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ONTOMETRY-BASED QUERY ANSWERING OVER DATALOG-EXPRESSIBLE RULE SETS IS UNDECIDABLE

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# Contents

1 Introduction 2

2 Preliminaries 4
   2.1 Syntax ................................. 4
   2.2 Semantics ............................. 5
   2.3 The chase ............................ 5
   2.4 Some computability theory .......... 6

3 OBQA over Datalog-expressible rule sets is undecidable 8
   3.1 The rule set .......................... 8
   3.2 $R_M$ simulates $M$ ................. 9
   3.3 $R_M$ is Datalog expressible ....... 16
      3.3.1 Skolem depth ..................... 17
      3.3.2 An axiomatization of equality ... 18
      3.3.3 Skolem-increasing derivations ... 22
      3.3.4 Some structure — The Fail predicate ... 25
      3.3.5 Controlling the chains .......... 26
      3.3.6 Skolem depth and Datalog-expressibility ... 30
Chapter 1

Introduction

To handle the ever-increasing amount of data available, and to process it efficiently, querying data has become a ubiquitous task. In some cases, one also needs to be able to reason over data. A standard use case is the harmonization of databases coming from different organizations. Indeed, to query data efficiently, it is necessary for those different organizations to agree on the vocabulary used, which may not necessarily be possible. Introducing a logical layer to simplify this harmonization is often more practical than convincing everyone to use a unique standard. This logical layer is usually called an ontology, giving rise to the problem of ontology-based query answering (OBQA).

There are many ways to express ontologies, the most usual being description logics. However, description logics are limited to unary and binary predicates, and can only encode knowledge in tree-like structures, which restricts their expressivity. Another language that is able to express more complex structures is Datalog, but it is limited in the sense that it cannot create any new individual: all the knowledge inferred is about already known individuals. Thus, to meet both those requirements, another framework has been studied, which is known as Existential rules. Existential rules extend Datalog rules with the ability to create new individuals. More precisely, an existential rule is a first order formula of the form $\text{body} \rightarrow \text{head}$, where $\text{body}$ and $\text{head}$ are both conjunctions of atoms, and variables appearing only in the head are existentially quantified.

While existential rules have both the ability to express complex structures and to infer the existence of new individuals, this expressivity comes with a cost: reasoning becomes semi-decidable. The usual reasoning task with existential rules, boolean conjunctive query (BCQ) entailment, can be summarized as the following: given a database and an ontology expressed as a set of existential rules, is a given query a logical consequence of the ontology if we take into account the facts that compose the database? In order to solve it, two main approaches have been developed.

The first approach to solve BCQ entailment is the chase. The chase is a family of algorithms that works by materializing new facts in the database using the rules in the ontology, until a fixpoint is reached. Then to solve BCQ entailment, it is enough to evaluate the query on the saturated database using traditional query evaluation algorithms. While this approach enables efficient query answering (through the use of standard database query evaluation over a query that stayed the same), it is not always feasible to modify the database,
either for security reasons, or because of size constraints.

The other standard way to solve BCQ entailment is through query rewriting. The idea is that instead of adding inferred knowledge to the database, one can modify the query to take into account the dependencies in the rule set, and then evaluate this query over the initial database. When starting from BCQs, using standard techniques, one ends up with a union of conjunctive queries (UCQ) as a rewriting, though other target languages have been studied. In this report, we focus particularly on Datalog rewritings, as it is a very natural restriction of existential rules, that ensures termination of the chase (as Datalog rules cannot create new individuals). Let us define these two kinds of rewritings. Take note however that to end up with Datalog rewritings, one not only modifies the query, but also the rule set.

**Definition 1.** The couple \((R', q')\) is a rewriting of a rule set \(R\) and a query \(q\) if \((R, D) |= q\) if and only if \((R', D) |= q'\) for all databases \(D\). An UCQ rewriting of a query \(q\) w.r.t. a rule set \(R\) is a rewriting \((\emptyset, q')\) where \(q'\) is a union of conjunctive queries. A Datalog rewriting of a rule set \(R\) and a query \(q\) is a rewriting \((R', q')\) where all the rules in \(R'\) are Datalog. A couple rule set-query is UCQ-expressible (resp. Datalog-expressible) if it admits a UCQ rewriting (resp. a Datalog rewriting).

An interesting characteristic of UCQ and Datalog rewritings is that query answering using these rewritings is decidable. Indeed, a UCQ rewriting does not feature a rule set so usual database theory algorithms work, and for Datalog rewritings, the chase terminates. Thus, from any rule set and query, if one can compute a UCQ or a Datalog rewriting, then one can solve query entailment in finite time. Thus, the question of finding these rewritings is of paramount interest, and gives rise to the following problems.

**Query answering over UCQ-expressible Rule Sets**

**Input:** A database \(D\), a rule set \(R\) and a query \(q\) that is UCQ-expressible w.r.t. \(R\)

**Question:** Do we have \((R, D) |= q\)?

**Theorem 2.** [3] Query answering over UCQ-expressible rule sets is decidable.

This means that we have an effective algorithm to compute UCQ rewritings. Though, the situation is very different for Datalog rewritings.

**Query answering over Datalog-expressible Rule Sets**

**Input:** A database \(D\), a couple rule set-query \((R, q)\) that is \(R\)-Datalog-expressible

**Question:** Do we have \((R, D) |= q\)?

**Theorem 3.** Query answering over Datalog-expressible rule sets is undecidable.

Our contribution is proving Theorem 3. To do so, we present a reduction from the halting problem to the problem of query answering over Datalog-expressible rule sets.
Chapter 2
Preliminaries

2.1 Syntax

We work in a first-order setting limited to predicates, constants, and variables. A term is a variable or a constant. To each predicate we associate a natural integer, called the arity of the predicate. A P-atom (or just an atom) is a first order formula of the form \( P(t_1, \ldots, t_n) \) where \( P \) is a predicate of arity \( n \) and \( t_1, \ldots, t_n \) are some terms.

In the following, we may also group variables into tuples (which are seen as sets when convenient). Let \( x_1, \ldots, x_n \) be pairwise disjoint tuples of variables. Then, \( X[x_1, \ldots, x_n] \) denotes a conjunction of atoms whose variables are among \( x_1 \cup \cdots \cup x_n \).

Definition 4. An (existential) rule \( R \) is a first-order formula of the following form:

\[
\forall \vec{x}\forall \vec{y}. \ B[\vec{x}, \vec{y}] \rightarrow \exists \vec{z}. \ H[\vec{x}, \vec{z}]
\]

where \( B[\vec{x}, \vec{y}] \) and \( H[\vec{x}, \vec{z}] \) are conjunctions of atoms called the body and the head of the rule, respectively. The set \( \vec{x} \), which is shared between the body and the head, is called the frontier of the rule and is denoted by \( \text{fr}R \). An existential rule where \( \vec{z} \) is empty is a Datalog rule.

For the sake of readability, we omit universal quantifiers when writing existential rules, and we denote conjunctions of atoms with commas instead of wedges. For instance, the rule \( \forall x, y. \ A(x) \land P(x, y) \rightarrow \exists z. \ P(y, z) \) will be written \( A(x), P(x, y) \rightarrow \exists z. \ P(y, z) \).

An instance is an existentially closed conjunction of atoms, and a database is an instance featuring only constants. It is usual to identify an instance with the corresponding set of atoms. For instance, the instance \( \exists x, y, z. \ A(x, y) \land B(x, z, y) \) is identified to the set \( \{A(x, y), B(x, z, y)\} \). A knowledge base is a tuple \( K = (R, D) \) where \( R \) is a rule set and \( D \) is an instance.

Definition 5. A conjunctive query is a conjunction of atoms. We call the free variables of a conjunctive query its answer variables. A Boolean conjunctive query is a conjunctive query that has no answer variable.

Note that by this definition, a Boolean conjunctive query (BCQ) is an instance.
In this setting, homomorphisms are often denoted as sets of individual variable mappings. For example, the homomorphism from \( \{x, y, z\} \) to \( \{a, b\} \) such that \( \sigma(x) = a, \sigma(y) = a \) and \( \sigma(z) = b \) can be denoted by \( \{x \mapsto a, y \mapsto a, z \mapsto b\} \).

**Definition 6.** A retraction \( r \) from a set of atoms \( D \) to \( D' \subseteq D \) is a homomorphism from \( D \) to \( D' \) such that \( r_{|D'} = \text{id}_{D'} \) and \( r(D) = D' \).

### 2.2 Semantics

We rely on classical first-order logic semantics. Indeed, the following definitions can be derived from the classical ones by considering the knowledge base \((\mathcal{R}, \mathcal{D})\) as the theory \(\mathcal{R} \cup \mathcal{D}\) (recall that an instance is a formula).

An instance \( \mathcal{D} \) satisfies (or models) a rule \( \mathcal{R} = B \rightarrow H \), denoted with \( \mathcal{D} \models \mathcal{R} \), if for every homomorphism \( \pi \) from \( B \) to \( D \), there is an extension \( \hat{\pi} \) of \( \pi \) to \( B \cup H \) such that \( \hat{\pi}(H) \subseteq D \). A model \( \mathcal{M} \) of a knowledge base \((\mathcal{R}, \mathcal{D})\) is a set of atoms such that \( \mathcal{D} \subseteq \mathcal{M} \) that satisfies all the rules in \( \mathcal{R} \). A model \( \mathcal{M} \) of a knowledge base \( \mathcal{K} \) is universal if for every model \( \mathcal{M}' \) of \( \mathcal{K} \), there is a homomorphism from \( \mathcal{M} \) to \( \mathcal{M}' \). An instance \( \mathcal{D}_1 \) entails an instance (or a BCQ) \( \mathcal{D}_2 \) if there is a homomorphism from \( \mathcal{D}_2 \) to \( \mathcal{D}_1 \). A knowledge base \((\mathcal{R}, \mathcal{D}_1)\) entails an instance (or a BCQ) \( \mathcal{D}_2 \) if every model of \((\mathcal{R}, \mathcal{D}_1)\) entails \( \mathcal{D}_2 \). In both cases, \( \mathcal{A} \) entails \( \mathcal{B} \) is denoted by \( A \models B \).

Note that by this definition, if \( \mathcal{U} \) is a universal model of a knowledge base \( \mathcal{K} \), then for every model \( \mathcal{M} \) of \( \mathcal{K} \), \( \mathcal{M} \models \mathcal{U} \). Thus, given a BCQ \( q \), if \( \mathcal{U} \models q \), then for any model \( \mathcal{M} \) of \( \mathcal{K} \), we have \( \mathcal{M} \models q \), and if \( \mathcal{U} \not\models q \), then there is a model of \( \mathcal{K} \) that does not model \( q \). Thus, \( \mathcal{K} \models q \) if and only if \( \mathcal{U} \models q \). This motivates the study of an algorithm to find universal models in order to solve BCQ entailment.

### 2.3 The chase

The chase is a family of algorithms mainly used to solve BCQ entailment, through repeated rule applications until a fixpoint is reached. The chase is indeed sound and complete [2], but since the problem of BCQ entailment is semi-decidable [1], it does not necessarily terminate. To define it properly, we first introduce the notion of a trigger.

**Definition 7.** A trigger \( t \) for an instance \( \mathcal{D} \) is a pair \((\mathcal{R}, \pi)\) consisting of a rule \( \mathcal{R} = B \rightarrow H \) and a homomorphism from \( B \) to \( \mathcal{D} \). We then define \( \pi^R \) as the extension of \( \pi \) that maps every existential variable \( z \) in \( \mathcal{R} \) to the fresh variable \( z_i \) that is unique for \( z \) and \( t \). A trigger \( t = (\mathcal{R}, \pi) \) is Datalog if \( \mathcal{R} \) is Datalog, and existential otherwise. The trigger \( t \) is applicable on \( \mathcal{D} \) if \( \pi^R(H) \not\subseteq \mathcal{D} \). We denote \( \pi(B) \) and \( \pi^R(H) \) by support(t) and output(t), and refer to them as the support and the output of \( t \), respectively.

Now, that we have a basic notion of applicability, we can define derivations, before refining the notion of applicability to exhibit different chase variants.

**Definition 8.** Let \( \mathcal{K} = (\mathcal{R}, \mathcal{D}) \) be a knowledge base. A derivation from \( \mathcal{K} \) is a (possibly infinite) sequence \( \mathcal{D} = \mathcal{D}_0, \mathcal{D}_1, \mathcal{D}_2, \ldots \) where \( \mathcal{D}_0 = \mathcal{D} \), and for each \( i > 0 \), \( \mathcal{D}_i \) is a trigger for the instance \( \mathcal{D}_{i-1} \) and \( \mathcal{D}_i = \mathcal{D}_{i-1} \cup \text{output}(t_i) \). The result of a derivation is the set \( \text{res}(\mathcal{D}) = \bigcup_i \mathcal{D}_i \).
Note that \( \text{res}(D) \) is well-defined for every derivation \( D = D_0, t_1, D_1, \ldots \) (finite or not) because \( \{D_i\}_{i \geq 0} \) is an increasing sequence for \( \subset \) for every derivation.

In the following it will be useful to distinguish between two variants of the chase, namely the oblivious chase (\( \mathcal{O} \)) and the restricted chase (\( \mathcal{R} \)). They differ from each other in how they constrain trigger applicability, as specified in the next definition.

**Definition 9.** Let \( \mathcal{K} = (\mathcal{R}, D) \) be a knowledge base, \( D = D_0, t_1, D_1, \ldots \) be a derivation from \( \mathcal{K} \), and \( t = (R, \pi) \) a trigger applicable on \( \text{res}(D) \). Then \( t \) is:

- \( \mathcal{O} \)-applicable on \( D \) if there is no \( i \) such that \( t = t_i \).
- \( \mathcal{R} \)-applicable on \( D \) if there is no retraction from \( \text{res}(D) \cup \text{output}(t) \) to \( \text{res}(D) \).

An \( \mathcal{X} \)-derivation (with \( \mathcal{X} \in \{\mathcal{O}, \mathcal{R}\} \)) is a derivation \( D = D_0, t_1, D_1, \ldots \) for which every trigger \( t_i \) is \( \mathcal{X} \)-applicable on \( D_{i-1} \). A Datalog-first \( \mathcal{X} \)-derivation is an \( \mathcal{X} \)-derivation \( D = D_0, t_1, D_1, \ldots \) such that for all \( i \), if \( t_i \) is existential, then there is no Datalog trigger \( \mathcal{X} \)-applicable on \( D_{i-1} \).

Datalog-first derivations consist of a succession of closure under Datalog rules and applications of a single existential trigger. Thus, in the following, we will write Datalog-first derivations from \( (\mathcal{R}, D) \) as \( D = D_0, t_1, D_1, \ldots \), where for all \( i \), \( t_i \) is an existential trigger and \( D_i \) is a derivation from \( (\mathcal{R}, \text{res}(t_i)) \) that features only Datalog triggers.

**Theorem 10.** If \( D \) is a chase sequence from a knowledge base \( (\mathcal{R}, D) \), then \( (\mathcal{R}, D) \models q \) if and only if \( \text{res}(D) \models q \), for all queries \( q \).

### 2.4 Some Computability theory

**Definition 11.** A Turing machine \( M \) is a tuple \( (Q, q_0, q_f, \delta) \) where \( Q \) is a set of states, \( q_0 \) and \( q_f \) are two special states called the initial and the final state, respectively, and \( \delta : (Q \setminus \{q_f\}) \times \{0, 1, B\} \to (Q \setminus \{q_0\}) \times \{0, 1, B\} \times \{\leftarrow, \rightarrow\} \) is a function called the transition function.

A configuration of a Turing machine is a triple \( (q, h, T) \) where \( q \) is a state, \( h \) is an integer called the position of the head, and \( T : \{0, 1, \ldots, n\} \to \{0, 1, B\} \) is the tape, that is such that \( T(n) = B \), and where \( n \) is an integer. We then say that the tape is of size \( n \). The start configuration \( C_0 \) of \( M \) on a word \( w \) (on the alphabet \( \{0, 1\} \) ) is \( (q_0, 0, T_0) \) where \( T_0 \) is a tape of size \( |w| \) such that for all \( i \) between 0 and \( |w| \), we have \( T_0(i) = w[i] \).

The run of \( M \) on a word \( w \) is a sequence \( C_0, C_1, \ldots \) of configurations such that \( C_0 \) is the start configuration of \( M \) on \( w \), and for all \( t \), if \( C_t = (q_t, h_t, T_t) \), then \( T_t \) is of size \( t \) and:

- If \( q_t = q_f \), then \( C_t \) is the last element of the run. In this case, we say \( M \) halts on \( w \) at step \( t \).
- If \( \delta(q_t, T_t(h_t)) = (q, c, \leftarrow) \) and \( h_t = 0 \), then we say \( M \) halts on \( w \) at step \( t \).
- If \( \delta(q_t, T_t(h_t)) = (q, c, \leftarrow) \) and \( h_t > 0 \), then \( C_{t+1} = (q, h_t - 1, T_{t+1}) \).
• If $\delta(q_t, T_t(h_t)) = (q, c, \rightarrow)$, then $C_{t+1} = (q, h_t + 1, T_{t+1})$.

where $T_{t+1}(h_t) = c$, $T_{t+1}(t + 1) = B$, and $T_{t+1}(i) = T_t(i)$ for all $i \neq h_t$ between 0 and $t$.

In the following, we denote the unique run from $M$ on the empty word as $r^M = C^M_0, C^M_1, \ldots$, with $C^M_t = (q_t, h_t, T_t)$ for all $t \geq 0$, and we write $M(i, t) = T_t(i)$, so $M(i, t)$ is the content of position $i$ of $M$’s tape at step $t$.

If $M$ halts on the empty word, we denote with $\text{time}_\varepsilon(M)$ the index at which it does. Otherwise, we define $\text{time}_\varepsilon(M) = \infty$.

Note that this definition of a Turing machine is a bit unusual, to make the representation using existential rules and the proofs a bit simpler. First, we do not consider acceptance or rejection, but only halting and not halting. In addition, instead of the usual “infinite tape” that Turing machines feature, we use a tape of unbounded size, but which is finite at each step. In addition, the size of the tape is not its real size: as a tape $T$ of size $n$ is a function from $\{0, 1, \ldots, n\}$ to our alphabet, it actually features $n + 1$ cases. This can be explained by the fact that we ask for $T(n)$ to be $B$, which ensures that the head of the Turing machine always has something to read (otherwise, when starting from the empty word $\varepsilon$, the head would not be able to the tape in the starting configuration). Though, the size of the word represented on the tape is indeed the size of the tape as we define it (the empty word has size 0).
Chapter 3

OBQA over Datalog-expressible rule sets is undecidable

We present a reduction that takes a Turing machine $M$ and produces a rule set $\mathcal{R}_M$ such that

1. The Turing machine $M$ halts on the empty word if and only if $(\mathcal{R}_M, \emptyset) \models \text{Goal}$.

2. The couple rule set-query $(\mathcal{R}_M, \text{Goal})$ is Datalog-expressible.

Provided we can construct such a reduction, if we assume, by the absurd, that there is an algorithm that decides entailment for Datalog-expressible rule sets, then we can decide if $M$ halts, which contradicts the undecidability of the halting problem. Thus, this is enough to prove Theorem 3. We then exhibit such a rule set, before proving it enjoys both these properties.

3.1 The rule set

**Definition 12.** For a TM $M$, let $\mathcal{R}_M$ be the rule set containing the following rules:

\[
\begin{align*}
\mathcal{R}_0 & : q_0(w_0, w_0) \\
\mathcal{R}_1 & : q_0(w_0, w_0) \rightarrow \exists w_1. N(w_0, w_1) \\
\mathcal{R}_{+1} & : N(w_i, w_{i+1}) \rightarrow N^+(w_i, w_{i+1}) \\
\mathcal{R}_{N^+} & : N(w_i, w_{i+1}), N^+(w_{i+1}, w_k) \rightarrow N^+(w_i, w_k) \\
\mathcal{R}_B & : q_0(w_0, w_0) \rightarrow B(w_0, w_0) \\
\mathcal{R}_8 & : q_0(w_0, w_0), N^+(w_0, w_i) \rightarrow B(w_i, w_i) \\
\mathcal{R}_{\text{Goal}} & : q_f(x, y) \rightarrow \text{Goal}
\end{align*}
\]
For every $q,q' \in Q$, $c,c' \in \{0,1,B\}$ such that $\delta(q,c) = (q',c',\leftarrow)$,

$$N(p_1,p_2), N(t_1,t_2), q(p_2,t_1), c(p_2,t_1), N^+(p_2,t_2) \rightarrow q'(p_1,t_2), c'(p_2,t_2)$$

($R^+_{q,c}$)

For every $q,q' \in Q$, $c,c' \in \{0,1,B\}$ such that $\delta(q,c) = (q',c',\rightarrow)$,

$$N(p_1,p_2), N(t_1,t_2), q(p_1,t_1), c(p_1,t_1), N^+(p_2,t_2) \rightarrow q'(p_2,t_2), c'(p_1,t_2)$$

($R^+_{q,c}$)

$$N(w_1,w_2), q(w_1,w_1), c(w_1, w_1) \rightarrow q'(w_2,w_2), c'(w_1,w_2)$$

($R^{\text{max}}_{q,c}$)

And the rules:

$$N(x,y), N(x,y') \rightarrow \text{Eq}(y,y')$$

($R^+_{\text{func}}$)

$$N(x,y), N(x',y) \rightarrow \text{Eq}(x,x')$$

($R^-_{\text{func}}$)

$$q_0(x,y), q_0(z,t) \rightarrow \text{Eq}(x,y), \text{Eq}(y,z), \text{Eq}(z,t)$$

($R^0_{q_0}$)

$$N^+(x,x) \rightarrow \text{Fail}$$

($R_{\text{cycle}}$)

$$N(w_{-1},w_0), q_0(w_0,w_0) \rightarrow \text{Fail}$$

($R_{-1}$)

$$N^+(x,y), q_1(x,t), q_2(y,t) \rightarrow \text{Fail} \quad \text{for every } q_1, q_2 \in Q$$

($R^0_{\text{step}}$)

$$q_1(x,t), q_2(x,t) \rightarrow \text{Fail} \quad \text{for every } q_1 \neq q_2 \text{ in } Q$$

($R^0_{\text{cell}}$)

$$c_1(x,t), c_2(x,t) \rightarrow \text{Fail} \quad \text{for every } c_1 \neq c_2 \text{ in } \{0,1,B\}$$

($R^0_{\text{cell}}$)

$$N^+(t,x), c(x,t) \rightarrow \text{Fail} \quad \text{for every } c \in \{0,1,B\}$$

($R^0_{\text{cell}}$)

$$\text{Fail} \rightarrow \text{Goal}$$

($R_{\text{Fail}}$)

$$\text{Eq}(x,y), \text{Eq}(y,z) \rightarrow \text{Eq}(x,z)$$

($R_{\text{trans}}$)

$$\text{Eq}(x,y) \rightarrow \text{Eq}(y,x)$$

($R_{\text{sym}}$)

For all predicates $P$ and integers $i$ between 1 and $\text{ar}(P)$, $P(x_1, \ldots, x_{\text{ar}(P)}), \text{Eq}(x_i,y_i) \rightarrow P(x_1, \ldots, y_i, \ldots, x_{\text{ar}(P)})$($R^0_{\text{rep}}$)

### 3.2 $\mathcal{R}_M \text{ simulates } M$

This section is dedicated to proving the following theorem.

**Theorem 13.** The Turing machine $M$ halts on the empty word if and only if $(\mathcal{R}_M, \emptyset) \models \text{Goal}$.

Before proving this theorem, we explain the relevant parts of the rule set. For this rule set, we use an encoding derived from the usual grid representation of Turing machines. In the grid representation of Turing machines, one would
usually consider a two-way infinite grid (isomorphic to \( \mathbb{N} \times \mathbb{N} \)), on which the position \((i, j)\) would represent the \(i\)-th cell of the machine’s tape at step \(j\). Then, to encode this representation in existential rules, one would have an individual for each cell and two binary predicates representing the relations “\(x\) is right below \(y\)” and “\(x\) is right at the left of \(y\)”. Finally, one would have a unary predicate for each state and for each tape symbol, and \(q(x)\) would mean that the head is on the cell represented by \(x\) and the Turing machine is at step \(q\) at this time, and \(c(x)\) means that \(x\) contains \(c\).

Here, we use the same representation, but we encode it differently: instead of using unary predicates for the content of the tapes, we use binary predicates. This means that we only need individuals representing \(\mathbb{N}\) and not the full \(\mathbb{N} \times \mathbb{N}\). In addition, we only use one successor predicate instead of two. In our case, this successor predicate is \(N\), and the rules that generate this encoding of \(\mathbb{N}\) are rules \(R_0, R_1\) and \(R_{+1}\). Then, the predicate \(N^+\) is \(N\)’s transitive closure, and is computed by rules \(R_{N^+}\) and \(R_{trans}^N\). In the following, we will refer to the elements of this representation of \(\mathbb{N}\) by \((z_n)_{n \in \mathbb{N}}\): \(z_0\) is the element that does not have a predecessor through \(N\), and \(z_{i+1}\) is \(z_i\)’s successor, for all \(i\).

Then, as we said, we model Turing machine simulation using a binary predicate for each state of the Turing machine and for each character that can appear on the tape. In more detail, we will show in Proposition \(16\) that if \(q(z_i, z_i)\) is in \(\text{chase}(R_M, \emptyset)\) for some state \(q\), then the Turing machine is in state \(q\) at step \(t\), and its head is on position \(i\). Similarly, if \(c(z_i, z_i)\) is in \(\text{chase}(R_M, \emptyset)\), then the character at position \(i\) of the tape at step \(t\) is \(c\). Rules \(R_0, R_0^c\) and \(R_b\) initialize this calculation, rules \(R_{q,c}^-\) and \(R_{q,c}^+\) move the head and change the character, and rules \(R_{q,c}^{\text{L}}\) and \(R_{q,c}^{\text{R}}\) propagate the symbols that do not change. Finally, rules \(R_{\text{Goal}}\) and \(R_{q,c}^{\text{sym}}\) generate \(\text{Goal}\) whenever the Turing machine encounters \(q_f\) or tries to move its head left when it is on position \(0\), that is to say whenever it halts. The remaining rules will not do much on the empty database, and will be useful later to ensure that the rule set is Datalog expressible. We will thus explain them later. We first show a quick lemma that will be useful in the proof of Theorem \(13\).

**Lemma 14.** Let \(D\) be an instance and \(t\) a term in \(D\). There is no trigger \((R, \pi)\) that is applicable on \(D\) and such that \(\text{Eq}(t, t) \in \pi(\text{body}(R))\).

**Proof.** Suppose for a contradiction that there is such a trigger. Then, since the only rules that feature an \(\text{Eq}\)-atom in their body are rules \(R_{\text{trans}}^t\), \(R_{\text{sym}}^t\) and \(R_{\text{cpt}}^t\), the rule \(R\) must be one of these three.

- If \(R = R_{\text{trans}}^t\), then two cases are possible. Either \(\pi(x) = \pi(y) = t\) and \(\pi(z) = u\) such that \(\text{Eq}(t, u) \in D\), and \((R, \pi)\) yields \(\text{Eq}(t, u)\) or \(\pi(y) = \pi(z) = t\) and \(\pi(x) = u\) with \(\text{Eq}(u, t) \in D\) and \((R, \pi)\) yields \(\text{Eq}(u, t)\). In either case, \(\text{output}(R, \pi) \subseteq D\) so the trigger is not applicable.

- If \(R = R_{\text{sym}}^t\), then \(\pi(x) = \pi(y) = t\), and \((R, \pi)\) yields \(\text{Eq}(t, t)\), which is by hypothesis in \(D \cup \{\text{Eq}(t, t)\}\), so this trigger is not applicable either.

- If \(R = R_{\text{cpt}}^t\), then there is an atom \(P(t_1, \ldots, t_{i-1}, t, t_{i+1}, \ldots, t_n)\) (with \(n = \text{art}(P)\)). Then, again, \((R, \pi)\) yields \(P(t_1, \ldots, t_{i-1}, t, t_{i+1}, \ldots, t_n)\), which is in \(D \cup \{\text{Eq}(t, t)\}\) by hypothesis, so \((R, \pi)\) is not applicable in this case either. \(\square\)
Then, to show Theorem 13, we will specify the result of Datalog-first derivations. We first define a few sets that will be useful to express this result.

**Definition 15.** For all \( n \), we define the following sets

\[
\begin{align*}
D_n^N &= \{ N(z_i, z_{i+1}) \mid 0 \leq i < n \} \\
D_n^{N^+} &= \{ N^+(z_i, z_j) \mid 0 \leq i < j \leq n \} \\
D_n^Q &= \{ q_t(z_i, z_t) \mid 0 \leq t \leq \min(n, \text{time}_c(M)) \} \\
D_n^\Sigma &= \{ \varepsilon(z_i, z_t) \mid 0 \leq t \leq \min(n, \text{time}_c(M)), 0 \leq i \leq t, M(i, t) = c \} \\
D_n^{\text{eq}} &= \{ \text{Eq}(z_i, z_t) \mid 0 \leq i \leq n \} \\
D_n^{\text{goal}} &= \{ \text{Goal} \} \text{ if } n \geq \text{time}_c(M) \text{ and } \emptyset \text{ otherwise.}
\end{align*}
\]

We can now formulate the following proposition.

**Proposition 16.** For a Datalog-first derivation \( D = D_{\text{init}}, t_0, D_0, t_1, D_1, \ldots \) from \((R_M, \emptyset)\), we have that:

- \( t_0 = ((R_0), \emptyset) \) and \( t_1 = (R_1, \{ w_0 \mapsto z_0 \}) \)
- For all \( n > 1 \), \( t_n = (R_{n+1}, \{ w_0 \mapsto z_0, w_i \mapsto z_{n-1} \}) \)
- For all \( n \in \mathbb{N} \), \( \text{res}(D_n) = D_n^N \cup D_n^{N^+} \cup D_n^Q \cup D_n^\Sigma \cup D_n^{\text{eq}} \cup D_n^{\text{goal}} \)

Proof. We proceed by induction on \( n \).

At step \( n = 0 \), on the database \( \emptyset \), only rules with an empty body are applicable. As \( R_0 \) is the only rule with an empty body, it is applicable, so \( D_{\text{init}} \) is empty and \( t_0 = (R_0, \emptyset) \), with \( \text{res}(t_0) = \{ q_0(z_0, z_0) \} \). Then, rules \( R_0^\emptyset \) and \( R_0 \) are applicable and yield \( B(z_0, z_0) \) and \( \text{Eq}(z_0, z_0) \), respectively. Finally, if \( \delta(q_0, B) = (q', c, \leftarrow) \) for some \( q', c \), then rule \( R_0^\emptyset, B \) is applicable, and if \( q_0 = q_f \), \( R_{\text{goal}} \) is applicable. In both these cases, the application yields \( \text{Goal} \), and by definition of a run, \( \text{time}_c(M) = 0 \). We then show that \( \text{res}(D_0) = D_0^N \cup D_0^{N^+} \cup D_0^Q \cup D_0^\Sigma \cup D_0^{\text{eq}} \cup D_0^{\text{goal}} \) by double inclusion. For the converse inclusion, note that \( D_0^N \) and \( D_0^{N^+} \) are empty, and by definition of a starting configuration, we have \( D_0^Q = \{ q_0(z_0, z_0) \} \) and \( D_0^\Sigma = \{ \text{Eq}(z_0, z_0) \} \). In addition, we also have \( D_0^{\text{eq}} = \{ \text{Eq}(z_0, z_0) \} \). Then, \( D_0^{\text{goal}} = \{ \text{Goal} \} \) if \( \text{time}_c(M) = 0 \) (case in which \( \text{Goal} \in \text{res}(D_0) \)), and \( D_0^{\text{goal}} = \emptyset \) otherwise. Thus, the converse inclusion holds.

Then, for the direct inclusion, we show that no Datalog rule is applicable on \( D_0^N \cup D_0^{N^+} \cup D_0^Q \cup D_0^\Sigma \cup D_0^{\text{eq}} \cup D_0^{\text{goal}} = \{ q_0(z_0, z_0), B(z_0, z_0) \} \cup D_0^{\text{goal}} \). First notice that all Datalog rules except \( R_{\text{goal}} \) can only be mapped into \( \{ q_0(z_0, z_0), B(z_0, z_0) \} \cup D_0^{\text{goal}} \) if \( \text{time}_c(M) = 0 \). Indeed, if rule \( R_{\text{goal}} \)'s body can be mapped, then there is \( q_f(x, y) \) in the database, so \( q_0 = q_f \), and if \( R_{q,c} \)'s body can be mapped, then \( q = q_0, c = B \) and \( \delta(q_0, B) = (q', c', \leftarrow) \). Thus, in both cases, \( \text{time}_c(M) = 0 \), so \( \text{Goal} \in D_0^{\text{goal}} \subseteq \text{res}(D_0) \), and these rules are not applicable.

Regarding rule \( R_{q,c} \), as it has already been applied with its body mapped to the only \( q_0 \)-atom, it is not applicable either. Rule \( R_{q_1,c_1}^\text{cell} \) (resp. \( R_{c_2}^\text{cell} \)) has two atoms that use distinct state (resp. character) predicates in its body. As there is
only one state (resp. character) atom in $\text{res}(D'_0) \cup D_0^{eq}$, rule $R^{cell}_{\text{cell}}$ (resp. $R^{cell}_{\text{cell}}$) is not applicable. As $\text{Fail} \notin \text{res}(D'_0)$, rule $R_{\text{Fail}}$ is not applicable either. Finally, if $t = (R, \pi)$ is a trigger such that $R \in \{ R^{\text{trans}}, R^{\text{sym}}, R^{\text{input}} \}$, then there must be an $Eq$-atom in $\pi(\text{body}(R))$. As $\text{Eq}(z_0, z_0)$ is the only $Eq$-atom in $\text{res}(D'_0) \cup D_0^{eq}$, it must be that $\text{Eq}(z_0, z_0) \in \pi(\text{body}(R))$, which by Lemma 14 means that $t$ is not applicable. Thus, the equality holds in the base case.

Before proving the inductive step, we prove that $t_1 = (R_1), \{ w_0 \mapsto z_0 \}$. Since $\text{res}(D_0) = \{ q_0(z_0, z_0) \}$, rule $R_{\text{Res}}$ is not applicable (it has a $N^+$-atom in its body). Since rule $R_0$ has already been applied with the only homomorphism possible, the only applicable rule is $R_{\text{1}}$, so $t_1 = (R_1), \{ w_0 \mapsto z_0 \}$.

Now, for the inductive step, assume that $n > 0$ and that the lemma is true for all $i < n$. We first prove that if $n > 1$, $t_n = (R_{n+1}), \{ w_1 \mapsto z_{n-1}, w_0 \mapsto z_0 \}$. By definition of a Turing machine, $q_0$ can only appear at step and position 0, so by induction hypothesis, the only term $x$ such that $q_0(x, z) \in \text{res}(D'_{n-1}) = z$. Thus, all the homomorphisms from the body of rule $R_{n+1}$ to $\text{res}(D'_{n-1})$ are of the form $\{ w_1 \mapsto z_j, w_0 \mapsto z_0 \}$ with $0 \leq j \leq n-1$. Again by induction hypothesis, all triggers $(R_{n+1}), \{ x_1 \mapsto z_j, w_0 \mapsto z_0 \}$ for $2 \leq j \leq n-2$ have been applied at earlier steps, so the only applicable existential trigger is $(R_{n+1}), \{ w_1 \mapsto z_{n-1}, w_0 \mapsto z_0 \}$.

We now come back to the more general case $n > 0$, and we prove that $D^n_0 \subseteq \text{res}(D'_n)$; by induction hypothesis, $D^{n-1}_0 \subseteq \text{res}(D'_{n-1}) \subseteq \text{res}(D'_n)$. Then, if $n = 1$, $\text{output}(t_1) = \{ N(z_0, z_1) \} = \{ N(z_{n-1}, z_n) \}$, and if $n > 1$, $\text{output}(t_n) = \{ N(z_{n-1}, z_n) \}$, so in either case, $D^n_0 \subseteq \text{res}(D'_n)$.

$D^{N^+}_n \subseteq \text{res}(D'_n)$ by induction hypothesis, $D^{n-1}_n \subseteq \text{res}(D'_{n-1}) 
\subseteq \text{res}(D'_n)$, so it is enough to show that for all $i$ such that $0 \leq i < n$, we have $N^+(z_i, z_n) \in \text{res}(D'_n)$, or equivalently that for all $i$ such that $1 \leq i \leq n$, we have $N^+(z_{n-1}, z_n) \in \text{res}(D'_n)$. We prove this last result by induction on $i$.

We first show that if $i = 1$, then $N^+(z_{n-1}, z_n) \in \text{res}(D'_n)$. As $D^n_0 \subseteq \text{res}(D'_n)$, we have $N(z_{n-1}, z_n) \in \text{res}(D'_n)$. Thus, since $\text{res}(D'_n)$ satisfies rule $R_{\text{Res}}$, the atom $N^+(z_{n-1}, z_n)$ is in $\text{res}(D'_n)$.

For the induction step, we show that if $1 < i \leq n$ and $N^+(z_{n-(i-1)}, z_n) \in \text{res}(D'_n)$, then $N^+(z_{n-1}, z_n) \in \text{res}(D'_n)$. Since $D^n_0 \subseteq \text{res}(D'_n)$, we have $N(z_{n-1}, z_n) \in \text{res}(D'_n)$. As $n - i + 1 = n - (i - 1)$, the atoms $N(z_{n-1}, z_{n-1})$ and $N^+(z_{n-1}, z_n)$ are both in $\text{res}(D'_n)$. Thus, since $\text{res}(D'_n)$ models rule $R^{\text{trans}}_{\text{Res}}$, $N^+(z_{n-(i-1)-1}, z_n) \in \text{res}(D'_n)$.

$D^{Q}_n \subseteq \text{res}(D'_n)$: First, notice that if $n > time_c(M)$, then $D^n_Q = D^Q_{n-1}$, so the induction hypothesis suffices. We thus only consider the case where $n \leq time_c(M)$ in the following. We then want to show that $q_n(z_{h_{n-1}}, z_n) \in \text{res}(D'_n)$. As $q_{n-1} \neq q_f$, there are $q_n, c, c', d$ such that $c = M(h_{n-1}, n - 1)$ and $\delta(q_n, c) = (q_f, c', d)$. By induction hypothesis, both the atoms $q_{n-1}(z_{h_{n-1}}, z_n)$ and $c(z_{h_{n-1}}, z_n)$ are in $\text{res}(D'_n)$. In addition, as $h_{n-1} \leq n - 1 < n$, we also have $N^+(z_{h_{n-1}}, z_n) \in \text{res}(D'_n)$, and we showed earlier that $N(z_{n-1}, z_n) \in \text{res}(D'_n)$. Thus:

- If $d \rightarrow$, as $h_{n-1} < n$, we have $N(z_{n-1}, z_{n-1}+1) \in \text{res}(D'_n)$. Thus, $t_{n-1} = (R_{q_{n-1}, c'}, \{ p_i \mapsto z_{h_{n-1}}, p_{i+1} \mapsto z_{h_{n-1}+1}, t_i \mapsto z_{n-1}, t_{i+1} \mapsto z_n \})$.
is applicable. In this case, by definition, \( h_n = h_{n-1} + 1 \), so this trigger yields the atoms \( q_n(z_{h_n}, z_n) \) and \( c'(z_{h_{n-1}}, z_n) \).

- If \( d = \leftarrow \), since \( n - 1 < t_{\text{ime}}(M) \), then \( h_{n-1} > 0 \), so we have \( \mathcal{N}(z_{h_{n-1}}, z_{h_{n-1}}) \in \text{res}(\mathcal{D}_n') \). Thus, the trigger

\[
t = (\mathcal{R}_{q_{n-1}, c}, \{ p_{i-1} \mapsto z_{h_{n-1}}, p_i \mapsto z_{h_{n-1}}, t_i \mapsto z_{n-1}, t_{i+1} \mapsto z_n \})
\]

is applicable. In this case, by definition, \( h_n = h_{n-1} - 1 \), so this trigger yields the atoms \( q_n(z_{h_n}, z_n) \) and \( c'(z_{h_{n-1}}, z_n) \).

Thus, in either cases, we have \( q_n(z_{h_n}, z_n) \) and \( c'(z_{h_{n-1}}, z_n) \) in \( \text{res}(\mathcal{D}_n') \), so \( \mathcal{D}_n^0 \subseteq \text{res}(\mathcal{D}_n') \).

1. If \( n_{\text{ime}}(M) \), then \( \mathcal{D}_n^0 = \mathcal{D}_n^{n-1} \), so the induction hypothesis suffices. In the following, we restrict ourselves to the case \( n \leq t_{\text{ime}}(M) \). We thus need to prove that \( c_i(z_i, z_n) \in \text{res}(\mathcal{D}_n') \) for all \( i \) such that \( 0 \leq i \leq n \) and \( M(i, n) = c_i \). There are four cases:

- If \( i < h_{n-1} \), then \( c_i = M(i, n) = M(i, n - 1) \). By induction hypothesis, the atoms \( q_i(z_i, z_{n-1}) \), \( q_{n-1}(z_{h_{n-1}}, z_{n-1}) \) and \( \mathcal{N}^+(z_i, z_{h_{n-1}}) \) are in \( \text{res}(\mathcal{D}_n') \). In addition, since \( \mathcal{D}_n^N \subseteq \text{res}(\mathcal{D}_n') \), we have \( \mathcal{N}(z_{n-1}, z_n) \in \text{res}(\mathcal{D}_n') \). Thus, as \( \text{res}(\mathcal{D}_n') \) satisfies rule \( R^L_{q_{n-1}, c} \), we have \( c_i(z_i, z_n) \in \text{res}(\mathcal{D}_n') \).

- If \( i = h_{n-1} \), as seen in the previous case, we have \( c_i'(z_{h_{n-1}}, z_n) \), with \( c' \) such that \( \delta(q_{n-1}, M(h_{n-1}, n - 1)) = (q', c', d) \). By definition of a run, \( c' = M(h_{n-1}, n) = c_i \), which concludes this case.

- If \( h_{n-1} < i < n \), then \( c_i = M(i, n) = M(i, n - 1) \). As \( i \leq n - 1 \), by induction hypothesis, the atoms \( q_i(z_i, z_{n-1}) \), \( q_{n-1}(z_{h_{n-1}}, z_{n-1}) \) and \( \mathcal{N}^+(z_i, z_{h_{n-1}}) \) are in \( \text{res}(\mathcal{D}_n') \). In addition, since \( \mathcal{D}_n^N \subseteq \text{res}(\mathcal{D}_n') \), we have \( \mathcal{N}(z_{n-1}, z_n) \in \text{res}(\mathcal{D}_n') \). Thus, as \( \text{res}(\mathcal{D}_n') \) satisfies rule \( R^L_{q_{n-1}, c} \), we have \( c_i(z_i, z_n) \in \text{res}(\mathcal{D}_n') \).

- If \( i = n \), a usual property of Turing machines states that \( M(n, n) = \mathcal{B} \), as a Turing machine can only move one step at a step and edit the bit its head was on at a previous step. As \( \mathcal{D}_n^{N^+} \subseteq \text{res}(\mathcal{D}_n') \), we have \( \mathcal{N}^+(z_0, z_n) \in \text{res}(\mathcal{D}_n') \). Thus, as \( \text{res}(\mathcal{D}_n') \) satisfies rule \( R_B \), the atom \( \mathcal{B}(z_n, z_n) \) is in \( \text{res}(\mathcal{D}_n') \).

\( \mathcal{D}_n^0 \subseteq \text{res}(\mathcal{D}_n) \): As we saw earlier, the atom \( \mathcal{N}(z_{n-1}, z_n) \) is in \( \text{res}(\mathcal{D}_n) \), so rule \( R^L_{q_{n-1}, c} \) is applicable by mapping \( x \) to \( z_{n-1} \), and \( y \) and \( y' \) to \( z_n \). This application yields the atom \( \mathcal{Q}(z_n, z_n) \), so \( \mathcal{D}_n^0 \subseteq \text{res}(\mathcal{D}_n) \) (as we already had \( \mathcal{D}_n^{n-1} \subseteq \text{res}(\mathcal{D}_n) \) by induction hypothesis).

\( \mathcal{D}_n^{\text{goal}} \subseteq \text{res}(\mathcal{D}_n) \): If \( n < t_{\text{ime}}(M) \), the result follows from the fact that \( \mathcal{D}_n^{\text{goal}} \) is empty in this case. Otherwise, if \( n \geq t_{\text{ime}}(M) \), then there are two cases:

- If \( q_{t_{\text{ime}}(M)} = q_f \), since \( \mathcal{D}_n^0 \subseteq \text{res}(\mathcal{D}_n) \), \( q_f(z_{t_{\text{ime}}(M)}, z_{t_{\text{ime}}(M)}) \) in \( \text{res}(\mathcal{D}_n') \). Thus, as \( \text{res}(\mathcal{D}_n') \) models rule \( R_{\text{goal}} \), \( \text{goal} \in \text{res}(\mathcal{D}_n') \).
Otherwise, we have \( h_{\text{time}_c(M)} = 0 \) and
\[
\delta(q_{\text{time}_c(M)}, M(0, \text{time}_c(M))) = (q, c, \leftarrow)
\]
for some \( q \) and \( c \). In this case, as \( D_n^Q \cup D_n^S \subseteq \text{res}(\mathcal{D}_n') \), the atoms
\( q_{\text{time}_c(M)}(z_0, z_{\text{time}_c(M)}) \) and \( c_0(z_0, z_{\text{time}_c(M)}) \) are in \( \text{res}(\mathcal{D}_n') \), with \( c_0 = M(0, \text{time}_c(M)) \). Thus, as \( \text{res}(\mathcal{D}_n') \) satisfies rule \( R_{q,c}^0, \text{Goal} \in \text{res}(\mathcal{D}_n') \).

This concludes the proof of the first inclusion. To show that the other inclusion holds, we will show that \( \mathcal{D} = D_n^N \cup D_n^N^+ \cup D_n^Q \cup D_n^S \cup D_n^R \cup D_n^\text{Goal} \) satisfies all the Datalog rules in \( \mathcal{R}_M \).

\( R_{N^+}^n \): Let \( i, j \) be such that \( N(z_i, z_j) \in D \). Then, by the definition of \( D_n^N \), we have \( 0 \leq i < n \) and \( j = i + 1 \), so \( 0 \leq i < j \leq n \). Thus, by the definition of \( D_n^N^+ \), \( N^+(z_i, z_j) \in D \), so \( R_{N^+}^n \) is satisfied by \( D \).

\( R_{N^+}^{\text{trans}} \): Assume that \( N(z_i, z_j) \) and \( N^+(z_j, z_k) \) are in \( D \), for some \( i, j, k \). Then, by the definition of \( D_n^N \), we have \( 0 \leq i < n \) and \( j = i + 1 \), so \( 0 \leq i < j \leq n \). In addition, by the definition of \( D_n^N^+ \), we have \( 0 \leq j < k \leq n \), so \( 0 \leq i < j \leq n \). In particular, we have \( 0 \leq i < k \leq n \), so \( \text{N}^+(z_i, z_j) \in D \), and \( R_{N^+}^{\text{trans}} \) is satisfied by \( D \).

\( R_0^0 \): The only term \( x \) such that \( q_0(x, x) \in D \) is \( z_0 \), and \( B(z_0, z_0) \in D \), so this rule is not applicable.

\( R_B \): As stated earlier, we have \( M(i, t) = B \) for all \( t \leq i \). In particular, \( M(i, i) = B \) for all \( i \leq n \). Thus, by the definition of \( D_n^S \), all \( 0 \leq i \leq n \), we have \( B(z_i, z_i) \in D \), so rule \( R_B \) is satisfied.

\( R_{\text{Goal}} \): If \( q_f(z_i, z_i) \in D \), for some \( i, t \), then by definition of \( D_n^Q \), \( q_t = q_f \), and thus \( \text{time}_c(M) = t \leq n \). As such, \( D_n^\text{Goal} = \{ \text{Goal} \} \), and rule \( R_{\text{Goal}} \) is satisfied.

\( R_{q,c}^0 \): As stated earlier, the only term \( x \) such that \( q_0(x, x) \in D \) is \( z_0 \). Assume that there are \( q, c \) and \( t \) such that \( \delta(q, c) = (q', c', \leftarrow) \) for some \( q', c', \leftarrow \), and \( q(z_0, z_i) \) and \( c(z_0, z_i) \) are in \( D \). Then, by the definitions of \( D_n^Q \) and \( D_n^S \), \( q_t = q \), \( h_t = 0 \), and \( M(h_t, t) = M(0, t) = c \). Thus, by definition of a run, \( \text{time}_c(M) = t \leq n \), and \( D_n^\text{Goal} = \{ \text{Goal} \} \), so rule \( R_{q,c}^0 \) is satisfied.

\( R_{q,c}^i \): Let \( q, q', c, c' \) and \( i, t \) be such that \( \delta(q, c) = (q', c', \leftarrow) \), and the atoms \( q(z_i, z_t), c(z_i, z_t) \) are in \( D \). Then, by definition of \( D_n^Q \) and \( D_n^S \), we have \( q_t = q \), \( h_t = i \), and \( M(h_t, t) = c \).

Now, assume that there is a homomorphism from \( \text{body}(R_{q,c}^i) \) to \( D \) that sends \( p_i \) to \( z_i \) and \( t_j \) to \( z_t \), and let \( j, t \) be such that \( p_{t-1} \) is mapped to \( z_j \) and \( t_{t+1} \) is mapped to \( z_t \). The atoms \( N(z_j, z_j) \) and \( N(z_t, z_t) \) must then be present in \( D \), so by definition of \( D_n^N \), we have \( 0 \leq j = i - 1 \) and \( t = t + 1 \). To show that \( R_{q,c}^i \) is satisfied, we then show that \( q'(z_{i-1}, z_{t+1}) \) and \( c'(z_{i-1}, z_{t+1}) \) are in \( D \). As \( 0 \leq j = i - 1 \), we have \( i > 0 \), so by definition of a run, we have \( q_{t+1} = M(h_t, t+1) = M(i, t+1) = c' \). Thus, by definition of \( D_n^Q \) and \( D_n^S \), the atoms \( q'(z_{i-1}, z_{t+1}) \) and \( c'(z_{i-1}, z_{t+1}) \) are in \( D \), and rule \( R_{q,c}^i \) is satisfied.
$R^+_{q,c}$: Let $q, q', c, c'$ and $i, t$ be such that $\delta(q, c) = (q', c', \leftarrow)$, and the atoms $q(z_i, z_t)$, $c(z_i, z_t)$ are in $D$. Then, by definition of $D^q_n$ and $D^c_n$, we have $q_t = q$, $h_t = i$ and $M(h_t, t) = c$, so by definition of a run, we have $q_{t+1} = q'$, $h_{t+1} = h_t + 1 = i + 1$ and $M(h_t, t + 1) = M(i, t + 1) = c'$. Now, assume that there is a homomorphism from body($R^+_{q,c}$) to $D$ that sends $p_i$ to $z_i$ and $t_j$ to $z_t$. By definition of $D^N_n$ (as seen in the previous case), $p_{i+1}$ is mapped to $z_{i+1}$ and $t_{j+1}$ is mapped to $z_{t+1}$. Then, rule $R^+_{q,c}$ is satisfied, as the atoms $q'(z_{i+1}, z_{t+1})$ and $c'(z_i, z_{t+1})$ are in $D$. Indeed, as $q_{i+1} = q'$ and $h_{t+1} = i + 1$, the first one is in $D$ by definition of $D^q_n$, and since $M(i, t + 1) = c'$, the second atom is in $D$ by definition of $D^c_n$.

$R^0_{q,c}$: Assume that the atoms $N^+(z_i, z_k)$, $N(z_i, z_{t+1})$, $q(z_k, z_t)$ and $c(z_i, z_t)$ are in $D$, for some $i, k, t$. Then, we have $h_t = k$, $M(i, t) = c$, and $i < k = h_t$ by definitions of $D^q_n$, $D^c_n$ and $D^{N^+}_n$, respectively. Thus, by definition of a run, $M(i, t + 1) = M(i, t) = c$, so $c(z_i, z_{t+1}) \in D$, and $R^0_{q,c}$ is satisfied.

$R^R_{q,c}$: Assume that the atoms $N^+(z_i, z_k)$, $N(z_i, z_{t+1})$, $q(z_k, z_t)$ and $c(z_i, z_t)$ are in $D$, for some $i, k, t$. Then, we have $h_t = i$, $M(k, t) = c$, and $h_t = i < k$ by definitions of $D^q_n$, $D^c_n$ and $D^{N^+}_n$, respectively. Thus, by definition of a run, $M(k, t + 1) = M(k, t) = c$, so $c(z_k, z_{t+1}) \in D$, and $R^R_{q,c}$ is satisfied.

$R^\text{func}_+$: Assume that $N(z_i, z_j)$ and $N(z_i, z_k)$ are in $D$, for some $i, j, k$. Then, by the definition of $D^N_n$, we have $j = k = i + 1$. Thus, since $\text{Eq}(z_{i+1}, z_{i+1}) \in D$, this rule is satisfied.

$R^\text{func}_-$: Assume that $N(z_i, z_k)$ and $N(z_j, z_k)$ are in $D$, for some $i, j, k$. Then, by the definition of $D^N_n$, we have $i = j = k = t = 0$. Since $\text{Eq}(z_0, z_0) \in D$, this rule is satisfied.

$R^{cyc}_{N^+}$: By definition of $D^{N^+}_n$, there is no $x$ such that $N^+(x, x) \in D$, so this rule is not applicable.

$R_{q_0}$: By the definition of $D^q_n$ and a Turing machine, there can only be one term that appears in a $q_0$-atom, which is $z_0$. Thus, if $q_0(z_i, z_j)$ and $q_0(z_k, z_l)$ are in $D$, then $i = j = k = l = 0$. Since $\text{Eq}(z_0, z_0) \in D$, this rule is satisfied.

$R_{-1}$: Again, the only $x$ such that $q_0(x, x) \in D$ is $z_0$. Thus, by definition of $N$, there is no $i$ such that $N(z_i, z_0) \in D$, so this rule is not applicable.

$R^\text{step}_{q_1, q_2}$: Assume that $q_1(z_i, z_t)$ and $q_2(z_j, z_t)$ are in $D$, for some $q_1, q_2, i, j, t$. By definition of $D^q_n$, we then have $i = j = h_t$. Thus, by definition of $D^{N^+}_n$, we do not have $N^+(z_{h_t}, z_{h_t})$, so this rule is never applicable (and thus satisfied).

$R^\text{cell}_{q_1, q_2}$: Assume that $q_1(z_i, z_t)$ and $q_2(z_j, z_t)$ are in $D$, for some $q_1, q_2, i, t$. By definition of $D^q_n$, we then have $q_1 = q_2 = q_t$, so $R^\text{cell}_{q_1, q_2}$ is not in $R_M$ (as it requires $q_1 \neq q_2$). Thus, by contrapositive, no rule $R^\text{cell}_{q_1, q_2}$ in $R_M$ is applicable.
Let $c_1, c_2, i, t$ be such that $c_1(z_i, z_t)$ and $c_2(z_j, z_t)$ are in $D$. By definition of $D^\Sigma_n$, we then have $c_1 = c_2 = M(i, t)$, so $R_{c_1, c_2}$ is not in $R_M$ (as it requires $c_1 \neq c_2$). Thus, by contrapositive, no rule $R_{c_1, c_2}$ in $R_M$ is applicable.

$R_{\text{Goal}}$: Let $c, i, t$ be such that $c(z_i, z_t)$ and $N^+(z_i, z_t)$ are in $D$. By definition of $D_n^\Sigma$, we then have $t < i$, and by definition of $D_n^\Sigma$, we have $i \leq t$, which is a contradiction.

$R_{\text{Fail}}$: As $\text{Fail} \notin D$ this rule is not applicable and thus satisfied.

$\{R_{\text{trans}}, R_{\text{sym}}, R_{\text{repl}}\}$: As all the $\text{Eq}$-atoms in $D$ are of the form $\text{Eq}(x, x)$, by Lemma 14, no trigger $t = (R, \pi)$ such that $\text{body}(R)$ features an $\text{Eq}$-atom in its body is applicable on $D$. As this is the case for these three rules, they are satisfied.

As $D$ satisfies all the Datalog rules in $R_M$, none of these rules is applicable on $D$. Since $D \subseteq \text{res}(D_n')$, we indeed have $\text{res}(D_n') = D$, which concludes the proof.

As the result of all derivations from $(R_M, \emptyset)$ is characterized by this proposition, Theorem 13, which we recall here, is easy to prove.

**Theorem 13.** The Turing machine $M$ halts on the empty word if and only if $(R_M, \emptyset) \models \text{Goal}$.

**Proof.** Consider a Datalog-first derivation $D = t_0, D_0, t_1, D_1, \ldots$ from $(R_M, \emptyset)$. If $(R_M, \emptyset) \models \text{Goal}$, then there is $n \in \mathbb{N}$ such that $\text{Goal} \in \text{res}(D_n')$. By Proposition 16, $\text{res}(D_n')$ contains $\text{Goal}$ if and only if $n \geq \text{time}_c(M)$. Thus, $\text{time}_c(M)$ is finite, and $M$ halts. If $M$ halts, then $\text{time}_c(M)$ is finite. Thus, $\text{res}(D_{\text{time}_c(M)})$ contains $\text{Goal}$ by Proposition 16, so $(R_M, \emptyset) \models \text{Goal}$.

### 3.3 $R_M$ is Datalog expressible

We now show the following theorem.

**Theorem 17.** The pair $(R_M, \text{Goal})$ is Datalog-expressible.

If $M$ halts on the empty word, then $(R_M, \emptyset) \models \text{Goal}$ by Theorem 13, and since entailment w.r.t. first-order theories is monotonic, $(R_M, D) \models \text{Goal}$ for all databases $D$. Thus, the query $(\{\rightarrow \text{Goal}\}, \text{Goal})$ is a rewriting of $R_M$. Now, if $M$ does not halt, while $R_M$ does not entail $\text{Goal}$ on $\emptyset$, there are databases on which $R_M$ entails goal, even if we only consider the rules of $R_M$ up to $R^{\Sigma}_{\text{Goal}}$, that were used for the simulation. For instance, if $D$ already contains $\text{Goal}$, or a $\text{qf}$-atom, then $(R_M, \emptyset) \models \text{Goal}$, but there are also more interesting (and problematic to find a Datalog rewriting for) databases on which the first part of $R_M$ would entail $\text{Goal}$ too.

We call databases on which the first part of $R_M$ entails $\text{Goal}$ even though $M$ does not halt on the empty word false starts. To control the structure of the database and to detect these false starts, we introduce a new predicate $\text{Fail}$, and the rules in the second part of $R_M$ (from $R^{\text{Func}}_{\text{func}}$ onwards). Then, the argument revolves around the notion of Skolem depth of a term.
3.3.1 Skolem depth

Definition 18. Consider a database $D$, a rule set $R$, and a derivation $D = D_0, t_1, D_1, \ldots$ from $(R, D)$. For all $n$, the Skolem depth $SkD(x)$ of a term $x$ appearing in $D_n$ is defined inductively as the following:

- If $x$ is a constant, then its Skolem depth is 0.
- If $x$ is a variable introduced by a trigger $t$, then its Skolem depth is $\max\{SkD(y) \mid y \in \text{support}(t)\} + 1$.

Then, the Skolem depth $SkD(E)$ of a set $E$ of terms is $\max\{SkD(y) \mid y \in E\}$. The Skolem depth of an atom or a trigger (or a set thereof) is then the Skolem depth of the set of variables appearing in it.

The rough idea behind this definition is that existential rules can be “Skolem-ized” by replacing their existential quantifiers with Skolem functions, and the Skolem depth of a term is the maximal depth of nested Skolem functions. This notion is interesting here because of Theorem 7 from [4], that we restate here.

Definition 19. A couple rule set-query has bounded depth if there is $k$ such that for all databases $D$, the following are equivalent:

- $(R, D) \models q$.
- There is a finite derivation $D$ such that $\text{res}(D) \models q$ and all the terms in $\text{res}(D)$ are of Skolem depth less than $k$.

Theorem 20. If $(R, q)$ has bounded depth, then it is Datalog-expressible.

Thus, in the following, we show that $(R_M, \text{Goal})$ has a bounded depth, and that the bound is one. To do so, we distinguish two cases: the databases that entail Fail and those that do not. For the databases that entail Fail, we show that they do it fast: we only need to close under Datalog to see if a database entails Fail. For the other databases, though, we show that (if Goal is not in them), then the body of rules that generate Goal cannot contain terms of Skolem depth greater than one. However, this is not enough to conclude: it could be the case that, for instance, there is a derivation that can entail $q_f(x, y)$ with $x$ and $y$ constants, but that this derivation needs terms of Skolem depth greater than one to generate this atom. Thus, we introduce the notion of Skolem-increasing derivation, a restriction of Datalog-first derivations in which after closing under Datalog, we apply the existential trigger that create the variable with the smallest Skolem depth.

Definition 21. A Skolem-increasing derivation is a Datalog-first derivation $D = D_{\text{init}}, t_0, D_0, \ldots$ such that for all $n$, there is no existential trigger $t$ applicable on $\text{res}(D_n)$ such that $SkD(t) < SkD(t_{n+1})$.

Note that Skolem-increasing derivations always exist, as the property that characterizes them is only a criterion for choosing which existential trigger to apply. We do not require for the sequence $(SkD(t_i))_{i \in N}$ to be increasing, even though we will see that it is indeed the case for our rule set. We also show another important property, which is that to generate an atom featuring terms of Skolem depth less than $n$, then the sequence of trigger applications that leads to it only features terms of depth less than $n$. 
Proposition 22. Let $D$ be a database and $\mathcal{D} = D_0, t_0, D_1, \ldots$ a Datalog-first derivation from $(\mathcal{R}_M, D)$. Then, the following holds for all terms $x$ and $y$ in $\text{res}(\mathcal{D})$:

1. If $N(x, y) \in \text{res}(\mathcal{D})$, then either $\text{SkD}(x) = \text{SkD}(y) = 0$ or $\text{SkD}(x) = \text{SkD}(y) + 1$.
2. If $N^+(x, y) \in \text{res}(\mathcal{D})$, then $\text{SkD}(x) \leq \text{SkD}(y)$.
3. For all states $q$, if $q(x, y) \in \text{res}(\mathcal{D})$, then $\text{SkD}(x) \leq \text{SkD}(y)$.
4. For all triggers $t$ in $\mathcal{D}$ and atoms $A \in \text{output}(t)$ not using $\text{Eq}$, we have $\text{SkD}(\text{support}(t)) \leq \text{SkD}(A)$.

To show this, we first prove a few results about the $\text{Eq}$ predicate. Let us first describe the role of the rules in which $\text{Eq}$ appears.

3.3.2 An axiomatization of equality

First, rules $R_{\text{Eq}}^{\text{trans}}$, $R_{\text{Eq}}^{\text{sym}}$ and $R_{\text{Eq}}^{\text{rep}}$ constitute an axiomatization of non-reflexive equality. Then, rules $R_{\text{func}}^{+}$ and $R_{\text{func}}^{-}$ ensure that $N$ is both functional and anti-functional, and rule $R_{\text{eq}}$ ensures that there is only one $q_0$-atom. We have already seen in Lemma 14 that making equality reflexive would not yield any new fact (and it is complicated to do properly with existential rules). Thus, we define an equivalence relation $\approx$ which is the reflexive closure of the $\text{Eq}$ predicate, and we show that this relation is indeed an axiomatization of equality.

Lemma 23. Let $D$ be a Datalog closed database w.r.t $\mathcal{R}_M$. The relation $\approx$ defined as:

$$x \approx y \quad \text{iff} \quad \text{Eq}(x, y) \in D \text{ or } x = y$$

is an equivalence relation. In addition, for all Datalog closed instances $D$, predicates $P$ of arity $n$ and variables $x_1, \ldots, x_n, y_1, \ldots, y_n$, if $x_i \approx y_i$ for all $i \leq n$, then $P(x_1, \ldots, x_n) \in D$ if and only if $P(y_1, \ldots, y_n)$.

Proof. Let us first prove that $\approx$ is an equivalence relation.

Symmetry: Let $x$ and $y$ be terms in $D$ such that $x \approx y$. If $x = y$, then $y = x$ so $y \approx x$. Otherwise, it means $\text{Eq}(x, y) \in D$. In this case, since $D$ satisfies rule $R_{\text{Eq}}^{\text{sym}}$, $\text{Eq}(y, x) \in D$. Thus, $y \approx x$.

Reflexivity: If $x$ is a term in $D$, then $x = x$ so $x \approx x$.

Transitivity: Let $x$, $y$ and $z$ be terms in $D$ such that $x \approx y$ and $y \approx z$. Then:

- If $x = y$, then since $y \approx z$, we have $x \approx z$.
- If $y = z$, then since $x \approx y$, we have $x \approx z$.
- Otherwise, we have both $\text{Eq}(x, y) \in D$ and $\text{Eq}(y, z) \in D$. Since $D$ is a model of rule $R_{\text{Eq}}^{\text{trans}}$, it means $\text{Eq}(x, z) \in D$, so $x \approx z$.

Thus, $\approx$ is indeed an equivalence relation. Now, for the second part of the lemma, assume that $P(x_1, \ldots, x_n) \in D$. We then show by induction on $i$ that $P(y_1, \ldots, y_i, x_{i+1}, \ldots, x_n) \in D$. 

18
If \( i = 0 \), by hypothesis we have \( P(x_1, \ldots, x_n) \in D \), so there is nothing to prove. Now, assume that \( i > 0 \) and \( P(y_1, \ldots, y_{i-1}, x_i, \ldots, x_n) \in D \). If \( x_i = y_i \), then the result follows immediately from the induction hypothesis. Otherwise, we have \( \text{Eq}(x_i, y_i) \in D \). Thus, since \( D \) is a model of rule \( R_{\text{repl}}^r \), we have \( P(y_1, \ldots, y_i, x_{i+1}, \ldots, x_n) \in D \).

In particular, this result is true for \( i = n \), meaning that \( P(y_1, \ldots, y_n) \in D \). \qed

We then consider the quotient of Datalog closed instances, and show that this quotient is also Datalog closed.

**Definition 24.** For \( D \) a Datalog closed instance w.r.t. \( R_M \), we denote by \([x] \) the class of a term \( x \) in \( D \) for the equivalence relation \( \approx \), and define \( D/\approx \) the quotient of \( D \) by \( \approx \) as the database such that:

- Its terms are the classes \([x]\) for all \( x \in D \).
- We have \( P([x_1], \ldots, [x_n]) \in D/\approx \) if and only if \( P(x_1, \ldots, x_n) \in D \).

**Lemma 25.** If \( D \) is a Datalog closed database w.r.t. \( R_M \), then \( D/\approx \) satisfies all the Datalog rules in \( R_M \) that do not feature an \( \text{Eq} \)-atom in its heads.

**Proof.** Let \( R = B(\vec{x}, \vec{y}) \rightarrow H(\vec{x}) \) be a rule in \( R_M \) not featuring an \( \text{Eq} \)-atom in its head, and \( \pi \) be a homomorphism from \( B(\vec{x}, \vec{y}) \) to \( \text{SC} \). As \( \pi(B(\vec{x}, \vec{y})) \in D/\approx \), if \( \pi(\vec{x}) = \vec{c} \) and \( \pi(\vec{y}) = \vec{d} \), then for all \( \vec{u} \in \vec{c} \) and \( \vec{v} \in \vec{d} \), we have \( B(\vec{u}, \vec{v}) \in D \). Thus, since \( D \) models \( R \), we also have \( H(\vec{u}) \in D \), so \( H(\vec{c}) = \pi(H(\vec{x})) \in D_{\text{SC}} \), and \( D_{\text{SC}} \) satisfies \( R \). \qed

Note that Lemma 23 and Lemma 25 are independent of the rules in \( R_M \) other that our axiomatization, and could be used in any rule set in which the same axiomatization of equality is. Though, since rule \( R_{\text{repl}}^r \) can create any atom, if we want to show that \( \text{Fail} \) cannot appear too late in our context, we need to show that the rules we just described do not equalize too many individuals. This informal intuition calls for the following result, and especially point (4).

**Lemma 26.** Let \( D \) be a database, and \( D = D_0, D_1, D_2, \ldots \) a Datalog-first restricted derivation from \( (R_M, D) \) (with \( D_0 = D \)), and \( D_n \) the prefix of \( D \) composed only of Datalog triggers. Then, the following claims hold for all \( n \):

1. All the atoms \( N(v, w) \) in \( D_n \) with \( w \) constant are in \( \text{res}(D_0) \).
2. If \( w \) is the variable created by an application of rule \( R_0 \), there is no \( v \) such that \( N(v, w) \in D_n \).
3. All \( q_0 \)-atoms in \( D_n \) either feature only constant and are in \( \text{res}(D_0) \), or feature a variable and are created by \( R_0 \).
4. If \( \text{Eq}(x, y) \in D_n \setminus \text{res}(D_0) \), then \( x = y \).

**Proof.** We show the claim by induction on \( n \). The base case is trivial. Indeed, in \( D \) there is no variable so (2) holds, and everything that is in \( D \) is in \( \text{res}(D_0) \), so the other points hold too. We then prove the induction step. Assume that all the points are true at step \( n - 1 \), and that \( t_n = (R_n, \pi_n) \).
First, regarding point (1), assume by contradiction that \( t_n \) creates an atom \( \mathcal{N}(v, w) \) with \( v \) and \( w \) a constant. Then, the rule \( R_n \) must be either \( R_{N, 1}^{rep} \) or \( R_{N, 2}^{rep} \), or \( w \) would be a variable. If \( R_n \) is \( R_{N, 1}^{rep} \), then the atoms \( \mathcal{N}(u, w) \) and \( \mathsf{Eq}(u, v) \) must be in \( D_{n-1} \), with \( u \) a term such that \( u \neq v \). Then, by point (4) of the induction hypothesis, we have \( \mathsf{Eq}(u, v) \in \text{res}(D_0) \). In addition, \( \mathcal{N}(u, w) \) is an \( \mathcal{N} \)-atom with a constant on second position in \( D_{n-1} \), so by point (1) of the induction hypothesis, we also have \( \mathcal{N}(u, w) \in \text{res}(D_0) \). Finally, since \( \text{res}(D_0) \) models rule \( R_{N, 1}^{rep} \), we have \( \mathcal{N}(v, w) \in \text{res}(D_0) \), which contradicts our hypothesis, so rule \( R_{N, 1}^{rep} \) cannot generate \( \mathcal{N}(v, w) \). An analogous argument proves that rule \( R_{N, 2}^{rep} \) cannot do so either, concluding the proof of this point.

Regarding point (2), assume that \( w \) is the variable introduced by an application of rule \( R_0 \), and that \( t_n \) creates the atom \( \mathcal{N}(v, w) \). First, rules \( R_1 \) and \( R_{+1} \) both create an \( \mathcal{N} \)-atom with an existentially quantified variable in its second position. Since \( w \) has already been introduced, it cannot be introduced again by these two rules. Rule \( R_{N, 1}^{rep} \) requires an atom \( \mathcal{N}(u, w) \) to be applicable, which is impossible as \( \mathcal{N}(v, x) \) is the first with \( w \) in second position. Finally, rule \( R_{N, 2}^{rep} \) requires an \( \mathsf{Eq} \)-atom involving \( w \) to be applicable, which by induction hypothesis does not exist, which concludes this point.

To show point (3), we first treat the constant case. Assume that \( t_n \) creates \( \mathcal{q}_0(v, w) \) with \( v \) and \( w \) constants. Then, as it only features constants, it must have been generated by rule \( R_{q_0, 1}^{rep} \) or \( R_{q_0, 2}^{rep} \). If \( R_n = R_{q_0, 1}^{rep} \), then there are \( \mathcal{q}_0(u, w) \) and \( \mathsf{Eq}(u, v) \) in \( D_n \), with a term \( u \) such that \( u \neq v \). Then, by point (4) of the induction hypothesis, we have \( \mathsf{Eq}(u, v) \in \text{res}(D_0) \). In addition, since \( \mathsf{Eq}(u, v) \in \text{res}(D_0) \), \( u \) is a constant, so \( q_0(u, w) \) is an \( \mathcal{q}_0 \)-atom over constants. Thus, by point (3) of the induction hypothesis, \( \mathcal{q}_0(u, w) \in \text{res}(D_0) \). Then, since \( \text{res}(D_0) \) is closed under rule \( R_{q_0, 1}^{rep} \), then \( \mathcal{q}_0(v, w) \in \text{res}(D_0) \). An analogous argument holds if \( R_n = R_{q_0, 2}^{rep} \), which concludes the constant case.

Then, for the variable case of point (3), assume that \( t_n \) creates the atom \( \mathcal{q}_0(v, w) \) with \( v \) or \( w \) a variable, and that \( R_n \neq R_0 \). If \( R_n = R_{q_0, 1}^{rep} \), then there must be \( \mathcal{q}_0(u, w) \) and \( \mathsf{Eq}(u, v) \) in \( D_{n-1} \), with \( u \) a term such that \( u \neq v \). Thus, \( u \) and \( v \) must be constants. Since we assume \( v \) or \( w \) is a variable, it must be that \( w \) is a variable. Thus, by induction hypothesis, the atom \( q_0(u, w) \) must have been created by rule \( R_0 \), so \( u = w \), and then \( u \) is both a constant and a variable, which is absurd. An analogous argument concludes this point if \( R_n = R_{q_0, 2}^{rep} \).

Then, to prove point (4), assume by contradiction that \( t_n \) is not in \( \text{res}(D_0) \), and creates an atom \( \mathsf{Eq}(x, y) \) with \( x \neq y \) two terms. We then do a case distinction on \( R_n \).

If \( R_n = R_{\text{func}}^+ \): In this case, there are atoms \( \mathcal{N}(z, x) \) and \( \mathcal{N}(z, y) \) in \( D_{n-1} \) with \( z \) a term, so that \( t \) is applicable. If \( x \) and \( y \) are constant, then both \( \mathcal{N}(z, x) \) and \( \mathcal{N}(z, y) \) are in \( \text{res}(D_0) \) by point (1) of the induction hypothesis, so by rule \( R_{\text{func}}^+ \), \( \mathsf{Eq}(x, y) \in \text{res}(D_0) \), contradicting our hypothesis. Then, for the case where \( x \) or \( y \) is a variable, assume that \( x \) is a variable \((x \text{ and } y \text{ are symmetric in this case}) \), and let \( t_k = (R_k, \pi_k) \) be the trigger that creates \( x \).

If \( R_k = R_0 \), then by point (2), the atom \( \mathcal{N}(z, x) \) cannot be in \( D_{n-1} \). Thus, \( R_k \) is either \( R_1 \) or \( R_{+1} \). In either case, \( t_k \) creates the atom \( \mathcal{N}(v, x) \) along with \( x \). We show that there is no atom \( \mathcal{N}(w, y) \) in \( D_{n-1} \) with \( w \in [v] \).
Assume by contradiction that the atom $N(w, y)$ is the first atom of this form created. We then study the rule that introduces $N(w, y)$.

If the rule that creates $N(w, y)$ is $R_1$ or $R_{+1}$, then there is $l$ such that $t_l$ introduces $N(w, y)$, and $l \neq k$. If $l < k$, then $\text{res}(D_l) \subseteq \text{res}(D_{k-1})$. As $\text{res}(D_k)$ is Datalog closed, by Lemma 23, $N(v, y) \in \text{res}(D_l)$, so $t_k$ is not applicable, which contradicts our hypothesis. If $l > k$, as $\text{res}(D_k)$ is Datalog closed, by Lemma 23, $N(w, x) \in \text{res}(D_k)$, so $t_l$ is not applicable. Thus, these rules cannot create $N(w, y)$.

Rule $R_{N,2}^{rep}$ requires an $\text{Eq}$-atom involving $y$ to produce $N(w, y)$, so $y$ has to be a constant. Then, by point (1), the atom $N(v, y)$ is in $\text{res}(D_0)$. Since $\text{res}(D_0)$ is Datalog closed, by Lemma 23, we have $N(v, y) \in \text{res}(D_0)$. Thus, $t_k$ is not applicable, as one can map $x$ to $y$.

For rule $R_{N,1}^{rep}$ to produce $N(w, y)$, there must be $N(u, y)$ and $\text{Eq}(u, w)$ in $D_{n-1}$ before it. Thus, $u \in [v]$, so since $N(w, y)$ is the first one, this rule cannot create it either.

Then, there is no atom $N(w, y)$ in $D_{n-1}$ with $w \in [v]$. As $v \in [v]$, the atom $N(v, y)$ is not in $D_{n-1}$ either, so $t$ is not applicable in this case. We can now show that for any $z$, the atoms $N(z, x)$ and $N(z, y)$ cannot exist at the same time. If the rule that generates $N(z, x)$ is $R_1$ or $R_{+1}$, then $z = v$ and we have shown that for all $w \in [v]$, including $v$ itself, $N(w, y) \notin D_{n-1}$. Then, $N(z, y) \notin D_{n-1}$, so these rules cannot create $N(z, x)$. If this rule is $R_{N,1}^{rep}$, then $z \approx v$, and by the same result $N(z, y) \notin D_{n-1}$. Finally, rule $R_{N,2}^{rep}$ requires an $\text{Eq}$-atom over $x$, a variable, so it cannot be used either. Thus, the atoms $N(z, x)$ and $N(z, y)$ cannot exist at the same time.

If $R_n = R_{N,1}^{fun}$: In this case, there are atoms $N(x, z)$ and $N(y, z)$ in $D_{n-1}$ with $z$ a term, so that $t$ is applicable. First notice that if $z$ is a constant, by point (1), $N(x, z)$ and $N(y, z)$ are in $\text{res}(D_0)$. Thus, the closure under rule $R_{N,1}^{fun}$ entails that $\text{Eq}(x, y) \in \text{res}(D_0)$, which contradicts our hypothesis. Thus, $z$ must be a variable, so the atoms $N(x, z)$ and $N(y, z)$ must have been created during the chase. The term $z$ being a variable also means that $R_{N,2}^{rep}$ cannot create any atom $N(v, z)$, as in this case $z$ would be a constant. Let $t_k = (R_{k}, \pi_k)$ be the trigger that created $z$.

If $R_k = R_0$, then by point (2), the atom $N(x, z)$ cannot be in $D_{n-1}$. Thus, $R_k$ must be either $R_1$ or $R_{+1}$. In either case, $t_k$ creates the atom $N(v, z)$. We show that for all $w \notin [v]$, the atom $N(w, z)$ is not in $D_{n-1}$. Assume by contradiction that $N(w, z)$ is the first of these atoms to appear in $D_{n-1}$. As $z$ is a variable created along the atom $N(v, z)$, only rules $R_{N,1}^{rep}$ and $R_{N,2}^{rep}$ can generate the atom $N(v, z)$. As we saw earlier, rule $R_{N,2}^{rep}$ cannot be used, so there is only rule $R_{N,1}^{rep}$. This rule requires the atoms $N(u, z)$ and $\text{Eq}(u, w)$ to be in $D_{n-1}$ for it to be applicable (for some $u$). As by hypothesis $N(w, z)$ is the first one with $w \notin [v]$, we have $u \notin [v]$ so $u \approx v$, but since we have $\text{Eq}(u, w)$, we also have $u \approx w$. Thus, by transitivity, we have $w \approx v$, so $w \in [v]$, which is a contradiction. Thus, the only $w$ such that $N(w, z) \in D_{n-1}$ are in $[v]$. Then, if we have $N(x, z)$ and $N(y, z)$
in \( D_{n-1} \), then \( x \approx v \approx y \) so as \( x \neq y \), we have \( \text{Eq}(x, y) \in D_{n-1} \), which contradicts our hypothesis.

If \( R_n = R_{q_0} \): In this case, in \( D_{n-1} \) there are either the atoms \( q_0(x, y) \) and \( q_0(v, w) \), or the atoms \( q_0(v, x) \) and \( q_0(y, w) \) (with \( v \) and \( w \) terms). In the first case, as \( x \neq y \), the terms \( x \) and \( y \) must both be constants. Then, \( q_0(x, y) \in \text{res}(D_0) \) by point (3). Thus, since \( \text{res}(D_0) \) is closed under rule \( R_{q_0} \), we have \( \text{Eq}(x, y) \in \text{res}(D_0) \), contradicting our hypothesis. Thus, there must be atoms \( A_x = q_0(v, x) \) and \( A_y = q_0(y, w) \) in \( D_{n-1} \). By point (3), there are four cases possible.

- If \( A_x \) and \( A_y \) both only feature constants, they are both in \( \text{res}(D_0) \), so rule \( R_{q_0} \) ensures that \( \text{Eq}(x, y) \) is in \( \text{res}(D_0) \) too, which contradicts our hypothesis.
- If \( A_x \) features constants and \( A_y \) a variable, then by rule \( R_{q_0} \), we have \( \text{Eq}(v, x) \in \text{res}(D_0) \), and by rule \( R_{q_0,1}^{rev} \), the atom \( q_0(x, x) \) is in \( \text{res}(D_0) \). Thus, rule \( R_0 \) is not applicable (one can map \( y \) to \( x \)), and \( A_y \) cannot appear.
- The case where \( A_y \) features constants and \( A_x \) a variable is symmetric to the previous one.
- Finally, if \( A_x \) and \( A_y \) both feature variables, then they are both created by rule \( R_0 \). As it has an empty body, it can be applied at most once, so as \( x \neq y \), this case is not possible either. \( \square \)

### 3.3.3 Skolem-increasing derivations

We are now equipped with the notions we need to show Proposition 22, which we recall here.

**Proposition 22.** Let \( D \) be a database and \( \mathcal{D} = D_0, D_1, D_2, \ldots \) a Datalog-first derivation from \((\mathcal{R}_M, D)\). Then, the following holds for all terms \( x \) and \( y \) in \( \text{res}(\mathcal{D}) \):

1. If \( N(x, y) \in \text{res}(\mathcal{D}) \), then either \( \text{SkD}(x) = \text{SkD}(y) = 0 \) or \( \text{SkD}(y) = \text{SkD}(x) + 1 \).
2. If \( N^+(x, y) \in \text{res}(\mathcal{D}) \), then \( \text{SkD}(x) \leq \text{SkD}(y) \).
3. For all states \( q \), if \( q(x, y) \in \text{res}(\mathcal{D}) \), then \( \text{SkD}(x) \leq \text{SkD}(y) \).
4. For all triggers \( t \) in \( \mathcal{D} \) and atoms \( A \) in \( \text{output}(t) \) not using \( \text{Eq} \), we have \( \text{SkD}(\text{support}(t)) \leq \text{SkD}(A) \).

**Proof.** For point (1), assume for a contradiction that there is a first atom \( N(x, y) \in \text{res}(\mathcal{D}) \) such that neither \( \text{SkD}(x) = \text{SkD}(y) = 0 \) nor \( \text{SkD}(y) = \text{SkD}(x) + 1 \). If \( y \) is a constant, then by point (1) of Lemma 26, \( x \) must also be a constant so \( \text{SkD}(x) = \text{SkD}(y) = 0 \). Otherwise, if \( y \) is a variable, then \( N(x, y) \) has been generated during the chase. Let \( t = (R, \pi) \) be the trigger that generates this atom.

If \( R \in \{R_1, R_{+1}\} \): Then \( t \) also creates \( y \) from \( x \), so \( \text{SkD}(y) = \text{SkD}(x) + 1 \).
If \( R \in \{ \text{ repl}_{R,N,1}, \text{ repl}_{R,N,2} \} \): Then there is a \( \mathcal{N}(z,t) \) with \( z \approx x \) and \( t \approx y \). Since \( y \) is a variable, it must be that \( t = y \) by Lemma 26. As \( \mathcal{N}(x,y) \) is the first \( \mathcal{N} \)-atom for which the statement does not hold, and \( \text{SkD}(y) \neq 0 \), it must be that \( \text{SkD}(y) = \text{SkD}(y) + 1 \). If \( x \) is a constant, then \( z \) is too so \( \text{SkD}(z) = 0 \) so \( \text{SkD}(y) = 1 \). Thus, as \( \text{SkD}(x) = 0 \), it is indeed the case that \( \text{SkD}(y) = \text{SkD}(x) + 1 \). Now, if \( x \) is a variable, then \( z = x \) so the atom \( \mathcal{N}(x,y) \) must be used to generate itself, which is a contradiction.

Thus, point (1) holds.

For point (2), assume for a contradiction that there is a first atom \( \mathcal{N}^+(x,y) \in \text{res}(\mathcal{D}) \) such that \( \text{SkD}(x) > \text{SkD}(y) \) for some \( x,y \). Then, \( x \) must be a variable so \( \mathcal{N}^+(x,y) \) must have been generated during the chase; let \( t = (R,\pi) \) be the corresponding trigger.

If \( R = \text{N}_{\pi:+} \): Then the atom \( \mathcal{N}(x,y) \) is in \( \text{res}(\mathcal{D}) \), so by point (1), \( \text{SkD}(x) \leq \text{SkD}(y) \).

If \( R = \text{N}_{\pi:trans} \): Then there are atoms \( \mathcal{N}(x,z) \) and \( \mathcal{N}^+(z,y) \) in \( \text{res}(\mathcal{D}) \). By point (1), we then have \( \text{SkD}(x) \leq \text{SkD}(z) \). In addition, as \( \mathcal{N}^+(x,y) \) is the first \( \mathcal{N}^+ \)-atom such that \( \text{SkD}(x) > \text{SkD}(y) \), we also have \( \text{SkD}(z) \leq \text{SkD}(y) \). Thus, by transitivity, we get \( \text{SkD}(x) \leq \text{SkD}(y) \).

If \( R \in \{ \text{ repl}_{\pi,1}, \text{ repl}_{\pi,2} \} \): Then there is an atom \( \mathcal{N}^+(z,t) \) with \( z \approx x \) and \( t \approx y \). As \( x \) is a variable, \( z = t \). Since \( \mathcal{N}^+(x,y) \) is the first \( \mathcal{N}^+ \)-atom such that \( \text{SkD}(x) > \text{SkD}(y), \text{SkD}(z) \leq \text{SkD}(t) \). Thus, as \( x = z \) and \( x \) is a variable, \( t \) must also be a variable, so \( t = y \), which means \( \mathcal{N}^+(x,y) \) is necessary to generate itself, a contradiction.

Thus, point (2) holds too.

Then, for point (3), assume for a contradiction that there is a first atom \( \mathcal{q}(x,y) \mathcal{N} \) such that \( \text{SkD}(x) > \text{SkD}(y) \) for some \( x,y,q \). Then, \( x \) must be a variable so \( \mathcal{q}(x,y) \) must have been generated during the chase; let \( t = (R,\pi) \) be the corresponding trigger.

If \( R = \text{N}_0 \): In this case \( x = y \) which is not compatible with them having different Skolem depth.

If \( R = \text{N}_{\pi:} \): Then there must be atoms \( \mathcal{N}(x,z) \) and \( \mathcal{N}^+(z,y) \) for some term \( z \) (among other atoms) in \( \text{res}(\mathcal{D}) \). Thus, by points (1) and (2), \( \text{SkD}(x) \leq \text{SkD}(z) \leq \text{SkD}(y) \).

If \( R = \text{N}_{\pi:trans} \): Then there must be an atom \( \mathcal{N}^+(x,y) \) in \( \text{res}(\mathcal{D}) \), so by point (2), \( \text{SkD}(x) \leq \text{SkD}(y) \).

If \( R = \text{N}_{\pi:trans}^{\max} \): Then \( x = y \) which is not compatible with them having different Skolem depth.

If \( R \in \{ \text{ repl}_{\pi,1}, \text{ repl}_{\pi,2} \} \): Then there must be an atom \( \mathcal{q}(z,t) \) with \( z \approx x \) and \( t \approx y \). Note that by Lemma 26, for all terms \( a \) and \( b \in [0] \), \( \text{SkD}(a) = \text{SkD}(b) \). Thus, as \( \mathcal{q}(z,t) \) must be in \( \text{res}(\mathcal{D}) \) before \( \mathcal{q}(x,y) \), \( \text{SkD}(z) \leq \text{SkD}(t) \), so \( \text{SkD}(x) \leq \text{SkD}(y) \).
Thus, such an atom cannot exist, so point (3) holds.

Finally, for point (4), let \( t = (R, \pi) \) be a trigger. As rules \( R_{\text{Goal}} \), \( R^0_{q,c} \), \( R_{\text{cycle}} \), \( R_{\text{step}} \), \( R_{\text{cell}} \), \( R_{\text{cell}}^{\text{ref}} \), \( R^{\text{copy}} \), and \( R_{\text{sym}} \) do not feature any variable in their heads, if \( R \) is among them, point (4) is vacuously true. The same holds for rules \( R_{\text{func}} \), \( R_{\text{rule}} \), \( R_{\text{Eq}} \), \( R_{\text{trans}} \) and \( R_{\text{sym}} \), which only introduce \( \text{Eq} \)-atoms. We then show that for all the other rules, point (4) holds by showing that for all the variables in their bodies, there is a variable in each atom of the head that has a greater Skolem depth. We establish the order between the variables’ Skolem depths using the previous points.

If \( R = R_0 \): This rule features no atoms in its body, so the condition is vacuously true.

If \( R = R_1 \): We have \( \text{SkD}(w_0) \leq \text{SkD}(w_1) \) and \( w_1 \) is in the only atom of the head.

If \( R = R_{i+1} \): We have \( \text{SkD}(w_0) \leq \text{SkD}(w_i) \leq \text{SkD}(w_{i+1}) \) and \( w_{i+1} \) is in the head.

If \( R = R_{N+} \): The same variables appear in the only atoms in the body and the head of this rule.

If \( R = R_{N+}^{\text{trans}} \): We have \( \text{SkD}(w_i) \leq \text{SkD}(w_{i+1}) \leq \text{SkD}(w_k) \) and \( w_k \) is in the head.

If \( R = R^{0}_{i} \): The same variable appear in the only atoms in the body and the head of this rule.

If \( R = R_{k} \): We have \( \text{SkD}(w_0) \leq \text{SkD}(w_i) \) and \( w_i \) is in the head.

If \( R = R^{\text{sym}}_{k} \): We have \( \text{SkD}(p_1) \leq \text{SkD}(p_2) \leq \text{SkD}(t_1) \leq \text{SkD}(t_2) \), and \( t_2 \) is in both the atoms in the head.

If \( R = R^{\text{max}}_{k} \): We have \( \text{SkD}(p_1) \leq \text{SkD}(p_2) \leq \text{SkD}(t_2) \) and \( \text{SkD}(p_1) \leq \text{SkD}(t_1) \leq \text{SkD}(t_2) \), so \( t_2 \) has the greatest Skolem depth of all these variables, and appears in both atoms in the head.

If \( R = R^{\text{trans}}_{k} \): We have \( \text{SkD}(w_1) \leq \text{SkD}(w_2) \), and \( w_2 \) appears in the head.

If \( R = R^{L}_{k} \): We have \( \text{SkD}(p_i) \leq \text{SkD}(p_k) \leq \text{SkD}(t_1) \leq \text{SkD}(t_2) \), and \( t_2 \) appears in the head.

If \( R = R^{R}_{k} \): We have \( \text{SkD}(p_i) \leq \text{SkD}(p_k) \) and \( \text{SkD}(p_i) \leq \text{SkD}(t_1) \leq \text{SkD}(t_2) \), and \( p_k \) and \( t_2 \) both appear in the head.

If \( R = R^{\text{copy}}_{j} \): The variables \( x_j \) for \( j \neq i \) all appear in the head. Regarding \( x_i \), by point 4, either it is a constant, and \( y_i \) is a constant too so they both have a Skolem depth of zero, or it is a variable and \( x_i = y_i \). Thus, either way, the head has a greater Skolem depth than the body.

We are now equipped to show that in Skolem-increasing derivations, all the facts entailed by the knowledge base about terms of depth \( k \) are in the database before a term of depth \( k + 1 \) is produced.

24
Proposition 27. Consider a database $D$, a Skolem-increasing derivation $\mathcal{D} = D_0, t_0, D_1$ from $(\mathcal{R}_M, D)$, and an atom $A$ not using $\mathit{Eq}$ such that $(\mathcal{R}_M, D) \models A$. Then, for all $n$, if $\text{SkD}(A) < \text{SkD}(t_{n+1})$, then $A \in \mathcal{D}_n$.

Proof. Assume for a contradiction that there is an atom $A$ that contradicts the proposition. Then, there must be a sequence of trigger $t^1, \ldots, t^k$ appearing in $\mathcal{D}$ such that $t^1 = t_0$, $A \in \text{output}(t^k)$, and for all $i < k$, $\text{support}(t^{i+1}) \cap \text{output}(t^i) \neq \emptyset$. As we saw in the proof of Proposition 22, all the rules either have only one atom in the head or both their atoms feature the variable with the greatest Skolem depth. Thus, for all $i < k$, $\text{SkD}(\text{output}(t^i)) \leq \text{SkD}(\text{support}(t^{i+1}))$ by point (4) of Proposition 22, for all $i \leq k$, $\text{SkD}(\text{support}(t^i)) \leq \text{SkD}(\text{output}(t^i))$. Thus, both these results together give by transitivity that $\text{SkD}(t^1) \leq \text{SkD}(t^k)$, which entails that $\text{SkD}(t_{n+1}) \leq \text{SkD}(A)$, and contradicts our hypothesis. \hfill \qed

Note that, on a side note, this also entails that the sequence $\text{SkD}(t_n)$ is increasing. Now that we have this fundamental result, we can go back to our dichotomy about the $\text{Fail}$ predicate.

3.3.4 Some structure — The $\text{Fail}$ predicate

First, we describe the rules that generate $\text{Fail}$, through a description of what a Datalog closed database without $\text{Fail}$ looks like. First, rule $R_{\text{N}_+}^{\text{Skide}}$ ensures that $\text{N}$, which is both functional and inverse functional, is without cycles. Thus, the graph formed by the equivalence classes by $\mathit{Eq}$ as nodes and $\text{N}$-atoms as edges is a disjoint union of what we call chains.

Definition 28. In a graph $G = (V, E)$, a chain $C$ of size $n$ is a sequence of vertices $v_1, \ldots, v_n$ such that for all $(v, w) \in E$, either there is $i$ such that $v = v_i$ and $w = v_{i+1}$, or $v$ and $w$ are both not in $C$.

Then, rule $R_{-1}$ ensure that the only $q_0$-atom is at the start of a chain. Finally, rules $R_{\text{step}}^{\text{N}, q_1, q_2}, R_{\text{cell}}^{w_1, w_2}$ and $R_{\text{GoB}}^{\text{N}, v_1, v_2}$ ensure that on each chain, there is only one Turing machine simulation at a step. We formalize this into the following proposition.

Definition 29. Consider an instance $D$ and a binary predicate $P$. Then, the $P$-graph associated with $D$, denoted with $G^P_D$, is the graph having as vertices the terms of $D$, and an edge between $x$ and $y$ if and only if $P(x, y) \in D$.

Proposition 30. Let $D$ be a Datalog closed instance that does not contain $\text{Fail}$. Then:

- The graph $G^\mathcal{N}_D/\approx$ is a union of chains.
- There is at most one $q_0$-atom in $D/\approx$, and if there is one, it is of the form $q_0([z_0], [z_0])$ with $z_0$ being the first element of a chain. We call this chain the starting chain.

Proof. We first show that $G^\mathcal{N}_D/\approx$ is a union of chain. First, we show that $\mathcal{N}$ is functional, that is that for all $c \in D/\approx$, there is at most one $d \in D/\approx$ such that $\mathcal{N}(c, d) \in D/\approx$. Indeed, if $d_1$ and $d_2$ are such that $\mathcal{N}(c, d_1)$ and $\mathcal{N}(c, d_2)$ are in $D/\approx$, let $x \in c, y_1 \in d_1$ and $y_2 \in d_2$. Then, we have $\mathcal{N}(x, y_1)$ and $\mathcal{N}(x, y_2)$ in $D$. Thus, since $D$ satisfies rule $R_{\text{func}}^+$, we have $\mathit{Eq}(y_1, y_2) \in D$, so $y_1 \approx y_2$.  

25
and \( d_1 = d_2 \). The same reasoning using rule \( R_{\text{func}} \) shows that \( N \) is also inverse functional in \( D/\approx \).

Then, to show that \( G_{D/\approx}^N \) is a union of chains, we must show that it is without cycles. Assume by the absurd that it contains a cycle \( c_1, \ldots, c_n \). Let \( x_i \) be a representative of \( c_i \) for all \( i \). Then, we have \( N(x_n, x_0) \) and \( N(x_i, x_{i+1}) \) in \( D \) for all \( i < n \). We then show by induction on \( i \) that for all \( i \), \( N^+(x_{n-i}, x_0) \in D \).

For the base case, since \( D \) is a model of rule \( R_{N^+} \), we have \( N^+(x_n, x_0) \) in \( D \). For the induction step, assume that \( N^+(x_{n-i+1}, x_0) \in D \). Then, since \( N(x_{n-i}, x_{n-i+1}) \in D \) and \( D \) models \( R_{N^+}^{\text{trans}} \), we have \( N^+(x_{n-i}, x_0) \in D \), which concludes the inclusion. Thus, in particular for \( i = n \), we have \( N^+(x_0, x_0) \in D \).

Since \( D \) models rule \( R_{\text{cycle}}^{\text{trans}} \), the predicate \( \text{Fail} \) is in \( D \), which contradicts our initial hypothesis. Thus, \( G_{D/\approx}^N \) contains no cycle, and is indeed a union of chains.

Now for the second point, if we have \( q_0(c_1, c_2) \in D/\approx \) and \( q_0(c_3, c_4) \in D/\approx \), let \( x_i \) be a representative of \( c_i \) for all \( i \), and then we have \( q_0(x_1, x_2) \in D \) and \( q_0(x_3, x_4) \in D \). As \( D \) is a model of \( R_{q_0} \), the atoms \( \text{Eq}(x_1, x_2), \text{Eq}(x_2, x_3) \) and \( \text{Eq}(x_3, x_4) \) are all in \( D \). Thus, \( x_1 \approx x_2 \approx x_3 \approx x_4 \), so \( c_1 = c_2 = c_3 = c_4 \).

Thus, there is at most one \( q_0 \)-atom in \( D/\approx \), which is of the form \( q_0(c_0, c_0) \). We then show that if it exists, there is no \( c \) such that \( N(c, c_0) \in D/\approx \). Indeed, if by contradiction we assume there is one, let \( x \in c \) and \( z_0 \in c_0 \). We then have \( N(x, z_0) \in D \). Since \( D \) models rule \( R_{-1} \), the predicate \( \text{Fail} \) is entailed, which contradicts our initial hypothesis, and concludes the proof.

We now are equipped to show that if the Datalog closure of a database \( D \) does not contain \( \text{Fail} \), and \( D = D_0, t_0, D_1, \ldots \) is a Datalog-first restricted derivation from \( (R_M, D) \), then \( \text{res}(D_n) \) does not contain \( \text{Fail} \) either. Thus, Proposition 30 applies on \( \text{res}(D_n) \) too, for all \( n \). Therefore, this structure is maintained through all derivations from databases that do not entail \( \text{Fail} \).

**Proposition 31.** Consider a database \( D \) and a Datalog-first restricted derivation \( D = D_0, t_1, D_1, \ldots \). If \( \text{Fail} \notin D_0 \), then for all \( n \), \( \text{Fail} \notin D_n \).

**Proof.** We proceed by induction on \( n \). The base case is trivial, so we focus on the induction step. Assume that \( \text{Fail} \notin D_{n-1} \). First, as \( t_n = (R_n, \pi_n) \) is an existential trigger, \( R_n \) must be among \( R_0, R_1, R_{-1} \). Thus, it follows from its \( R \)-applicability that \( t_n \) can only either create a starting chain of length one if there is none, or add one element at the end of a chain. Then, by point (4) of Lemma 26 and the fact that no other rule can create \( q_0 \)-atoms or \( N \)-atoms, this structure cannot change during \( D_n \). Thus, rules \( R_{\text{cycle}}^{\text{trans}} \) and \( R_{-1} \) cannot fire and entail \( \text{Fail} \).

Regarding the other four rules, they follow the same pattern: if they were applicable on \( \text{res}(D_n) \), then their supports must have been introduced at a previous step, which is not possible by induction hypothesis.

### 3.3.5 Controlling the chains

We then come back to our result through several lemmas. The main idea is that since Datalog closed databases are composed of chains, we then show that each chain is well-behaved, and that nothing inconvenient happens between chains. We start with the starting chain, by showing that it behaves exactly like the chase on \( (R_M, \emptyset) \).
Lemma 32. Consider $D$ be a Datalog closed instance that neither contain Fall nor Goal, and such that $D/\approx$ has a starting chain. Then, let $\mathcal{D} = D_0, D_1, \ldots$ be a Datalog-first derivation from $(\mathcal{R}_M, \emptyset)$, and $D_{SC}$ be the instance obtained by removing all the classes in $D/\approx$ that are not on the starting chain, and all the atoms in which such a term appears. Finally, let $n$ be the number of classes on the starting chain. Then, $D_{SC}$ and $\text{res}(D_{n-1})$ are isomorphic.

Proof. First, by Proposition 30, $G^N_{D_{SC}}$ is also a chain of size $n$. We thus denote the elements of $\text{res}(D_{n-1})$ and $D_{SC}$ as $z_i$ and $d_i$, respectively, where $i$ is $z_i$ and $d_i$’s position in the chain (and ranges from 0 to $n-1$). Then we show that the map $h$ that sends $z_i$ to $d_i$, which is a bijection, is an isomorphism.

Let us start by showing that $h(\text{res}(D_{n-1})) \subseteq D_{SC}$. More precisely, we show by induction on $i$ that for all atoms $A \in \text{res}(D_{n-1})$ featuring only variables among $\{z_j | 0 \leq j \leq i\}$, we have $h(A) \in D_{SC}$.

For the base case, the atoms in $\text{res}(D_{n-1})$ featuring only $z_0$ are $q_0(z_0, z_0)$ and $B(z_0, z_0)$. Then, $q_0(d_0, d_0) \in D_{SC}$ since $D_{SC}$ is the starting chain in $D/\approx$. Finally, as $q_0(d_0, d_0) \in D_{SC}$, since $D_{SC}$ models rule $R^0_q$ by Lemma 25, we have $B(d_0, d_0) \in D_{SC}$, which concludes the base case.

For the inductive step, assume that for all atoms $A \in \text{res}(D_{n-1})$ featuring only variables among $\{z_j | 0 \leq j \leq i\}$, we have $h(A) \in D_{SC}$, and let $A$ be an atom in $\text{res}(D_{n-1})$ featuring only variables among $\{z_j | 0 \leq j \leq i+1\}$. If it only features variables among $\{z_j | 0 \leq j \leq i\}$, then the induction hypothesis suffices, so we assume that it features $z_{i+1}$. As by Proposition 16 we have $\text{res}(D_{n-1})$ characterized, we now exactly which atoms fulfill this specification.

$N(z_i, z_{i+1})$: As we said earlier, the graph $G^N_{D_{SC}}$, is a chain, so our naming convention ensures that $N(d_i, d_{i+1}) \in D_{SC}$.

$N^+(z_j, z_{i+1})$ for $j \leq i$: By the previous point, $N(d_i, d_{i+1}) \in D_{SC}$, so by rule $R^+_{N}$, we have $N^+(d_i, d_{i+1}) \in D_{SC}$. Then, if by induction we assume that $N^+(c_{j+1}, d_{i+1}) \in D_{SC}$, as by induction hypothesis $N(c_j, c_{j+1}) \in D_{SC}$, then $N^+(c_j, d_{i+1}) \in D_{SC}$.

$q_{i+1}(z_{h_{i+1}}, z_{i+1})$: As we saw earlier, the atom $N(d_i, d_i+1)$ is in $D_{SC}$. Then, as for all $t$ we have $h_t \leq t$, in particular we have $h_i \leq i$, so by induction hypothesis the atoms $q_t(c_{h_t}, d_i)$, $N^+(c_{h_t}, d_{i+1})$ and $c(c_{h_t}, z_i)$ with $c = M(h_t, i)$ are all in $D_{SC}$. We also have $h_{i+1} \leq i+1$, so the atom $N(c_{h_{i+1}}, c_{h_{i+1}})$ or $N(c_{h_t}, c_{h_{i+1}})$ is in $D_{SC}$, depending on whether $\delta(q_i, c) = (q_{i+1}, c', \leftarrow)$ or $\delta(q_i, c) = (q_{i+1}, c', \rightarrow)$. Thus, by rules $R^2_{q,c}$ and $R^2_{q,c}$, we have $q_{i+1}(c_{h_{i+1}}, d_{i+1})$ and $c'(z_{h_t}, z_{i+1})$ in $D_{SC}$, with $c' = M(h_t, i+1)$.

$c_j(z_j, z_{i+1})$ for $j \leq i+1$, with $c_j = M(j, i+1)$: By the previous case, if $j = h_i$, this atom is in $D_{SC}$, so we assume $j \neq h_i$ in the following. The atom $N(z_i, z_{i+1})$ is in $D_{SC}$, and by induction hypothesis, the atoms $q_t(d_i, d_i)$ and $c_j(d_j, z_i)$ are in $D_{SC}$, since for all $j \neq h_i$, $M(j, i) = M(j, i+1)$. Then, if $j < h_i$, we have $N^+(d_j, d_{h_i}) \in D_{SC}$ so by rule $R^2_{q,c}$, the atom $c_j(z_j, z_{i+1})$ is in $D_{SC}$. If $j > h_i$, we reach the same conclusion using rule $R^2_{q,c}$ instead.

Thus, this concludes the proof that for all $i$, and all atoms $A \in \text{res}(D_{n-1})$ featuring only variables among $\{z_j | 0 \leq j \leq i\}$, we have $h(A) \in D_{SC}$. Thus, in particular, $h(\text{res}(D_{n-1})) \subseteq D_{SC}$.
We then prove that $h^{-1}$ is a homomorphism. Assume by contradiction that $A$ is an atom in $D_{SC}$ such that $h^{-1}(A) \notin \text{res}(D_{n-1})$. First note that we assumed that $\text{Fail}$ and $\text{Goal}$ were not in $D$, so they are not in $D_{SC}$, and since $G_{DSC}^{N}$ and $G_{\text{res}(D_{n-1})}^{N}$ are both chains, $A$ cannot use the predicate $N$. Then, we show that $D_{SC}$ must contain $\text{Fail}$, contradicting our initial hypothesis on $D$.

If $A = N^{+}(d_{i}, d_{j})$: As $h^{-1}(A) = N^{+}(z_{i}, z_{j}) \notin \text{res}(D_{n-1})$, it must then be that $j \leq i$. We then show by induction on $i-j$ that if $N^{+}(z_{i}, z_{j}) \in D_{SC}$ with $j \leq i$, then $\text{Fail} \in D_{SC}$. For the base case, if $i-j = 0$, then $j = i$. Since $D_{SC}$ models rule $R^{\text{cycle}}_{N^{+}}$, $\text{Fail}$ must then be in $D_{SC}$. Otherwise, if $i-j > 0$, then $j < i$, so $N(d_{i-1}, d_{i}) \in D_{SC}$. Thus, by rule $R^{\text{trans}}_{N^{+}}$, $N(d_{j}, d_{i-1}) \in D_{SC}$. Then, $(i-1) - j = (i-j) - 1$, so by induction hypothesis, we have $\text{Fail} \in D_{SC}$.

If $A = q(d_{i}, d_{j})$: As $\text{time}_{c}(M) = \infty$, for all $j$, we have $q_{j}(z_{h_{j}}, z_{j}) \in \text{res}(D_{n-1})$, so by the previous point, $q_{j}(d_{h_{j}}, d_{j}) \in D_{SC}$. Since $h^{-1}(A) \notin \text{res}(D_{n-1})$, the atom $A$ must be different from $q_{j}(d_{h_{j}}, d_{j})$. If $h_{j} \neq i$, then either $N^{+}(d_{h_{j}}, d_{i})$ or $N^{+}(d_{i}, d_{j})$ is in $D_{SC}$. In either case, since $D_{SC}$ models rule $R^{\text{cell}}_{q_{i}, d_{j}}$, $\text{Fail}$ is in $D_{SC}$. Otherwise, if $i = h_{j}$, it must be that $q \neq q_{j}$. Thus, as $D_{SC}$ models rule $R^{\text{cell}}_{q_{i}, d_{j}}$, $\text{Fail}$ is again in $D_{SC}$.

If $A = c(d_{i}, d_{j})$: First, if $j < i$, then $N^{+}(z_{i}, z_{j}) \in \text{res}(D_{n-1})$, so $N^{+}(d_{j}, d_{i}) \in D_{SC}$. Thus, as $D_{SC}$ models rule $R^{\text{cell}}_{c_{i}, c_{j}}$, $\text{Fail}$ is in $D_{SC}$. We then assume that $i \leq j$. As by hypothesis, $\text{time}_{c}(M) = \infty$, for all $i \leq j$, the atom $c_{i}(z_{i}, z_{j})$ is in $\text{res}(D_{n-1})$, with $c_{j} = M(i, j)$. Thus, by the previous point, $c_{j}(d_{i}, d_{j}) \in D_{SC}$. Since $h^{-1}(A) \notin \text{res}(D_{n-1})$, the atom $A$ must be different from $c_{j}(d_{i}, d_{j})$, so $c \neq c_{i}$. Thus, since $D_{SC}$ models rule $R^{\text{cell}}_{c_{i}, c_{j}}$, $\text{Fail}$ is in $D_{SC}$.

Thus, $\text{res}(D_{n-1})$ and $D_{SC}$ are indeed isomorphic.

Now, since we assume that $M$ does not halt on the empty word, by Theorem 13, we have $(R_{M}, \emptyset) \not\models \text{Goal}$, so what happens on the starting chain alone cannot entail $\text{Goal}$. We then show that the non-starting chains cannot grow much.

**Lemma 33.** Let $D$ be a database, and $D = D_{0}, t_{0}, D_{1}, \ldots$ a Datalog-first restricted derivation from $(R_{M}, D)$. Then, for all $n \in \mathbb{N}$, if $\text{res}(D_{0})$ does not contain $\text{Fail}$, then:

1. If $x$ or $y$ is a variable and $N^{+}(x, [y]) \in \text{res}(D_{n})/\approx$, then $[x]$ and $[y]$ are on the same chain.
2. All non-starting chains only feature classes of Skolem depth at most one.

**Proof.** For point (1), assume for a contradiction that $N^{+}(x, y)$ is the first $N^{+}$-atom in $\text{res}(D_{n})$ featuring a variable, and such that $x$ and $y$ are two terms on different chains. Then, there is a trigger $t = (R, \pi)$ that created $N^{+}(x, y)$.

If $R = R_{N^{+}}$: Then the atom $N(x, y)$ is in $\text{res}(D_{n})$, so $x$ and $y$ are on the same chain.
If $R = R^{trans}$: Then the atoms $N(x, z)$ and $N^+(z, y)$ must be in $\text{res}(\mathcal{D}_n)$ for some term $z$. First, since $N(x, z)$ is in $\text{res}(\mathcal{D}_n)$, then $x$ and $z$ are on the same chain. It remains to show that $z$ and $y$ are on the same chain.

If $y$ is a variable, then $N^+(z, y)$ is an $N^+$-atom containing a variable created before $N^+(x, y)$, so $z$ and $y$ are on the same chain by induction hypothesis.

If $z$ is a constant, then by point (1) of Lemma 26, we have $N(x, z) \in \text{res}(\mathcal{D}_0)$, so $x$ is a constant. Thus, $y$ has to be a variable, and $N^+(z, y)$ is again an $N^+$-atom containing a variable created before $N^+(x, y)$, so $z$ and $y$ are on the same chain by induction hypothesis.

Thus, in both cases, the result holds.

If $R \in \{R^{exp}_{N^+, 1}, R^{exp}_{N^+, 2}\}$: Then there must be $N^+(z, t)$ in $\text{res}(\mathcal{D}_n)$ with $z \approx x$ and $t \approx y$. Then, if $x$ is a variable, by point (4) of Lemma 26, $[x] = \{x\}$, so $z \approx x$ and $N^+(z, t)$ is an $N^+$-atom featuring a variable introduced before $N^+(x, y)$, so $z$ and $t$ are on the same chain. The same reasoning applies if $y$ is a variable. Thus, in both cases, $z$ and $t$ are on the same chain, so $x$ and $y$ are on the same chain too.

Thus, no rule can generate such an atom, which then cannot exist, so point (1) holds.

We then prove point (2). Let $y$ be a variable on a non-starting chain, and let $t = (R, \pi)$ be the rule that created it. We then prove that its Skolem depth must be one. As $y$ is on a non-starting chain, we cannot have $q_0(y, y) \in \text{res}(\mathcal{D}_n)$, so $R \neq R_0$. In addition, for the same reason, $R \neq R_1$, as otherwise there would be a term $x$ such that $q_0(x, x)$ and $N(x, y)$ are in $\text{res}(\mathcal{D}_n)$, so $y$ would be on the starting chain. Thus, it must be that $R = R_{n+1}$. Then, there are some terms $z_0$ and $x$ such that $q_0(z_0, z_0)$, $N^+(z_0, x)$ and $N(x, y)$ are in $\text{res}(\mathcal{D}_n)$. As $y$ is on a non-starting chain, $z_0$ is not on the same chain as $y$, and thus as $x$. Thus, by point (1), $z_0$ and $x$ must both be constants, so $\text{SkD}(y) = 1$, concluding the proof.

Finally, we need to control what happens between chains. What happens between non-starting chains is not an issue as all the terms involved are of Skolem depth at most one by Lemma 33, but if state and character atoms are between a non-starting and a starting chain, there could be a false start that is allowed to grow enough to entail $\text{Goal}$ using terms of unbounded depth. To prevent this, we show that there can be no atom using a state predicate and terms of Skolem depth greater than one on different chains.

**Lemma 34.** Let $\mathcal{D}$ be a database, and $\mathcal{D} = \mathcal{D}_0, t_0, \mathcal{D}_1, \ldots$ a Datalog-first restricted derivation from $(\mathcal{R}_M, \mathcal{D})$. Then, for all $n \in \mathbb{N}$, if $\text{res}(\mathcal{D}_0)$ does not contain $\text{Fail}$, and $q(x, y) \in \text{res}(\mathcal{D}_n)$ for some state $q$ and terms $x, y$ where $x$ or $y$ is a variable, then $x$ and $y$ are on the same chain.

**Proof.** Assume for a contradiction that there is a first atom $q(x, y) \in \text{res}(\mathcal{D}_n)$ for some state $q$ and terms $x$ and $y$ on different chains with $x$ or $y$ a variable. This atom must have been generated by some trigger $t = (R, \pi)$, as it features a variable.

If $R = R_0$: Then $x = y$ so $x$ and $y$ are on the same chain.
If $R = R_{q_0}^{\text{var}}$: Then there are atoms $N(x, z)$ and $N^+(z, y)$ in $\text{res}(D_n)$ for some term $z$. By point (1) of Lemma 26, if $z$ is a constant, then $x$ has to be a constant too, so $y$ must be a variable. Thus, in all cases, the atom $N^+(z, y)$ features a variable, so $z$ and $y$ must be on the same chain by point (1) of Lemma 33. Thus, as $x$ and $z$ are on the same chain, $x$ and $y$ must be too.

If $R = R_{q_1}^{\text{var}}$: Then there must be an atom $N^+(x, y)$ in $\text{res}(D_n)$, so $x$ and $y$ must be on the same chain by point (1) of Lemma 33.

If $R = R_{q,\text{max}}$: Then again $x = y$ so $x$ and $y$ are on the same chain.

If $R \in \{ R_{q_1}^{\text{eq}}, R_{q_2}^{\text{eq}} \}$: Then there must be an atom $q(z, t)$ with $z \approx x$ and $t \approx y$. Since this atom has to come before $q(x, y)$, and $x$ or $y$ is a variable, so either $z = x$ or $t = y$ by (26), $z$ and $t$ must be on the same chain. As being on the same chain is a notion invariant through $\approx$, $x$ and $y$ are on the same chain too.

\[ \Box \]

### 3.3.6 Skolem depth and Datalog-expressibility

We now are fully equipped to show that $(R_M, \text{Goal})$ has bounded depth.

**Theorem 35.** If $M$ does not halt on the empty word, then $(R_M, \text{Goal})$ has bounded depth.

**Proof.** Let $D$ be a database and $D = D_0, t_1, D_1, \ldots$ any Skolem-increasing derivation. Then, assume that $(R_M, D) \models \text{Goal}$, and let $n$ be the smallest integer such that $\text{Goal} \in \text{res}(D_n)$. We then show that all the terms appearing in $\text{res}(D_n)$ are of Skolem depth at most one. Notice that this is enough to show that $(R_M, \text{Goal})$ has bounded depth, as the other direction is trivial.

First, if $n = 0$, as $\text{res}(D_0)$ only contains constants (of Skolem depth zero), the statement holds. Thus, in the following, we assume $\text{Goal} \notin \text{res}(D_0)$. As $\text{res}(D_0)$ models rule $R_{\text{Fail}}$, this also means that $\text{Fail} \notin \text{res}(D_0)$, which by Proposition 31 entails that $(R_M, D) \not\models \text{Fail}$. Let $n$ be the smallest integer such that $\text{Goal} \in \text{res}(D_n)$. Then, $\text{Goal}$ must have been introduced by some trigger $t = (R, \pi)$ during $\text{res}(D_n)$. As $(R_M, D) \not\models \text{Fail}$, it must be that $R \neq R_{\text{Fail}}$.

If $R = R_{q_0}$, then an atom $q_f(x, y)$ must be in $\text{res}(D_n)$. As $\text{Goal} \notin \text{res}(D_0)$, by Proposition 27, $x$ or $y$ must be a variable. Thus, by Lemma 34, $x$ and $y$ are on the same chain. In addition, as $M$ does not halt on the empty word, by Lemma 32, $x$ and $y$ cannot be on the starting chain, so they are both on a non-starting chain. By Lemma 33, $\text{SkD}(x)$ and $\text{SkD}(y)$ are both less than one. Thus, by the contrapositive of Proposition 27, $\text{res}(D_n)$ only contains terms of Skolem depth less than one.

If $R = R_{q_1}^{\text{eq}}$, then atoms $q_0(x, x)$, $q(x, y)$ and $c(x, y)$ must be in $\text{res}(D_n)$ (with $\delta(q, c) = (q', c', \leftarrow)$ for some $q'$, $c'$). As $\text{Goal} \notin \text{res}(D_0)$, by Proposition 27, $x$ or $y$ must be a variable. Thus, by Lemma 34, $x$ and $y$ are on the same chain. In addition, as $M$ does not halt on the empty word, by Lemma 32, $x$ and $y$ cannot be on the starting chain, so they are both on a non-starting chain. By Lemma 33, $\text{SkD}(x)$ and $\text{SkD}(y)$ are both less than one. Thus, by the contrapositive of Proposition 27, $\text{res}(D_n)$ only contains terms of Skolem depth less than one. \[ \Box \]
Theorem 17. The pair \((R_M, \text{Goal})\) is Datalog-expressible.

Proof. If \(M\) halts on the empty word, then by Theorem 13, \((R_M, \emptyset) \models \text{Goal}\). Thus, by monotonicity of first-order entailment, for all databases \(D\), \((R_M, D) \models \text{Goal}\), so \((\{\rightarrow \text{Goal}\}, \text{Goal})\) is a suitable Datalog rewriting.

If \(M\) does not halt on the empty word, then by Theorem 35, it has bounded depth, so by Theorem 20, it is Datalog expressible. \qed

We can finally prove the main result.

Theorem 3. Query answering over Datalog-expressible rule sets is undecidable.

Proof. Assume for a contradiction that query answering over Datalog-expressible rule sets is decidable, and consider a Turing machine \(M\). Then, by Theorem 17, the couple \((R_M, \text{Goal})\) is Datalog-expressible. Thus, we can decide if \((R_M, \emptyset) \models \text{Goal}\). By Theorem 13, \((R_M, \emptyset) \models \text{Goal}\) if and only if \(M\) halts on the empty word. Thus, we are able to decide the halting problem, which is absurd. \qed
Bibliography


