbf{constants} \rightarrow \textbf{term } \tau \\ | \textbf{ variableDL : } \tau.\textbf{vars } \rightarrow \textbf{term } \tau \\ | \textbf{deriving DecidableEq} \end{array}
```

As we want to use these objects in practical algorithms we need a way to see if two terms are the same to e.g. replace a variable by a constant. We use Leans ability to automatically create a decidable function for equality for our inductive types and structure from the given functions for the equality of the types from the signature. This allows us to use statements like  $\mathbf{a} = \mathbf{b}$  for atoms  $\mathbf{a}$ ,  $\mathbf{b}$  in the program we describe in the later sections.

For atoms we have to make sure that the amount of terms matches the arity of the relation symbol. Therefore the structure has an additional element that is a proof of this property. Two atoms are equal if all fields in the structure are equal. Since propositions as this proof are always equal, it is enough to show that the terms and the symbols are equal.

```
structure atom where  (\text{symbol: } \tau.\text{relationSymbols}) \\ (\text{atom\_terms: List (term } \tau \ )) \\ (\text{term\_length: atom\_terms.length} = \tau.\text{relationArity symbol}) \\ \text{deriving DecidableEq} \\ \\ \text{lemma atomEquality (a1 a2: atom } \tau): \\ \\ \text{a1 = a2} \leftrightarrow \text{a1.symbol} = \text{a2.symbol} \land \text{a1.atom\_terms} = \text{a2.atom\_terms}
```

Rules and programs can be expressed relatively straight forward. For programs we use abbrev, which introduces program as an alias for Finset(rule  $\tau$ ) from mathlib, instead of defining a new type as this allows us to use the common set operations without the need to redefine them.

```
structure rule where  (\text{head: atom } \tau) \\ (\text{body: List (atom } \tau)) \\ \text{deriving DecidableEq}   \text{abbrev program := Finset (rule } \tau)
```

We have previously introduced ground atoms as atoms whose terms are only constants. There are at least two options to represent them here. Firstly we could define a structure for ground atoms that extends atoms by a predicate that shows that there are only constants present. The second option is to define an entirely new structure similar to atoms but allow only constants instead of terms. The first options show directly that every ground atom is an atom which we would have to establish separatedly in the second option. The second option allows directly to define the functions on a list of constants instead of having to cast the list of terms of a ground atom directly to a list of constants and allows to use the complete induction schema when defining functions on ground atoms. The second option seemed to offer more advantegous and was therefore chosen.

```
structure groundAtom where symbol: \tau.relationSymbols atom_terms: List (\tau.constants) term_length: atom_terms.length = \tau.relationArity symbol deriving DecidableEq
```

Now we need a function that maps groundAtom back to atom. For this we can map the atom\_terms list in groundAtom with term.constant to term. Additionally we need to show that the term\_length property is preserved. Luckily, this is already proven in mathlib.

```
lemma listMapPreservesTermLength (ga: groundAtom \tau):
(List.map term.constant ga.atom_terms).length =
\tau.relationArity ga.symbol :=
by
    rw [List.length_map]
    apply ga.term_length

def groundAtom.toAtom (ga: groundAtom \tau): atom \tau:=
{
    symbol:=ga.symbol,
    atom_terms:= List.map term.constant ga.atom_terms,
    term_length:= listMapPreservesTermLength ga
}
```

Additionally, we need later that two groundAtom are equal iff the result of toAtom is equal. Similarly, we can define ground rules and functions to convert them to rules.

For now we have only seen

We formalize two semantics here. Firstly, we need the proof-theoretic semantics. Proof trees are a good way to show why an element must be in the solution and output already by multiple datalog engines. There is however to the best of our current knowledge no short certificate similar to proof trees to show the absence of elements. In order to show that a solution is complete we need another method. Both the fixed-point and the model-theoretic semantics offer help in this case. Both are the least element of some set (of fixed-point or of models respectively). Therefore it is enough to show that it is a member of this set for the other direction.

For the semantics we need the concept of the database. We do not want to deal with the implementation details of a database. We consider it as a black box that returns for a ground atom whether it is in the database. It is a function that returns Bool, because we want computable databases.

```
class database (\tau: signature) [DecidableEq \tau.vars] [DecidableEq \tau.relationSymbols] [DecidableEq \tau.constants]:= (contains: groundAtom \tau \to \text{Bool})
```

We start by defining the proof-theoretic semantics. For this we need to formalize trees. The tree is supposed to start from the facts and then expand upwards by the application of rules. As the body of rules is in general unbounded, we also require trees with an unbounded number of children, which

we realize via lists.

```
inductive tree (A: Type)
| node: A \rightarrow List (tree A) \rightarrow tree A
```

In contrast to binary trees, we will need to use functions for lists to define functions on trees. Most interesting function will however need a proof of termination due to this tree model.

```
\mathtt{def} root: tree A \rightarrow A
| tree.node a _ => a
def children: tree A \rightarrow List (A)
| tree.node _ 1 => List.map root 1
\mathtt{def} listMax {A: Type} (f: A 
ightarrow \mathbb{N}): List A 
ightarrow \mathbb{N}
| [] => 0
| (hd::tl) =>
     if f hd > listMax f tl
     then f hd
     else listMax f tl
def height: tree A 
ightarrow N
| tree.node a l =>
     1 + listMax (fun \langle x, h \rangle \Rightarrow height x) l.attach
termination_by height t => sizeOf t
decreasing_by
     simp_wf
     apply Nat.lt_trans (m:= sizeOf 1)
     apply List.sizeOf_lt_of_mem _h
     simp
```

Height is recursively called on the elements of in the list via the listMax function. Lean can not identify that this terminates so we have to provide a proof of termination. This is done in Lean by providing a well-founded relation that takes part of the input and show that the recursive calls of the function are only on elements that are smaller in this relation. Due to the well-foundedness there are no infinite descending chains and the function must terminate. We use the sizeOf function that is built in for any inductive type and maps an element to the successor of the sum of the sizeOf values of the elements used in the successor. If we show that this always decreases then the function will terminate as the natural numbers are well-founded.

In contrast to just using the list, we call listMax on List.attach instead. List.attach takes a list l and creates a new list consisting of pairs of the original elements and a proof that the element is in l. This proof can be later used when proving termination.

We have to show a statement of the form  $\mathtt{sizeOf} x < 1 + \mathtt{sizeOf} a + \mathtt{sizeOf} l$ . We use the transitivity property of the linear order to show this via showing first that  $\mathtt{sizeOf} x < \mathtt{sizeOf} l$  and secondly that  $\mathtt{sizeOf} l < 1 + \mathtt{sizeOf} a + \mathtt{sizeOf} l$ . This second statement is obviously true and can be found by  $\mathtt{simp}$ . For the first statement we can use the fact that the size of a member of a list is smaller than the size of the list. Due to using 1.attach we have a proof for this available and finish the proof. This way of proving termination is the standard way we use in this model and will be omitted for further tree functions.

Proof trees are then trees that have groundAtom as it vertices and we can formulate the validness criteria. There are two cases. If we are at leaf, i.e. the list of children is empty, then we simply check the database. Else there must exist a rule r from the program and a grounding g so that applying g to r matches the rule created from the current node and its children. Additionally all child trees must be valid as well.

```
abbrev proofTree' (\tau: signature) := tree (groundAtom \tau)

def isValid(P: program \tau) (d: database \tau) (t: proofTree \tau):

Prop :=

match t with

| proofTree.node a 1 =>
(\exists(r: rule \tau) (g:grounding \tau),

r \in P \land

ruleGrounding r g = groundRuleFromAtoms a (List.map root 1)

\land 1.attach.All<sub>2</sub> (fun \langlex, _h\rangle => isValid P d x))

\lor (1 = [] \land d.contains a)
```

The proof-theoretic semantics is then simply the set of ground atoms that are the root of a valid proof tree.

```
def proofTheoreticSemantics (P: program \tau) (d: database \tau): interpretation \tau:= {a: groundAtom \tau | \exists(t: proofTree \tau), root t = a \land isValid P d t}
```

After that we define the model-theoretic semantics. We choose the model-theoretic semantics over the fixed points semantics as we can directly construct the model and do not have to show that a fixed-point exists. Checking them in practice seems to be similar.

An interpretation is a set of ground atoms, that may be a model. A model of a program over a database is an interpretation that contains every database element and fulfills every rule. Choosing the database to be a part of the model simiplifies grounding later, as there is only one place to check for matches. Additionally, we want to show that both defined semantics are equal. From the definition above one can see that any database element has a valid proof tree and is therefore in the proof-theoretic semantics.

```
abbrev interpretation (\tau: signature) := Set (groundAtom \tau)
```

```
def ruleTrue (r: groundRule \tau) (i: interpretation \tau): Prop := groundRuleBodySet r \subseteq i \to r.head \in i def model (P: program \tau) (d: database \tau) (i: interpretation \tau):= (\forall (r: groundRule \tau), r \in groundProgram P \to ruleTrue r i) <math>\land \forall (a: groundAtom \tau), d.contains a \to a \in i
```

The usual way of defining the model-theoretic semantics is via the model intersection property. If we have two models for a datalog program, then their intersection is again a model. Intersecting all models yields therefore the minimal model. In order to use  $\bigcap$  in lead we would need to transform the set of models firstly into an indexed set. We instead used the following more simple notion. We know that an element a is a member of  $X \cap Y$  iff a is a member of X and a member of Y. Consequently, a is a member of  $\bigcap_{M \in models(P,d)} M$ , if it is a member in all models.

```
def modelTheoreticSemantics (P: program \tau) (d: database \tau):= {a: groundAtom \tau | \forall (i: interpretation \tau), model P d i \rightarrow a \in i}
```

This describes the same set, but does not offer yet the minimal model property, which we still have to prove.

We start by showing that it is a subset of every model.

```
lemma leastModel (P: program \tau) (d: database \tau) (i: interpretation \tau) (m: model P d i): modelTheoreticSemantics P d \subseteq i := by unfold modelTheoreticSemantics rw [Set.subset_def] intro a rw [Set.mem_setOf] intro h apply h apply m
```

This follows quickly from the definition. We have to show that if some arbitrary ground atom a is in the model-theoretic semantics then it is in i from the subset definition. a is in the model-theoretic semantics, if it is in every interpretation that is a model. Specifically, it must be a member of i, which is a model by assumption.

While the previous lemma is called leastModel, we still have to show that it is a model.

```
lemma modelTheoreticSemanticsIsModel (P: program \tau) (d: database \tau):
```

**Lemma 1.** Let P be a program and d be a database.

Then the modelTheoreticSemantics of P over d is a model for P over d.

Proof. We show that both conditions hold and start by showing that any rule must be rule. Let r be a arbitrary rule the ground program of P. Assume that the body of r is a subset of the modelTheoreticSemantics. If not, then the rule is already true since the body is not true. We assume for a contradiction that the head of the rule is not in the modelTheoreticSemantics. From the definition we know that there must exists a model i, which does not contain the rule head. We do know however that the body is a subset of the modelTheoreticSemantics and therefore also a subset of i. Then the rule r would not be true and i would not be a model and we have reached a contradiction.

After defining both semantics we finally want to show that they are equal, i.e. the following theorem.

```
theorem SemanticsEquivalence (P: program \tau) (d: database \tau): proofTheoreticSemantics P d = modelTheoreticSemantics P d
```

This is supposed to be done via the anti-symmetric property of the subset relation, i.e.  $\forall X, Y.X \subseteq Y \land Y \subseteq X \rightarrow X = Y$ .

First we want to show that the proof-theoretic semantics are a subset of the model-theoretic semantics. We show the bit stronger statement, that all element in the proof-theoretic semantics are in every model. As the modeltheoretic semantics are a model, the first direction follows.

**Lemma 2.** Let P be a program, d be a database and i a model of P over d. Then proofTheoreticSemantics P d is a subset of i

*Proof.* We want to show that every ground atom in proofTheoreticSemantics P d is also in i. A ground atom a is in the proof-theoretic semantics if there exists a valid proof tree that has the root a, so that we can instead prove that the root of any valid proof tree t is in i.

We do this using strong induction on the height of t for arbitrary valid proof trees t. There are two possiblities for valid proof trees. The first is that it only contains the root, which is a database element. As any model must contain the database, the root of this tree must be in i.

The second possiblity is that the root of t and the direct children of the root represent a ground rule r of P. In this case all subtrees must be valid as well and have from the definition of the height of a tree a smaller height. Therefore we can apply the induction hypothesis and conclude that the root for all direct subtrees of t is in i. This set is however exactly the body of r. Since i is a model and r is a rule from ground(P) whose body is already in i, the head of of this rule must be in i as well. The head of r is exactly the root of t which finishes the proof.

For the second direction, we need to show that the modelTheoreticSemantics is a subset of the proofTheoreticSemantics. As we know that the model-theoretic semantic is the least model it suffices to show that the proof-theoretic semantic is a model as well.

**Lemma 3.** Let P be a program and d a database. Then proofTheoreticSemantics P d is a model.

*Proof.* We have to show that the conditions for a model hold.

Firstly, that the database is a subset of the proof-theoretic semantics. For every ground atom in the database we can construct a tree with no children that has only this element as the node. This is valid and has the database element as its head, so that the condition is fulfilled.

Secondly, we have to show that every rule is fulfilled. Let r be a ground rule from ground(P) and assume that the body of r is a subset of proof-theoretic semantics of P over d. Then we have to show that head(r) is also in the proof-theoretic semantics of P over d. We do this by constructing a proof for head(r). In order to do we require a list l of valid proof trees such that mapping this list with root yields body(r). Then we can create the new proof tree with the node head(r) and the children l. This proof tree is valid as all trees in l are valid and head(r) and l are the rule grounding of some rule  $r' \in P$ . Since r is a ground rule from ground(P), such r' and grounding g must exists.

Finally, we have to show that such a list l really exists. We do this by proving the more general lemma.

**Lemma 4.** Let A and B be two types. Let l' be a list of type B and f be a function of  $A \to B$  and valid be a function from B to Prop. Let S be a finite set such that every member of l' is a member of S. Additionally, for any a in S exists a valid b with f(b) = a. Then exists a list l with mapping f on l yields l' and that all members of l are valid.

*Proof.* We proof this by induction on l'. If l' is the empty list, then we use again the empty list. Any member of the empty list is valid and the mapping condition holds as well, because the empty list is mapped to the empty list.

Now we consider l' to be of the form hd :: tl. Since hd is a member of l', it is also a member of S and therefore a valid element  $hd_b$  exists with  $f(hd_b) = hd$ . For tl we aquire such a list  $tl_b$  from the induction hypothesis, since any member of tl is a member of l' and by that a member of S. Then  $hd_b :: tl_b$  is the required list.

Letting l' be the body of r and S be the finite set consisting of the members of l, we fulfill the first requirement. We set f as the root function and valid as funt => isValidPdt. Then by assumption for any element a of S a valid proof tree with the root a exists, since body(r) is already in proofTheoreticSemantics P d. The lemma then presents us the required list of valid proof trees for the body.

#### 4 Soundness

After introducing the problem and modelling in Lean, we now describe the algorithm to verify a solution. In this chapter we deal with the soundness, which means here that every atom in the interpretation is actually in the semantics. For this we use the proof trees as the certificate and the proof theoretic semantics.

A ground atom is in the proof theoretic semantics if there exists a valid proof tree, that has this ground atom as its head. We were provided with all the proof trees and checking the heads is rather easy, so what remains to be checked is the validness of a proof tree, that was defined in the previous chapter.

```
def isValid(P: program \tau) (d: database \tau) (t: proofTree \tau):

Prop :=

match t with

| proofTree.node a l =>
( \exists(r: rule \tau) (g:grounding \tau),

r \in P \land

ruleGrounding r g = groundRuleFromAtoms a (List.map root l)

\land l.attach.All<sub>2</sub> (fun \langlex, _h\rangle => isValid P d x))

\lor (l = [] \land d.contains a)
```

The second part of this disjunction consists of a database check and an easy check of list emptyness. The first part is more interesting. Since we use there existential quantifiers, we have to implement something to check this. As the program is given as a list of rules, we can simply iterate over this list. For the grounding we however can something more sophisticated, but groundings are not our object of choice for that.

#### 4.1 Substitutions

A grounding is function from variables to constants. This mean that we always need to specify for every variable a constant that it is mapped to. This was good in the definitions to ensure that we always get a ground atom, but raises in the unification case problems as the following example demonstrates.

**Example 1.** Consider the signature consisting of  $C = \{a, b, c\}$ ,  $V = \{x, y, z\}$  and  $R = \{R\}$ . Suppose we want to match a list of terms with a list of constant. The first term is  $t_1 = x$  and the first constant is a. We might use the the grounding  $g = x \mapsto a, y \mapsto a, z \mapsto a$ .

Now we want to use this result and match another term  $t_2 = y$  with the constant b. The variable y is already mapped to a different constant, but we cannot say whether this is due to a previous matching process or simply because we needed to define a value for every input.

Instead, we want to use substitutions that were already introduced in [?]. A substitution is a partial mapping from variables to constants. We implement this by mapping to an Option of constant.

```
def substitution (\tau: signature):= \tau.vars \rightarrow Option (\tau.constants)
```

This allows us to only specify what is necessary. If we apply a substitution to a term, we only replace a variable by a constant, if the substitution is defined for this variable and the constant will be the result of the substitution in this case.

def applySubstitutionTerm (s: substitution  $\tau$ ) (t: term  $\tau$ ): term  $\tau$  match t with

```
| term.constant c => term.constant c
| term.variableDL v =>
    if p: Option.isSome (s v)
    then term.constant (Option.get (s v) p)
    else term.variableDL v
```

:=

We can use similar defintions as previously for groundings to apply substitutions to atoms or rules.

The main result we want to prove is the following.

```
theorem groundingSubstitutionEquivalence [Nonempty \tau.constants] (r: groundRule \tau) (r': rule \tau): (\exists (g: grounding \tau), ruleGrounding r' g = r) \leftrightarrow (\exists (s: substitution \tau), applySubstitutionRule s r'= r)
```

This allows us to replace the grounding check by a substitution check, when trying to validate trees and by this we can bypass the problems that were illustrated in the example above.

For the forward implication, we can transform any grounding in a simple way to a substitution. In this substitution every value is defined with the value of the grounding.

```
def groundingToSubstitution (g: grounding \tau): substitution \tau := fun x => Option.some (g x)
```

It is very easy to prove that this is equivalent on every rule.

For the back direction, we need additionally that the set of constants is nonempty. We can ensure this during the input phase by adding a fresh constant symbol to the constant symbols similar to Herbrand universes. This symbol does not appear in any proof trees and does not influence the results. Since we only look at safe programs, it will also not introduce any new ground atoms to the model.

The following example shows the problems that occur without the non-emptyness assured.

```
Example 2. Consider the program P = \{p \leftarrow, q \leftarrow p\} and the signature C = \emptyset, V = \{x, y, z\} and R = \{p, q\}
```

Any rule in P is already a ground rule and there exists a substitution, the empty substitution that maps all variables to none, so that the rule is equal to itself as a ground rule.

There is however no grounding that can achieve this. We cannot define a grounding since we have no constant available, but have variables that need to be mapped somewhere. Therefore the equivalence does not hold here.

Since the set of constants is non-empty, we can use the axiom of choice to get values for which the substitution is not defined.

```
noncomputable def substitutionToGrounding

[ex: Nonempty \tau.constants] (s: substitution \tau): grounding \tau :=

fun x => if p:Option.isSome (s x)

then Option.get (s x) p

else Classical.choice ex
```

When introducing substitutions, we had the goal to only add what is needed to a substitution and usually we want the smallest possible substitution. In order to formalize this, we want to define a linear relation on substitutions, that is denoted by  $\subseteq$ 

Firstly, we define the substitution domain of a substitution as the set of variables for which the substitution is defined.

A substitution  $s_1$  is then a subset of a substitution  $s_2$ , if both substitutions agree on the substitution domain of  $s_1$ . Outside of this  $s_1$  is never defined, whereas  $s_2$  might be, so that we view  $s_1$  as smaller.

```
def substitution_subs (s1 s2: substitution \tau): Prop := \forall (v: \tau.vars), v \in substitution_domain s1 \rightarrow s1 v = s2 v
```

This can be proven to be a partial order.

#### 4.2 Unification

We know that instead of finding a grounding, it suffices to find a substitution. Now we want to describe an algorithm that tells us whether the ground rule that is formed from a node of the proof tree is the substituted rule of some rule of the program. For this we take inspiration from the unification problem of first-order logic.

In the unification problem we are given a set of equations between first-order terms and are required to present the most-general unifier.

Our problem is similar. The equations will not be between terms, but between an object and a ground object of the same corrosponding type and we require a substitution that solves all equations and is minimal in our subset relation.

An algorithm to solve the first-order unfication problem is the algorithm of Martelli and Montanari [?] and is depicted below:

#### Algorithm 1 Algorithm of Martelli and Montanari

while There exists some equation for which a transformation is possible do Pick this equation e and do one of the following steps if applicable

- 1. If e is of the form t = t, then delete this equation from the set.
- 2. If e is of the form  $f(t_1,...,t_n) = f(s_1,...,s_n)$ , then delete e and add n new equations of the form  $t_i = s_i$
- 3. If e is of the form  $f(t_1,..,t_n) = g(s_1,..,s_m)$  with  $g \neq f$ , then stop and reject.
- 4. If e is of the form  $f(t_1,...,t_n) = x$  for a variable x and delete e and add an equation with the swapped order to the set
- 5. If e is of the form x = t for some variable x, then check if x occurs in t. If it does, then stop and reject. If not map all x to t in the set.

#### end while

This algorithm offers a good starting point for our own algorithm, but we certain transformation can't occur in the limited syntactic form we operate in. Additionally, we want to output a substitution instead of just answering whether a substitution exists. It is sufficient to do it here, but will later be important. Instead of mapping all x to t as done there in step 5, we will add  $x\mapsto t$  to a substitution that is presented as an input. If a variable occurs on the left side, we will check whether it is already in the domain of the substitution and if so check if its current value is consistent with the right side. As function symbols appart from constant symbols are not allowed, we can simplify steps 2 and 3, as we never add new equations and instead only check if the constant symbol matches. Finally, as the one side of the equation is always a ground object there will never be a variable on this side, so that we do not have to swap the equation as in step 4.

We will start with matching a term to a constant with the following algorithm.

```
def matchTerm (t: term \tau)(c: \tau.constants) (s: substitution \tau): Option (substitution \tau) := match t with | term.constant c' => if c = c' then Option.some s else Option.none
```

```
| term.variableDL v =>
   if p:Option.isSome (s v)
   then if Option.get (s v) p = c
        then
        Option.some s
   else
        Option.none
   else extend s v c
```

We are given a term t, a constant c and a current substitution s and want to return the minimal substitution s' so that  $s \subseteq s'$  and applying s' to t will make it equal to c or none if no such s' exists.

This is done by case distinction. If t is a constant, then we either return s if t is equal to c, or return none as two different constants can not be unified by a substitution. If t is variable, we check if t is in the domain of s. If it is already defined we check if the value matches the required value. If it is not defined we extend s with the new mapping  $v \mapsto c$ . Formally extend is defined in the following way:

```
def extend (s: substitution \tau) (v: \tau.vars) (c: \tau.constants) : substitution \tau := fun x => if x = v then Option.some c else s x
```

We know formally prove the correctness of this algorithm. The first result is that if  $\mathtt{matchTerm}$  returns a substitution s' that s' is indeed a solution, i.e. that applying s' to t results in t0 and that t1 is an extension of t2.

```
lemma matchTermFindsSolution (t: term \tau) (c: \tau.constants) (s: substitution \tau) (h: Option.isSome (matchTerm t c s)): applySubstitutionTerm (Option.get (matchTerm t c s) h) t = c \wedge s \subseteq (Option.get (matchTerm t c s) h)
```

*Proof.* The proof is done via case distinction. Suppose firstly that t is a constant c'. Since matchTerm returned a substitution we must have that c and c' are the same constant and therefore s' is s. Applying a substitution to a constant does not change it, so s't = s'(c') = c' = c. Additionally since  $\subseteq$  is a linear order and s' = s, we have that  $s \subseteq s'$ 

Now we assume that t is a variable v. Now we do another case distinction on whether sv is defined or not. If it is defined, v must already be mapped to c and we return s as this is a solution as seen previously. If it would be mapped to something else, then match Term would return none, which would be in violation to our assumptions. If it is not defined, we use extend. After that v is mapped to c, so that s't will be equal to c. Now we finally have to show that  $s \subseteq extend$ 

 $s\ v\ c$ . We only change the value of v. Since v was not defined earlier, for any variable in the domain of s, s and extend  $s\ v\ c$ , so that it is fulfilled.  $\Box$ 

We have proven so far the matchTerm returns a solution, but it might not be a minimal solution. When we want to match atoms with ground atoms, we need to match a list of terms with a list of constants. There it is important that the returned substitution is indeed minimal to conclude whether a solution exists as the following example shows.

**Example 3.** Consider the list of terms  $l_1 = [x, y, x]$  with the variables x and y and the list of constants  $l_2 = [a, b, c]$ . We want to find a substitution that we can apply to  $l_1$  to gain  $l_2$  if possible. We start with the empty substitution and first want to match the first elements of  $l_1$  and  $l_2$ . If we receive a solution s, then we continue with the next elements of  $l_1$  and  $l_2$ , but this time the matching extends s instead of the empty substitution.

Now suppose the procedure  $P_1(t, c, s)$  that takes a term, a constant and a substitution does not always return a minimal solution. So it might return for x, a and the empty substitution the substitution  $s = x \mapsto a, y \mapsto a$ .

Now we again call  $P_1$  with y, b and s.  $P_1$  will not return anything, because y is already mapped to something else. From this fact we cannot conclude that there exists no solution at all however. In fact, the non-minimality of the results of  $P_1$  prevents this reasoning.

If we have a second procedure  $P_2(t,c,s)$  that always returns the minimal solution we solve the matching process for the first two list elements of each list to return  $s' = x \mapsto a, y \mapsto y$ . Now we want to match x with c and  $P_2$  will return none. We can conclude that no solution exists since any substitution from  $P_2$  is minimal. If there exists a solution to the list then  $l_2$ , it necessarily must match the first to elements of both lists. Since s' is the minimal solution of a process that started with the empty substitution and always returned minimal solution, any solution to the list must extend s'. Therefore it must agree on the domain of s' and therefore it must map x to a and therefore no solution can exist.

```
lemma matchTermFindsMinimalSolution' (t: term \tau) (c: \tau.constants) (s: substitution \tau) (h: Option.isSome (matchTerm t c s)):

\forall (s': substitution \ \tau), (s \subseteq s' \land applySubstitutionTerm \ s' \ t = c) \rightarrow (Option.get (matchTerm t c s) h) \subseteq s' :=
```

*Proof.* This is again done via case distinction on the type of t. If t is constant, then s' must be equal to s. For any  $s^*$  with  $s \subseteq s^* \land s^*t = c$  we have b that  $s' \subseteq s^*$  by the assumption of the property of  $s^*$ 

Now we consider the case of t being a variable v and do a case distinction whether sv is defined. If it was already defined, then s' must again be equal to s, so that the claim is fulfilled by the argument above. If sv was not defined,

we have to show that extend s v c is a subset of any such  $s^*$ . We assume for a contradiction that this is not the case. Then there must be a variable in the domain of extend s v c such that extend s v c and  $s^*$  differ. Suppose this variable is v. Then  $s^*$  would either not be defined for v or map v to some other constant c'. In both cases  $s^*v \neq c$ , so that  $s^*$  would not be a solution and we would have reached a contradiction. If it is some other variable v', then the value of extend s v c is simply the value of s. Since  $s^*$  maps v to a different value compared s, s would not be a subset of  $s^*$  and we have reached another contradiction.

So we know that if matchTerm returns a substitution then it is a minimal solution. We additionally have to prove that if matchTerm does not return a substitution that then no solution exists.

```
lemma matchTermNoneImpNoSolution (t: term \tau)
(c: \tau.constants) (s: substitution \tau)
(h: Option.isNone (matchTerm t c s)):

\neg (\exists(s': substitution \tau), s \subseteq s'\landapplySubstitutionTerm s' t = c)
```

*Proof.* This is again done via case distinction on the type of t. If t is a constant c', then c' must be different from c, so that matchTerm returns none. Then no substitution can map t to c.

If t is a variable v, then sv must be defined and mapped to a different value compared to c. Then again no such s' can exist. If s would be a subset of s', then s' would not unify t with c and if s' would unify t with c then s would not be a subset of s'.

After proving the correctness for terms we now want to move up to atoms. Unfortunately, we cannot use recursion directly on the term list of an atom. An atom requires a proof that the length of the list is equal to the arity of the relation symbol, which fails when we do recursion on the list. Therefore we first establish a new procedure that matches a list of terms with a list of constants, if possible.

```
def matchTermList (s: substitution \( \tau ) \) (11: List (term \( \tau ) )
  (12: List (\( \tau \).constants )): Option (substitution \( \tau ) := \)
match 11 with
  | List.nil => some s
  | List.cons hd tl =>
    match 12 with
  | List.nil => none
  | List.cons hd' tl' =>
    let s' := matchTerm hd hd' s
    if p: Option.isSome s'
    then matchTermList (Option.get s' p) tl tl'
```

Here we are given as previously a substitution as an input with the two lists. For the correctness it is required that both lists have the same length, but this is the case for atoms. If the first list is empty we return the substitution. If instead it has a first element and the second list has as well a first element, we match these elements using matchTerm and if this results in a solution, we return the result of matchTermList with the remaining lists and the resulting substitution.

As previously, we have to prove the correctness of this algorithm. We again want to show that the algorithm returns the minimal solution iff it exists. We require for these results that both lists are the same length. If the list of constants is longer than the list of terms, the matchTermList function may return a solution eventhough the lists will never be equal. As we only want to use this to match atoms, this is however not a problem. No substitution can change the symbol, so that we will only try to match atoms with ground atoms that have the same symbol. The symbol determines the number of terms so that both lists will have the same length.

```
lemma matchTermListFindsSolution (s: substitution \tau)
(11: List (term \tau)) (12: List (\tau.constants))
(len: 11.length = 12.length)
(h:Option.isSome (matchTermList s 11 12)):
List.map (applySubstitutionTerm (Option.get (matchTermList s 11 12) h)) 11

= List.map term.constant 12
 \land s \subseteq (Option.get (matchTermList s 11 12) h ) :=
```

*Proof.* We prove this by induction on  $l_1$  for arbitrary s and  $l_2$ . In the base case  $l_1$  is the empty list. Since both lists have the same length  $l_2$  must also be the empty list. matchTermList then returns s. Applying this to an empty list returns an empty list. Therefore the base case is complete.

In the induction step we have that  $l_1$  is of the form hd :: tl and we can similarly assume that  $l_2$  is of the form hd' :: tl' and that tl and tl' have the same length by our assumption. Since matchTermList returned a substitution, matchTerm hd hd' also must return a substitution  $s^*$ . We then use this as an input to gain s' from matchTermList  $s^*$  tl tl'. By the induction hypothesis  $s^* \subseteq s'$  and applying s' to tl results in it being equal to tl'. To show that both lists are equal, we just have to show that after applying s' the heads will be equal. We know that applying  $s^*$  to hd will result in it being equal to hd'. Since  $s^* \subseteq s'$  and our previous result that if a substitution maps a term to a constant then extension of this substitution will also map the term to the same constant, we have this. Lastly, we have to show that  $s \subseteq s'$ . From the correctness proof of matchTerm we know that  $s \subseteq s^*$  and from the induction hypothesis we know that  $s^* \subseteq s'$ . Since  $\subseteq$  is transitive, the result follows.

After proving that it is a solution, we prove that the solution is minimal.

```
lemma matchTermListFindsMinimalSolution (s: substitution \tau) (l1: List (term \tau)) (l2: List (\tau.constants)) (len: l1.length = l2.length) (h: Option.isSome (matchTermList s l1 l2)): \forall (s': substitution \tau), List.map (applySubstitutionTerm s') l1 = List.map term.constant \land s \subseteq s' \rightarrow (Option.get (matchTermList s l1 l2) h ) \subseteq s' :=
```

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*Proof.* We prove this again via induction on  $l_1$  for arbitrary  $l_2$  and s. If  $l_1$  is empty, we return s and the claim is true by assumption.

In the induction step we have that  $l_1$  has the form hd :: tl and we can assume that  $l_2$  has the form hd' :: tl' and that tl and tl' have the same length. Additionally, we know that matchTerm hd hd' s returns a substitution  $s^*$ . From the induction hypothesis we know that matchTermList  $s^*$  tl tl'  $\subseteq \hat{s}$  for any substitution  $\hat{s}$  that extends  $a^*$  and maps tl to tl'. Since  $s^*$  is a minimal solution for hd and hd' and  $s^*$  only extends it, we know that it is a solution for the whole list. We also know from the minimality of  $s^*$  that  $s \subseteq s^*$ . From the induction hypothesis, we get that  $s^* \subseteq \hat{s}$ . Transitivity tells us that  $s \subseteq \hat{s}$  as

Finally the negative case that confirms that the return value of none does indeed state that there is no solution.

```
lemma matchTermListNoneImplNoSolution (s: substitution \tau) (11: List (term \tau)) (12: List (\tau.constants)) (len: l1.length = l2.length) (h: Option.isNone (matchTermList s l1 l2)): \forall (s': substitution \tau), s \subseteq s' \rightarrow \neg List.map (applySubstitutionTerm s') l1 = List.map term. constant l2 :=
```

*Proof.* We prove this again via induction on  $l_1$  for arbitrary  $l_2$  and s. If  $l_1$  is the empty list, we cannot return none. As the prerequisite is not fulfilled, the statement is correct.

In the induction step we have that  $l_1$  has the form hd :: tl and we can assume that  $l_2$  has the form hd' :: tl' and that tl and tl' have the same length. There are two cases where matchTermList can return none. The first case is when matchTerm hd hd' s returns none. If that is the case there is no s' with  $s \subseteq s'$  and applying s to hd will make it equal to hd'. Therefore the two lists cannot be equal either and the proof is finished.

If matchTerm hd hd' s returns a substitution  $s^*$ , then matchTermList  $s^*$  tl tl' must return none. From the induction hypothesis we know that there is no substitution s' with  $s^* \subseteq s'$  and applying s' to tl bringing it equal to tl'. Since

 $s^*$  is already the minimal solution to match hd with hd' there cannot exist a solution here.

This can be used to create a matchAtom procedure. We are given an atom and a ground atom and check if the symbols are equal. If they are, we also get that their term lists must be equal as the length of the term list is equal to the arity of the relation symbol. The same symbol implies the same length. If the symbols are different, we will never unify them.

```
def matchAtom (s: substitution \tau) (a: atom \tau) (ga: groundAtom \tau): Option (substitution \tau) :=
    if a.symbol = ga.symbol
    then
        matchTermList s a.atom_terms ga.atom_terms
    else none
```

The correctness proofs follow from the proofs of matchTermList since we already established the same length of both lists from the symbol.

Now we can create a matchAtomList function similarly to matchTermList and use this to define a matchRule function. We first try match the head of the rule with the head of the ground rule. If this returns a solution, we use this as the start for matching the bodies. If not, we will not find a solution and return none.

```
def matchRule (r: rule \tau) (gr: groundRule \tau):
   Option (substitution \tau):=
   let s := matchAtom emptySubstitution r.head gr.head
   if p: Option.isSome s
   then matchAtomList (Option.get s p) r.body gr.body
   else none
```

We know prove again that if this returns a substitution then this is a solution and if none is return then there is no solution using our previous results. For both these results we assume that both bodies have the same length, but determining the length of a list can be done in the tree validation process. We want a statement with the quantifier to combine it with the theorem about the equivalence between groundings and substitutions. We can prove this statement by using the result of matchRule as a witness for the quantifier. For the back direction, we see that this statement implies that a solution exists, which we always find with matchRule

```
theorem matchRuleIsSomeIffSolution (r: rule \tau) (gr: groundRule \tau) (len: r.body.length = gr.body.length):
Option.isSome (matchRule r gr) \leftrightarrow
\exists (s: substitution \tau), applySubstitutionRule s r = gr
```

We now have a method to replace this quantifier by a computable function and can finally devise the check for tree validation.

#### 4.3 Tree validation

We have so far introduced introduced substitutions and have shown a way to decide whether a substitution exists that maps a rule to a ground rule. Now we want to finally show a way to validate trees. As the first step we want to find whether a ground rule gr we gain from the tree is in the ground program, i.e. that there exists a grounding g (or from the previous results a substitution s) and a rule r from the program P, so that applying g to r yields gr. We want to use the matchRule function defined earlier for this. This function required that both bodies of the rules to have the same length in order to work properly. Instead of just computing the length we want to do a bit more. We previously noted that substitutions (or groundings) never change the symbol of an atom, so that we do not have to try to match rules whose symbols differ. The symbols of a rule are expressed in the symbol sequence.

```
def symbolSequence (r: rule \tau): List \tau.relationSymbols := r.head.symbol::(List.map atom.symbol r.body)
```

We can now compare the symbol sequence of a rule and the symbol sequence of a ground rule. If they are equal, we see that the bodies have the same length, since we just map each body element and attached for both the head at the front. If they are however not equal, then no substitution can be applied to the rule so that it will yield the ground rule.

We can use this to check whether a ground rule gr is in the ground program of P. We simply compare the symbol sequence of all rules in P with gr and try to match those whose symbol sequences are equal. As soon as we find a substitution using matchRule we return ok. If no rule matches we return an error displaying this.

```
def checkRuleMatch (P: List (rule \tau)) (gr: groundRule \tau) (ruleToString: rule \tau \to String): Except String Unit := match P with | List.nil => Except.error ("No match for " ++ (ruleToString gr.toRule)) | List.cons hd tl => if symbolSequence hd = symbolSequence gr.toRule then if Option.isSome (matchRule hd gr) then Except.ok () else checkRuleMatch tl gr ruleToString else checkRuleMatch tl gr ruleToString
```

# 5 Completeness

In the previous chapter we described a method why an atom is in the datalog semantics. This criteria is however not sufficient to recognize a solution. The empty list passes this test for any program while not being the semantics in most cases. Proof trees were a method to recognize why a ground atom is part of the semantics, but we are not aware of any simple way to describe why a ground atom is not in the semantics. Instead we want to show that the set of elements in the proof trees, S are complete in the sense that nothing else can derived from it any more. This is the case when the  $T_P$  operator has a fixed-point for S or alternatively when S is a model. In this chapter we are going to create a certified model checker to show the completeness. If S passed the tree validation algorithm and is a model the following statements hold:

 $S\subseteq \texttt{proofTheoreticSemantics} \; \mathsf{P} \; \mathsf{d} = \mathsf{modelTheoreticSemantics} \; \mathsf{P} \; \mathsf{d} \subseteq S$ 

# 5.1 Partial ground rules

We defined the model property on the ground program ground(P). In order to check if a set of ground atoms is a model for a program we therefore have to ground the program. We want to avoid simply grounding all the rules at once and instead do it in a more intelligent way. For this we introduce a new data structure, the partial ground rule. This bears some similarities to the rules we defined in chapter 3. It has a head that is an atom. The body is split into two lists. The first list contains the ground atoms and represents the atoms in the rule we already grounded, whereas the second list consists of the so far ungrounded atoms in the rule body. We want to move the ungrounded atoms one by one into the grounded list by applying substitutions, which map all variables of this atom to constants, so that we can transform this atom into a ground atom.

```
Structure partialGroundRule (\tau: signature) where head: atom \tau groundedBody: List (groundAtom \tau) ungroundedBody: List (atom \tau)

Example 4. A rule r := q(X) : -r(a,b), t(X,c), s(c,d), u(d,X). may be viewed as the following partial ground rule pgr_1 = \{ bead := q(X), \\ groundedBody := [], \\ ungroundedBody := [r(a, b), t(X, c), s(c, d), u(d, X)] \}
```

This representation does not look any different to the rule itself as we do not use the grounded body at all. We can however move ground atoms from the ungrounded body into the grounded body. The order of the atoms in the body does not matter semantically as we use a set definition when defining the criteria for a rule being true, so that we can simply move all ground atoms in the grounded body.

```
{
    head:= q(X),
    groundedBody := [r(a, b), s(c, d)],
    ungroundedBody := [t(X, c), u(d, X)]
}
```

We can transform any rule into a partial ground rule by setting the head as the head, the body as the ungrounded body and setting the grounded body to be empty.

```
def partialGroundRuleFromRule (r: rule \tau): partialGroundRule \tau := {
    head := r.head,
    groundedBody := [],
    ungroundedBody := r.body
}
```

Example 5.  $pgr_1$  is exactly the result of partialGroundRuleFromRule r.

We choose this representation instead of the approach used for  $pgr_2$  as this does not require iterating over the whole body to find ground atoms. As we will apply multiple substitutions in the grounding process, we will create anyways ground atoms in different place to the atom in the body we are currently trying to ground.

Any partial ground rule can also be transformed back into a rule by concatenating the grounded and ungrounded body and combining creating first a partial ground rule from a rule and then transforming the resulting partial ground rule yields the original rule. This does not hold if we swap the operations as we do not explicitly move atoms without variables from the start of the body into the grounded body.

```
def partialGroundRule.toRule (pgr: partialGroundRule \tau)
: rule \tau :=
{
   head:= pgr.head,
   body := (List.map (groundAtom.toAtom) pgr.groundedBody)
   ++ pgr.ungroundedBody
}
```

```
lemma partialGroundRuleToRuleInverseToFromRule (r: rule \tau):
r = partialGroundRule.toRule (partialGroundRuleFromRule r)
```

**Example 6.** The application of partial GroundRule. to Rule on  $pgr_1$  yields r as predicted by the lemma.

If we swap both functions and first apply partialGroundRule.toRule to a partial ground rule and then convert the resulting rule back to a partial ground rule, we see that this is no longer equal. Applying partialGroundRule.toRule to  $pgr_2$  results in the rule q(X): -r(a,b), s(c,d), t(X,c), u(d,X). Converting this back into a partial ground rule with partialGroundRuleFromRule we gain

```
{
    head:= q(X),
    groundedBody := [],
    ungroundedBody := [r(a, b), s(c, d), t(X, c), u(d, X)]
}
```

which is different from pgr<sub>2</sub>

Using the transformation to rules we can lift defintions like safety or being true to partial ground rules.

```
def partialGroundRule.isSafe (pgr: partialGroundRule \tau) := pgr.toRule.isSafe def partialGroundRule.ruleTrue (pgr: partialGroundRule \tau) (i: interpretation \tau) := ruleTrue pgr.toRule i
```

So far we only split the body into two parts and have the goal of applying substitutions to move everything into the grounded body. This is not to different to just applying groundings directly. This process allows us to potentially stop early. If the substitutions we applied so far resulted in a ground atom that is not part of the interpretation i we already know that the rule is true. No matter how the remaining variables are mapped, the body will never be a part of i and therefore the antecedent is false and the rule is therefore true. We call a partial ground rule  $active\ in\ an\ interpretation\ i$  where all ground atoms in the groundedBody

```
def active (pgr: partialGroundRule \tau) (i: interpretation \tau):= \forall (ga: groundAtom \tau), ga \in pgr.groundedBody \rightarrow ga \in i
```

#### 5.2 Explore grounding