Assessing Achievability of Queries and Constraints

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Abstract. Assessing and improving the quality of data in data-intensive systems are fundamental challenges that have given rise to numerous applications targeting transformation and cleaning of data. However, while schema design, data cleaning, and data migration are nowadays reasonably well understood in isolation, not much attention has been given to the interplay between the tools that address issues in these areas. Our focus is on the problem of determining whether there exist sequences of data-transforming procedures that, when applied to the (untransformed) input data, would yield data satisfying the conditions required for performing the task in question. Our goal is to develop a framework that would address this problem, starting with the relational setting.

In this paper we abstract data-processing tools as black-box procedures. This abstraction describes procedures by a specification of which parts of the database might be modified by the procedure, as well as by the constraints that specify the required states of the database before and after applying the procedure. We then proceed to study fundamental algorithmic questions arising in this context, such as understanding when one can guarantee that sequences of procedures apply to original or transformed data, when they succeed at improving the data, and when knowledge bases can represent the outcomes of procedures. Finally, we turn to the problem of determining whether the application of a sequence of procedures to a database results in the satisfaction of properties specified by either queries or constraints. We show that this problem is decidable for some broad and realistic classes of procedures and properties, even when procedures are allowed to alter the schema of instances.

1 Introduction

A common approach to ascertaining and improving the quality of data is to develop procedures and workflows for repairing or improving data sets with respect to quality constraints. The community has identified a wide range of problems that are vital in this respect, leading to the creation of several lines of research, which have normally been followed by the development of toolboxes that practitioners can use to solve their problems.
As a result, organizations facing data-improvement problems now have access to a variety of data-management tools to choose from; the tools can be assembled to construct what can be called workflows of data operations. However, in contrast to the considerable body of research on specific operations or entire business workflows (see, e.g., [17,10,16,5]), previous research appears to have not focused explicitly on the assembly process itself nor on providing guarantees that the desired data-quality constraints will be satisfied once the assembled workflow of procedures has been applied to the data.

We investigate constructing workflows from available procedures. That is, we consider a scenario in which an organization needs to meet a certain data-quality criterion or goal using available data-improvement procedures. The problem is to understand whether the procedures can be assembled into a workflow in a way that would guarantee that the data produced by the workflow will meet the desired quality goal.

Motivating example: Suppose a medical analyst wishes to know the emergency rooms that are used by patients with a certain medical insurance. The data owned by the analyst reside in a relation \( \text{LocVisits} (\text{facility}, \text{pId}, \text{timestp}) \), with the attributes standing, respectively, for the id of the facility where the emergency room is, the social-security number of a patient, and a timestamp marking the date of the emergency visit.

The analyst has also been given two procedures he can execute as-is but not modify: A procedure \( P_{\text{migrate}} \), which is supposed to migrate data into \( \text{LocVisits} \) from relation \( \text{EVisits} \) owned by another analysis company, and a procedure \( P_{\text{insur}} \), which augments the relation \( \text{LocVisits} \) with an attribute \( \text{insId} \) containing the insurance of patients, and whose data are drawn from relation \( \text{Patients}(\text{pId}, \text{insId}) \) owned by the local authority.

Given an insurance id \( I \), the analyst can capture the desired information via query
\[
\text{SELECT facility FROM LocVisits WHERE insId = I, posed over LocVisits}
\]
with an additional attribute \( \text{insId} \) containing the insurance of patients. It is natural for the analyst to ask: Can I use any or all of the above procedures to transform my data so that this query can be posed on my database? Or is there a way to apply these procedures so that I can guarantee that my database satisfies certain quality criteria?

1.1 Contributions

Our specific focus is on the problem of determining whether there exist sequences of data-transforming procedures that, when applied to the given data, would yield data satisfying certain given conditions.

We propose a formal framework in which data-processing tools are abstracted as black-box procedures, describing them by means of the following information:

- A specification of which parts of the database the procedure is modifying;
- A set of conditions that need to be satisfied in order for the procedure to be applied;
A set of conditions that are guaranteed to be satisfied once the procedure has been applied; and

In some cases, additional guarantees that certain pieces of data will not be deleted or modified.

We also define the notion of outcome of applying a procedure to an instance of data, and consider sets of such outcomes. As our goal is to reason about workflows of data-processing procedures, we also study the notion of outcome (and sets of outcomes) of a sequence of applications of procedures.

These definitions naturally lead us to two fundamental decision problems in our framework. The first problem is applicability: Given an instance and a sequence of procedures, is one guaranteed to be able to apply successive procedures in the sequence? The second problem is non-emptiness: Is one guaranteed to obtain at least one outcome of applying a given sequence of procedures? We show that our definitions are too general to guarantee efficient algorithms for these problems, but also identify interesting and realistic classes of procedures that lead to the tractability of these basic problems.

Next, for sequences of procedures belonging to the well-behaved classes we have identified, we focus on representing the sets of their outcomes. We show that these sets can be represented by a knowledge base in which the knowledge is given by tuple-generating dependencies, and some of the relations are closed to adding more data. We show that such knowledge bases form a strong representation system, in the sense of [25], for application of procedures. We also show how to reason about such knowledge bases, studying in particular the problems of query answering and constraint satisfaction.

Finally, we use our toolbox to study what we call the data-readiness problem: Given an instance \( I \), a set \( \Pi \) of procedures, and a specification of a property over instances, is there a way to construct a workflow with procedures from \( \Pi \) so that each instance in the outcome satisfies this property? Once again, while undecidable in its general form, we show that this problem is decidable for some broad classes of procedures.

Structure of the Exposition. To simplify the formal exposition, in this paper we restrict our attention to relational data. The general methods, however, seem promising for application to other forms of data as well, including semistructured and text data.

Within the scope of relational data, in most of the discussion in this paper we further restrict our attention to transformations of data that do not change the schema. In this setting, one can formalize many types of data-adequacy conditions in terms of dependencies, and treat the above planning task in terms of chase. We also briefly consider transformations that change both the schema and contents of the data, and sketch the use of such transformations in treating schema updates.
1.2 Related Work

Data quality: Numerous works treat issues in the broad spectrum of data quality. [40] provides a widely acknowledged study on eliciting and defining specific dimensions of quality of the data; see also [26,32]. In this space, many works view data-quality measures as objective properties unconnected to specific uses of the data. The role of purpose in determining data quality is more visible in [30,39,14], where quality data are regarded as being fit for their intended use, taking both context and use (i.e., tasks to be performed) into account when evaluating and improving the quality of data.

Task dependence: Recent efforts have put an emphasis on data-quality policies and strategies w.r.t. specific tasks to be performed on the data. [30] presents general information-quality policies that structure decisions on information, and [38] presents an improvement cycle for data quality. [31] moves toward integration of process measures with information-quality measures. Our work in the present paper differs from these lines of research in that we assume that task-oriented data-quality requirements are already given in the form of constraints on the data, and that procedures for improving data quality are also specified and available.

Data preparation: The work [24] introduces a unified framework covering formalizations and approaches for a range of problems in data extraction, cleaning, repair, and integration, and also supplies an excellent survey of related work in these areas. More recent work in data preparation includes [9,8,29,35,34].

Workflows: Research on business processes [16] studies both the environment in which data are generated and transformed, including processes, users of data, and goals of using the data, and automatic composition of services into business processes under the assumption that the assembly needs to follow a predefined workflow of executions of actions or services [5,6,7]. Our work, in contrast, begins with the data properties that the workflow should ensure, rather than with the outlines of the workflow itself. In that sense, our work is in line with the efforts of, e.g., [13], while differing from those works in the nature of the specifications and of the components from which workflows are assembled. The work of [17,10] stands closer to reasoning about static properties of business-process workflows, but does not pursue the goal of constructing workflows.

Some recent systems work, e.g., [28], emphasizes the importance of data-transforming workflows assembled from individual procedures, while advocating for users to choose from sets of preassembled workflows. In this paper, we focus on providing tools for assembling individual data-transforming workflows as needed, which complements nicely the efforts of the line of work of [28].

2 Preliminaries

2.1 Schemas and Instances

Assume a countably infinite set of attribute names $\mathcal{A} = \{A_1, A_2, \ldots\}$ totally ordered by $\leq_\mathcal{A}$, a countably infinite domain of values (or elements) $D$ disjoint
from $\mathcal{A}$, and a countably infinite set of relation names $\mathcal{R} = \{R_1, R_2, \ldots\}$ disjoint from both $\mathcal{A}$ and $\mathcal{R}$. A relational schema over $\mathcal{A}$ and $\mathcal{R}$ is a partial function $\mathcal{S} : \mathcal{R} \to 2^\mathcal{A}$ with finite domain, which associates a finite set of attributes with a finite set of relation symbols. Abusing the notation, we say that $R$ is in $\mathcal{S}$ if $\mathcal{S}(R)$ is defined.

An instance $I$ of schema $\mathcal{S}$ assigns a set $R^I$ of tuples to each relation $R$ in $\mathcal{S}$, so that if $\mathcal{S}(R) = \{A_1, \ldots, A_n\}$, then $R^I \subseteq D^n$, with the set of tuples structured so that the elements of each tuple $(a_1, \ldots, a_n)$ appear in the assumed attribute order, that is, $A_1 <_\mathcal{A} \cdots <_\mathcal{A} A_n$.

Regarding instances as sets of tuples as above suffices when we consider data transformations that do not change the schema. When treating transformations that change the schema of the data, we can no longer treat the functions in $R^I$ as lists of values in $D$, and must replace this unnamed perspective with a named perspective that explicitly notes the attributes connected with each tuple element. Following [1], we regard $R^I$ as a set of functions from $\mathcal{S}(R)$ to $D$, and each tuple $t$ in $R^I$ as a sequence of functions $t = t(A_1), \ldots, t(A_n)$ that lists the values in the attribute order, writing $t(A_i)$ to denote the element of $t$ corresponding to attribute $A_i$. In the named perspective, we denote a tuple $t : \{A_1, \ldots, A_n\} \to D$ using an expression of the form $(A_1 : d_1, \ldots, A_n : d_n)$.

2.2 Queries and Constraints across Schemas

Queries are usually defined with a particular schema in mind, but in preparing and transforming data one sometimes has to deal with queries that might be valid for several schemas. Consider, for instance, the relation LocVisits introduced in Section 1. In languages such as SQL, one can retrieve the IDs of the facilities in LocVisits by issuing the query $\text{SELECT facility from locVisits}$. This query can be applied over instances of multiple schemas, as long as the schema has a relation LocVisits with attribute facility.

Since our goal is to model a framework where schemas may change depending on which procedures are applied to the data, we need the flexibility of being able to specify queries that may be posed over multiple schemas. To formalize such queries, we assume the named perspective on schemas and data, as is explained next.

Named atoms: A named atom is an expression of the form $R(A_1 : x_1, \ldots, A_k : x_k)$, where $R$ is a relation name, each $A_i$ is an attribute name, and each $x_i$ is a variable. We say that the variables mentioned by such an atom are $x_1, \ldots, x_k$, and the attributes mentioned are $A_1, \ldots, A_k$. A named atom $R(A_1 : x_1, \ldots, A_k : x_k)$ is compatible with schema $\mathcal{S}$ if $\{A_1, \ldots, A_k\} \subseteq \mathcal{S}(R)$.

Given a named atom $R(A_1 : x_1, \ldots, A_k : x_k)$, an instance $I$ of schema $\mathcal{S}$ that is compatible with the atom, and an assignment $\tau : \{x_1, \ldots, x_k\} \to D$ assigning values to variables, we say that $(I, \tau)$ satisfies $R(A_1 : x_1, \ldots, A_k : x_k)$ if there is a tuple $\bar{a} : \mathcal{A} \to D$ matching values in $\tau$ with attributes in $R$, in the sense that $\bar{a}(A_i) = \tau(x_i)$ for each $1 \leq i \leq k$. (Under the unnamed perspective, we would require the presence of a tuple $a$ in $R^I$ such that its projection $\pi_{A_1, \ldots, A_k} \bar{a}$ over $A_1, \ldots, A_k$ is precisely the tuple $\tau(x_1), \ldots, \tau(x_k)$.)
**Conjunctive queries:** A conjunctive query (CQ) is an expression of the form \( \exists \bar{z} \phi(\bar{z}, \bar{y}) \), where \( \bar{z} \) and \( \bar{y} \) are tuples of variables, and \( \phi(\bar{z}, \bar{y}) \) is a conjunction of named atoms that use the variables in \( \bar{z} \) and \( \bar{y} \). A CQ is compatible with \( S \) if all its named atoms are compatible.

The usual semantics of conjunctive queries is obtained from the semantics of named atoms in the usual way. Given a conjunctive query \( Q \) that is compatible with \( S \), the result \( Q(I) \) of evaluating \( Q \) over \( I \) is the set of all the tuples \( \tau(x_1), \ldots, \tau(x_k) \) such that \((I, \tau)\) satisfy \( Q \).

**Total queries:** A total query, which we define to be an expression of the form \( R \) for some relation name \( R \), extracts all the tuples stored in \( R \), regardless of the schema and arity of \( R \), as is done in SQL with \( \text{SELECT} * \text{ FROM} \ R \). A total query of this form is compatible with schema \( S \) if \( S(R) \) is defined and the result of evaluating this query over an instance \( I \) over a compatible schema \( S \) is the set of all (unnamed) tuples in \( R \).

**Data constraints:** We consider data constraints that are (i) tuple-generating dependencies (tgds), i.e., expressions of the form \( \forall \bar{x}(\exists \bar{y}\phi(\bar{x}, \bar{y}) \rightarrow \exists \bar{z}\psi(\bar{x}, \bar{z})) \), for CQs \( \exists \bar{y}\phi(\bar{x}, \bar{y}) \) and \( \exists \bar{y}\psi(\bar{x}, \bar{z}) \), and (ii) equality-generating dependencies (egds), i.e., expressions of the form \( \forall \bar{x}(\exists \bar{y}\phi(\bar{x}, \bar{y}) \rightarrow x = x') \), for a CQ \( \exists \bar{y}\phi(\bar{x}, \bar{y}) \) and variables \( x, x' \) in \( \bar{x} \). As usual, for readability we sometimes omit the universal quantifiers of tgds and egds.

An instance \( I \) satisfies a set \( \Sigma \) of tgds and egds, written \( I \models \Sigma \), if (1) each CQ in each dependency in \( \Sigma \) is compatible with the schema of \( I \), and (2) every assignment \( \tau : \bar{x} \cup \bar{y} \rightarrow D \) such that \((I, \tau) \models \phi(\bar{x}, \bar{y})\) can be extended into a \( \tau' : \bar{x} \cup \bar{y} \cup \bar{z} \rightarrow D \) such that \((I, \tau') \models \psi(\bar{x}, \bar{z})\).

A tdg is full if it does not use existentially quantified variables on the right-hand side, and acyclic if none of the relations on the right-hand side appear on the left-hand side. A set \( \Sigma \) of tgds is full if each tdg in \( \Sigma \) is full. \( \Sigma \) is acyclic if an acyclic graph is formed by representing each relation mentioned in a tdg in \( \Sigma \) as a node and by adding an edge from node \( R \) to \( S \) if a tdg in \( \Sigma \) mentions \( R \) on the left-hand side and \( S \) on the right-hand side.

## 3 Procedures under static schemas

In this section we formalize the notion of procedures that transform data. We view procedures as black boxes, and assume no knowledge of or control over their inner workings. Our reasoning about procedures is based on the following information: The input conditions, or preconditions, on the state of the data that must hold for a procedure to be applicable; the output conditions, or postconditions, on the state of the data that must hold after an application of the procedure; and the set of relations affected by the application. To specify that some of the data will not be deleted, we also allow the inclusion of some queries whose answer needs to be preserved during the application of the procedure.

**Example 1.** Let us return to the procedure \( P_{\text{migrate}} \) outlined in Section 1. The intent of \( P_{\text{migrate}} \) is to define migration of data from relation \( \text{EVisits} \) into \( \text{LocVisits} \). \( P_{\text{migrate}} \) can be described by the following information:
Scope: Since \( P_{\text{migrate}} \) migrates tuples into \( \text{LocVisits} \), we specify that the procedure only changes this relation.

Precondition: We specify that \( P_{\text{migrate}} \) requires a schema with relations \( \text{LocVisits} \) and \( \text{EVisits} \), both with attributes \( \text{facility} \), \( \text{pId} \) and \( \text{timestp} \).

Postcondition: After \( P_{\text{migrate}} \) is applied, it must be that each tuple in \( \text{EVisits} \) is in \( \text{LocVisits} \).

Preserved queries: The existing tuples in \( \text{LocVisits} \) are not deleted during the migration process. We specify this by stating that the answers to the query \( \text{SELECT} \ \text{facility}, \ \text{ssn}, \ \text{timestp} \ \text{FROM} \ \text{locVisits} \) are preserved in each application of \( P_{\text{migrate}} \).

In the following we present notation for formally defining these types of procedures. We start by introducing “structure constraints,” which we use to define the scopes of procedures. We will also use these in Section 7, when working with schema-altering procedures.

3.1 Structure Constraints

A structure constraint is a formula of the form \( R[\bar{s}] \) or \( R[\ast] \), where \( R \) is a relation symbol, \( \bar{s} \) is a tuple of attributes names from \( A \), and \( \ast \) is a symbol not in \( A \) or \( R \) intended to function as a wildcard. A schema \( S \) satisfies a structure constraint \( R[\bar{s}] \), denoted by \( S | R[\bar{s}] = \), if \( S(R) \) is defined and each attribute in \( \bar{s} \) belongs to \( S(R) \). The schema satisfies the constraint \( R[\ast] \) if \( S(R) \) is defined.

Given a set \( C \) of structure constraints and a schema \( S \), we denote by \( Q_{S \setminus C} \) the conjunctive query formed by the conjunction of the following atoms:

- For each relation \( R \) such that \( S(R) = \{A_1, \ldots, A_m\} \) but \( R \) is not mentioned in \( C \), \( Q_{S \setminus C} \) includes an atom \( R(A_1 : z_1, \ldots, A_m : z_m) \), where \( z_1, \ldots, z_m \) are fresh variables.

- For each \( T \) mentioned in \( C \) but such that \( T[\ast] \) is not in \( C \), \( Q_{S \setminus C} \) includes an atom \( T(B_1 : z_1, \ldots, B_k : z_k) \), where \( \{B_1, \ldots, B_k\} \) is the set of all the attributes in \( S(T) \) that are not mentioned in any constraint of the form \( T[\bar{s}] \) in \( C \), and \( z_1, \ldots, z_k \) are fresh variables.

Intuitively, \( Q_{S \setminus C} \) is intended to retrieve the projection of the entire database over all the relations and attributes not mentioned in \( C \). Note that \( Q_{S \setminus C} \) is unique up to the renaming of variables and order of conjuncts.

As an example, let schema \( S \) have relations \( R, S, \) and \( T \), such that \( R \) has attributes \( A_1 \) and \( A_2 \), \( T \) has attributes \( B_1, B_2, \) and \( B_3 \), and \( S \) has \( A_1 \) and \( B_1 \). Let set \( C \) comprise constraints \( R[\bar{s}] \) and \( S[B_1] \). Then \( Q_{S \setminus C} \) is the query \( T(B_1 : z_1, B_2 : z_2, B_3 : z_3) \land S(A_1 : w_1) \).

3.2 Formal Definition of Procedures

We define procedures w.r.t. a class \( \mathcal{C} \) of FO constraints and a class \( \mathcal{Q} \) of queries, but we mostly consider tgds, egds, structure constraints, and CQ queries.
Definition 1. A procedure $P$ over $\mathbb{C}$ and $\mathbb{Q}$ is a tuple $(\text{Scope}, C_{\text{in}}, C_{\text{out}}, Q_{\text{pres}})$, where

- $\text{Scope}$ is a set of structure constraints that defines the scope (i.e., the relations and attributes) within which the procedure operates;
- $C_{\text{in}}$ and $C_{\text{out}}$ are constraints in $\mathbb{C}$ that describe the pre- and postconditions of $P$, respectively; and
- $Q_{\text{pres}}$ is a set of queries in $\mathbb{Q}$ that serve as a preservation guarantee for the procedure.

Example 2 (Example 1 continued). The procedure $P_{\text{migrate}}$ is formally described as follows:

$\text{Scope}$: The scope is the constraint $\text{LocVisits}[^*]$.  
$C_{\text{in}}$: We use the structure constraints $\text{EVisits}[\text{facility}, pId, timestp]$ and $\text{LocVisits}[\text{facility}, pId, timestp]$, to ensure that the data have the correct attributes.  
$C_{\text{out}}$: The postcondition comprises the tgd  
$\text{EVisits}(\text{facility}: x, pId : y, timestp : z) \rightarrow \text{LocVisits}(\text{facility}: x, pId : y, timestp : z)$.  

This says that, once $P_{\text{migrate}}$ has been applied, the projection of $\text{EVisits}$ over attributes $\text{facility}$, $pId$, and $\text{timestp}$ must be a subset of the respective projection of $\text{LocVisits}$.  
$Q_{\text{pres}}$: We use the query $\text{LocVisits}(\text{facility}: x, pId : y, timestp : z)$, whose intent is to state that all the answers to this query on $\text{LocVisits}$ that are present before the application of $P_{\text{migrate}}$ must be preserved.

Semantics: A procedure $P = (\text{Scope}, C_{\text{in}}, C_{\text{out}}, Q_{\text{pres}})$ is applicable on an instance $I$ over schema $S$ if (1) Each query in $Q_{\text{pres}}$ is compatible with $S$; and (2) $I \models C_{\text{in}}$. We can now proceed with the semantics of procedures.

Definition 2. Let $I$ be an instance over schema $S$. An instance $I'$ over $S$ is a possible outcome of applying procedure $P$ to $I$ if all of the following holds:

1. $P$ is applicable on $I$;  
2. $I' \models C_{\text{out}}$;  
3. The answers of the query $Q_{S \setminus \text{Scope}}$ do not change: $Q_{S \setminus \text{Scope}}(I) = Q_{S \setminus \text{Scope}}(I')$; and  
4. The answers to each query $Q$ in $Q_{\text{pres}}$ over $I$ are preserved: $Q(I) \subseteq Q(I')$.

Example 3 (Example 2 continued). Recall procedure $P_{\text{migrate}} = (\text{Scope}, C_{\text{in}}, C_{\text{out}}, Q_{\text{pres}})$ defined in Example 2. Consider instance $I$ over schema $S$ with relations $\text{EVisits}$ and $\text{LocVisits}$, each with attributes $\text{facility}$, $pId$, and $\text{timestp}$, as shown in Figure 1(a). Note first that $P_{\text{migrate}}$ is indeed applicable on $I$. When applying $P_{\text{migrate}}$ to $I$, we know from $\text{Scope}$ that the only relation whose content can change is $\text{LocVisits}$, while $\text{EVisits}$ is the same across all possible outcomes. Furthermore, we know from $C_{\text{out}}$ that in all possible outcomes the projection of $\text{EVisits}$ over attributes $\text{facility}$, $pId$, and $\text{timestp}$ must be the same as the
Fig. 1. Instance I of Example 3 (a), a complete possible outcome of applying $P_{\text{migrate}}$ to I (b), and the relation LocVisits of two other possible outcomes, one in which LocVisits contains additional tuples not mentioned in EVisits (c), and one where an extra attribute is added to LocVisits (d).

As seen in Example 3, in general the number of possible outcomes that result from applying a procedure is infinite. Thus, we are generally more interested in properties shared by all possible outcomes, which motivates the following definition.

**Definition 3.** The outcome set of applying a procedure P to I is defined as the set:

$$\text{outcomes}_p(I) = \{ I' \mid I' \text{ is a possible outcome of applying } P \text{ to } I \}.$$
The outcome of applying a procedure $P$ to a set of instances $\mathcal{I}$ is the union of the outcome sets of applying $P$ to all the instances in $\mathcal{I}$:

$$\text{outcomes}_P(\mathcal{I}) = \bigcup_{I \in \mathcal{I}} \text{outcomes}_P(I).$$

Finally, since in general we are interested in (perhaps repeated) applications of multiple procedures, we extend the definitions to enable talking about the outcomes of sequences of procedures.

**Definition 4.** The outcome of applying a sequence $P_1, \ldots, P_n$ of procedures to instance $I$ is the set

$$\text{outcomes}_{P_1, \ldots, P_n}(I) = \text{outcomes}_{P_n}(\text{outcomes}_{P_{n-1}}(\cdots(\text{outcomes}_{P_1}(I))\cdots)).$$

## 4 Fundamental Decision Problems

As promised, we begin our study with two decision problems on outcomes of sequences of procedures.

### 4.1 Applicability of Procedures

In our proposed framework, the focus is on transformations of data sets given by sequences of procedures. Because we treat procedures as black boxes, the only description we have of the results of these transformations is that they ought to satisfy the output constraints of the procedures. In this situation, how can one guarantee that all the procedures in a given sequence will be applicable? Suppose that, for instance, we wish to apply procedures $P_1$ and $P_2$ to instance $I$ sequentially: First $P_1$, then $P_2$. The problem is that, since output constraints do not fully determine the outcome of $P_1$ on $I$, we cannot immediately guarantee that this outcome would satisfy the preconditions of $P_2$.

Given that the set of outcomes is in general infinite, our focus is on guaranteeing that any possible outcome of applying $P_1$ to $I$ will satisfy the preconditions of $P_2$. This gives rise to our first problem of interest:

**Applicability**: 

**Input:** A sequence $P_1, \ldots, P_n$ of procedures and a schema $\mathcal{S}$; 

**Question:** Can $P_n$ be applied to each instance in $\text{outcomes}_{P_1, \ldots, P_{n-1}}(I)$, regardless of the choice of instance $I$ of $\mathcal{S}$?

The Applicability problem is intimately related to the problem of implication of dependencies, defined as follows: Given a set $\Sigma$ of dependencies and an additional dependency $\lambda$, is it true that all the instances that satisfy $\Sigma$ also satisfy $\lambda$?
\(\lambda\) — that is, does \(\Sigma\) imply \(\lambda\)? Indeed, consider a class \(\mathcal{L}\) of constraints for which the implication problem is known to be undecidable. Then one can easily show that the applicability problem is also undecidable for those procedures whose pre- and postconditions are in \(\mathcal{L}\); Intuitively, if we let \(P_1\) be a procedure with a set \(\Sigma\) of postconditions, and \(P_2\) a procedure with a dependency \(\lambda\) as a precondition, then it is not difficult to come up with proper scopes and preservation queries so that the set \(\text{outcomes}_{P_1}(I)\) satisfies \(\lambda\) for every instance \(I\) over schema \(\mathcal{S}\) if and only if \(\lambda\) is true in all the instances that satisfy \(\Sigma\).

However, as the following result shows, the \textsc{Applicability} problem is undecidable already for very simple procedures, and even when we consider the \textit{data-complexity} view of the problem, that is, when we fix the procedure and take a particular input instance.

\textbf{Proposition 1.} There are fixed procedures \(P_1\) and \(P_2\) that only use tgds for their constraints, and such that the following problem is undecidable: Given an instance \(I\) over schema \(\mathcal{S}\), is it true that all the instances in \(\text{outcomes}_{P_1}(I)\) satisfy the preconditions of \(P_2\)?

The proof of Proposition 1 is by reduction from the embedding problem for finite semigroups, shown to be undecidable in [27].

There are several lines of work aiming to identify practical classes of constraints for which the implication problem is decidable, and we believe that the corresponding results can be applied in our framework. However, we opt for a stronger restriction, by focusing on procedures without preconditions. In this setting, we have the following trivial result.

\textbf{Fact 1} If \(P_1, \ldots, P_n\) do not have preconditions, then \textsc{Applicability} is always true, regardless of the schema.

When studying schema-altering procedures in Section 7, we extend this class of procedures to include structure constraints as a means for specifying that certain procedures must be applied on schemas with certain properties. We do not do it here because structure constraints as preconditions do not make much sense under the static semantics of procedures.

### 4.2 Nonemptiness

The other important problem is determination of whether the outcome of a sequence of procedures will be nonempty. We remark that even without preconditions, the outcome of a procedure may be empty if it is not possible to transform an instance in a way that would satisfy the postconditions of a procedure (and to ensure that the scope and preservation queries are respected). Perhaps surprisingly, we can show that this problem is undecidable even if we just have one fixed procedure.

\textbf{Proposition 2.} There exists a procedure \(P\) that does not use preconditions and uses only tgds in its postconditions, such that the following is undecidable: Given an instance \(I\), is the set \(\text{outcomes}_{P}(I)\) nonempty?
The proof of this result makes use of arbitrary tgds. What is even more striking is that we can reproduce the undecidability proof even when considering acyclic tgds, albeit this time we need two fixed procedures.

**Proposition 3.** There exist procedures $P_1$ and $P_2$ that do not use preconditions and only use acyclic tgds in their postconditions, such that the following problem is undecidable: Given an instance $I$, is the set outcomes$_{P_1,P_2}(I)$ nonempty?

The idea of the proof is to manipulate the scope of procedures to create cases when we force some procedures to take care of transformations specified in subsequent procedures. We illustrate this idea with the following example.

**Example 4.** Consider two procedures $P_1$ and $P_2$, where $P_1 = (\text{Scope}^1, C_{\text{in}}^1, C_{\text{out}}^1, Q_{\text{pres}}^1)$, with $\text{Scope}^1 = \{R[s], T[s]\}$, $C_{\text{in}}^1 = \emptyset$, $C_{\text{out}}^1 = \{R(A : x) \rightarrow T(A : x)\}$, and $Q_{\text{pres}}^1 = R(A : x) \land T(A : x)$; $P_2$ has empty scope, preconditions, and preservation queries, and has the postcondition set $\{T(A : x) \rightarrow R(A : x)\}$. Let $I$ be an instance over schema with relations $R$ and $T$, each with attribute $A$. By definition, the possible outcomes of applying $P_1$ to $I$ are all the instances $J$ that extend $I$ and satisfy $R(A : x) \rightarrow T(A : x)$. Now the set outcomes$_{P_1,P_2}(I)$ corresponds to all the instances $I'$ that extend $I$ and satisfy both $R(A : x) \rightarrow T(A : x)$ and $T(A : x) \rightarrow R(A : x)$. (In other words, we can use $P_2$ to filter out all those instances $J$ where $T^I \not\subseteq R^J$.) Intuitively, this happens because the outcome set of applying $P_2$ to any instance not satisfying $T(A : x) \rightarrow R(A : x)$ is empty, and we define outcomes$_{P_1,P_2}(I)$ as the union of all the sets outcomes$_{P_2}(K)$ for each $K \in \text{outcomes}_{P_1}(I)$.

**Procedures with safe scope:** We could continue restricting the types of constraints we allow in procedures (for example, nonemptiness is decidable if we allow procedures made just from full, acyclic constraints). However, we choose to adopt a different strategy: We restrict the interplay between the postconditions of procedures, their scope, and their preservation queries. This will allow us to rule out the undesirable behaviours illustrated in Example 3, and will become crucial at the time of reasoning about sequences of procedures.

We say that procedure $P = (\text{Scope}, C_{\text{in}}, C_{\text{out}}, Q_{\text{pres}})$ has safe scope if the following holds:

- $C_{\text{in}}$ is empty;
- $C_{\text{out}}$ is an acyclic set of tgds;
- The set $\text{Scope}$ contains exactly one constraint $R[s]$ for each relation $R$ that appears on the right-hand side of a tgd in $C_{\text{out}}$; and
- The set $Q_{\text{pres}}$ contains one total query $R$ for each constraint $R[s]$ in $\text{Scope}$.

That is, it binds precisely all the relations in the scope of $P$.

Note that the procedure $P_{\text{migrate}}$ of Example 2 is not a procedure with safe scope, but can easily be transformed into a procedure with safe scope. Once again we have an easy result that makes a case for the good behaviour of procedures with safe scope.

**Proposition 4.** For every instance $I$ and sequence $P_1, \ldots, P_n$ of procedures with safe scope, the set outcomes$_{P_1,\ldots,P_n}(I)$, is not empty.
5 Analyzing the outcomes of procedures

We have seen that deciding properties of outcomes of sequences of procedures (or even of a single procedure) can be a nontrivial task. One of the reasons is that procedures do not completely define their outcomes: We do not really know the outcome of applying a sequence \( P_1, \ldots, P_n \) of procedures to an instance \( I \), we just know that it will be an instance from the collection \( outcomes(P_1, \ldots, P_n)(I) \). This collection may well be of infinite size, but can it still be represented finitely? The backdrop to this question is the variety of formalisms that have been developed by the community for representing sets of instances, from tables with incomplete information [25] to knowledge bases (see, e.g., [11]).

We now focus on developing a representation for outcomes of (sequences of) procedures, so that the usual data-oriented tasks could be performed over these outcomes. In pursuing this objective, we also connect our framework with the important topics of knowledge bases and incomplete information. We also show how our framework can be used to formalize and study new natural problems related to these areas.

Due to the results in the previous sections, we shall focus mostly on procedures with safe scope.

5.1 Representing Outcomes and Evolution of Knowledge Bases

The first question we ask is related to the representation of the outcome of a sequence of procedures: Is it possible to represent the set \( outcomes(P_1, \ldots, P_n)(I) \) for an instance \( I \) and sequence \( P_1, \ldots, P_n \) of procedures?

In representing instances, we use the notion of representation system, understood as finite representation of an infinite set of instances. Following [25], a representation system is a set \( W \) of representatives and a function \( \text{rep} \) that assigns a set of instances to each representative in \( W \). For now, we will assume that the function \( \text{rep} \) is uniform, in the sense that for each \( W \in W \) the function \( \text{rep}(W) \) maps \( W \) to instances of the same schema. We then say that a set \( I \) of instances can be represented by a representation system \( (W, \text{rep}) \) if there is a representative \( W \in W \) such that \( \text{rep}(W) = I \).

To represent outcomes of procedures, we extend the usual notion of knowledge base, so that we can define a relational scope over knowledge bases. That is, we use the following representation system:

**Definition 5.** A scoped knowledge base (SKB) over a schema \( S \) is a tuple \( K = (I, \Gamma, \text{Scope}) \), where \( I \) is an instance over \( S \), \( \Gamma \) is a set of constraints, and \( \text{Scope} \) is a set of relation names in \( S \). Intuitively, \( K \) represents all possible extensions of \( I \) that satisfy \( \Gamma \) and does not modify relations not in the scope. That is,

\[
\text{rep}(K) = \{ J \mid I \subseteq J, J \models \Gamma \}
\]

and \( R^I = R^J \) for each relation \( R \notin \text{Scope} \).
The first observation is that SKBs are an appropriate representation system for capturing the outcomes of procedures with safe scope.

**Proposition 5.** Let \( P = (\text{Scope}, \emptyset, \Gamma, Q_{\text{pres}}) \) be a procedure with safe scope, and \( I \) an instance such that \( P \) can be applied over \( I \). Then \( \text{outcomes}_P(I) = \text{rep}(K) \), where \( K \) is the scoped knowledge base \((I, \Gamma, \text{Scope})\).

However, we can do much more with SKBs, as this formalism is also appropriate for representing the outcomes of sequences of procedures with safe scope. We show this next for the case of procedures with safe scope whose constraints are given by full tgds.

**Theorem 1.** Let \( P_1, \ldots, P_n \) be a sequence of procedures with safe scope, and such that each of \( P_1, \ldots, P_n \) uses only full tgds. Then for every instance \( I \), the set \( \text{outcomes}_{P_1, \ldots, P_n}(I) \) can always be represented by an SKB. Furthermore, this SKB can be computed in exponential time from \( P_1, \ldots, P_n \) and \( I \).

A natural question at this point is whether scoped knowledge bases are closed under the operations expressed by procedures: If we start with an SKB \( K \) and apply a procedure \( P \) to each instance represented by \( K \), is it possible to represent \( \text{outcomes}_P(\text{rep}(K)) \)? Surprisingly, it turns out that the answer is positive, as long as the procedures and the scoped knowledge base satisfy the requirements of Proposition 1. An SKB \((I, \Gamma, \text{Scope})\) is full if \( \Gamma \) is a set of full tgds, acyclic if \( \Gamma \) is acyclic, and safe if \( \text{Scope} \) contains at least all the relations on the right-hand side of the tgds in \( \Gamma \). The next result shows that full acyclic safe SKBs are a strong representation system for the outcomes of such procedures.

**Theorem 2.** Let \( P \) be a procedure with safe scope using only full tgds. The for every full acyclic safe SKB \( K \), the set \( \text{outcomes}_P(\text{rep}(K)) \) can always be represented by a full acyclic safe SKB.

The proof relies on the fact that each application of a procedure not only changes the scope, but also forces us to update or drop some of the knowledge that we had before. The following example illustrates this issue:

**Example 5.** Consider two procedures with safe scope, \( P_T \) with scope \( T[^*] \) and postcondition \( \Gamma_T = \{ R(x) \rightarrow T(x), S(x) \rightarrow T(x) \} \), and \( P_R \) with scope \( R[^*] \) and postcondition \( \Gamma_R = \{ R(x) \rightarrow R(x) \} \).

Consider instance \( I \) with \( T^I = S^I = \emptyset \) and \( R^I = \{1\} \). We can show that all the instances in \( \text{outcomes}_{P_T}(I) \) must satisfy \( \Gamma_T \). One possible outcome of applying \( P_T \) to \( I \) is instance \( J \) with \( R^J = T^J = \{1\} \) and \( S^J = \emptyset \).

Consider now \( \text{outcomes}_{P_T, P_R}(I) \); it may include instances that do not satisfy the tgd \( R(x) \rightarrow T(x) \). For example, one can verify that the instance \( K \) given by \( R^K = \{1,2\} \), \( T^K = \{1\} \), \( S^K = \emptyset \) is a possible outcome of applying to \( I \) the procedure \( P_T \) followed by \( P_R \).

What happens here is that, in a sense, we lose the information given by \( R(x) \rightarrow T(x) \) when applying \( P_R \), because \( R \) is in the scope of \( P_R \). The set \( \text{outcomes}_{P_T, P_R}(I) \) is represented by the SKB \( K = (J, \Gamma, \{R,T\}) \), where \( \Gamma \) contains both \( S(x) \rightarrow T(x) \) and \( S(x) \rightarrow R(x) \).
To the best of our knowledge, this interaction between knowledge bases, scopes, and relational procedures has not been studied before. We do not know whether there are other languages with the above property, or to what degree Theorem 2 can be extended to more expressive languages. We believe these are interesting questions to study in future work. We finish with a remark about the unavoidable exponential blowup when representing outcomes of procedures with SKBs.

**Proposition 6.** There is an instance $I$, a procedure $P'$, and a family $(P_i)_{i \geq 1}$ of procedures, all with safe scope, such that every SKB $(J, \Gamma; \text{Scope})$ representing outcomes $P_i, P'(I)$ is such that $J$ has at least $2^i$ tuples.

### 5.2 Reasoning About Incomplete Instances With Open and Closed Relations

Another important problem is to reason about properties satisfied by the outcomes of (sequences of) procedures. With Theorem 1 at hand, we focus on scoped knowledge bases, as these are sufficient for capturing the outcomes of a wide range of procedures. However, our results are of independent interest as they go beyond full acyclic and safe SKBs. We study the following problem:

**SATISFACTION OF CONSTRAINTS:**

**Input:** Acyclic scoped knowledge base $K$ and constraint $\sigma$, both over a schema $S$;

**Question:** Is $\sigma$ satisfied on each instance in $\text{rep}(K)$?

In this paper we focus on the cases of the above problem where $\sigma$ is an egd or a tgd. Just as with applicability, we know that we need some restrictions on $\Gamma$ in SKBs, because allowing arbitrary tgds would make the problem undecidable. For the next sections, we choose to go with acyclic sets of tgds. However, note that our results do not need tgds to be full or SKBs to be safe.

**Satisfaction of egds.** Our first result is positive, stating that SKBs are as well behaved as other representation systems as far as reasoning about equality-generating dependencies is concerned.

**Proposition 7.** The problem SATISFACTION OF EGDS is coNP-complete when restricted to acyclic SKBs.

As with the problem of implication of egds over other forms of incomplete databases, the proof consists on showing that $\sigma$ is not valid on every instance in $\text{rep}(K)$ if and only if there is a small instance constructed from $I$ and the frozen body of $\sigma$ where $\sigma$ does not hold. The difference is that we need to be more careful when constructing the frozen body of $\sigma$, to take into account the scope of the SKB.

**Satisfaction of tgds.** For the case of tgds we cannot immediately adapt previous results, as the scope of SKBs prevents us from applying the chase in a direct...
way. On the other hand, the problem becomes much easier once we disallow unsafe knowledge bases.

**Proposition 8.** The problem satisfaction of Tgds is in $\Pi^p_2$ when restricted to acyclic SKBs. It is NP-complete if further restricted to safe SKBs.

The proof follows from the results of [15], which explores the decidability and complexity of determining containment of CQ queries in presence of materialized views and of dependencies on the instance that generates the materialized views. The results of [15] build on [42] and are obtained for the closed-world case, i.e., all the given materialized views are exact. In the proof of Proposition 8 in this paper, we explore a setting that is partially closed world, as we use a particularly simple case of exact materialized views to model relations that are not in the scope of an SKB. At the same time, our results differ from, and extend in part, those of [15], as our setting is also partially open world, as expressed by the relations that are in scope in the given SKB.

We remark that both Propositions 7 and 8 continue to hold if we allow the knowledge set $\Gamma$ in SKBs to be given by more expressive formalisms such as weakly acyclic [23] sets of tgds and even including egds, or virtually any other formalism that guarantees presence of polynomial-length witnesses of chase sequences.

**Query Answering.** The final task we consider is query answering: Given an instance $I$, a sequence $P_1, \ldots, P_n$ of procedures, and a query $Q$, we would like to find the answers to $Q$ over the outcomes of applying $P_1, \ldots, P_n$ to $I$. To simplify the presentation, we consider only boolean CQ queries. As usual in cases that deal with infinite sets of instances, we are interested in the certain (or unambiguous) answers, which in our framework translate into the answers that hold over any possible outcome of applying $P_1, \ldots, P_n$ to $I$.

More formally, let $\text{certain}_{P_1, \ldots, P_n}(Q, I)$ denote the intersection

$$\bigcap_{J \in \text{outcomes}_{P_1, \ldots, P_n}(I)} Q(J).$$

**QUERY ANSWERING**

**Input:** Instance $I$, boolean CQ $Q$, and sequence $P_1, \ldots, P_n$ of procedures;

**Question:** Is $\text{certain}_{P_1, \ldots, P_n}(Q, I)$ nonempty?

The complexity of query answering is not high when compared to similar reasoning tasks in other similar scenarios such as data exchange or ontology-based query answering. The problem is even in polynomial time if we consider the data complexity of the problem.

**Proposition 9.** Query answering is in NExptime when restricted to sequences of procedures with safe scope. It is in Exptime if the procedures involved contain only full tgds, and in polynomial time if $P_1, \ldots, P_n$ and $Q$ are fixed.
Interestingly, this result extends the settings we can represent with Theorem 1 as we allow any sequence of procedures with safe scope. The reason we can work with more expressive outcomes is that for computing certain answers to conjunctive queries, we only need to keep the set of minimal instances in the set of outcomes, instead of representing the complete outcome space of a sequence of procedures. We show that this set of minimal instances can be represented with an extension of conditional tables, and for each subsequent application of a procedure we update this set by chasing the conditional table, as is done in, e.g., [3]. Although we can easily get \( P^{\text{space}} \)-hardness from a reduction from the query answering problem for non-recursive datalog [37], we do not know if the bounds presented above are tight.

6 The data-readiness problem

We now address the problem of assessing achievability of data-quality constraints, which we describe informally as follows. We start with an instance \( I \) and have a set \( \Pi \) of procedures. We are also given a property \( \alpha \) over instances (specified, for example, as a boolean query or a set of constraints) that does not hold in \( I \). The question we ask in this setting is whether we can apply to \( I \) some or all the procedures in \( \Pi \) so that all the instances in the outcome satisfy \( \alpha \):

\[
\text{DATA READINESS:} \quad \text{Input:} \quad \text{An instance } I, \text{ a set } \Pi \text{ of procedures, and a property } \alpha; \\
\text{Question:} \quad \text{there a sequence } P_1, \ldots, P_n \text{ of procedures in } \Pi \text{ such that all the instances in } \text{outcomes}_{P_1, \ldots, P_n}(I) \text{ satisfy } \alpha? 
\]

The length of \( n \) of the assembled workflow is not part of the input, but instead needs to be derived from the system as well. This implies a striking difference between readiness and the problems we study in Section 5, and will lead us to the undecidability of problems that would instead be decidable if \( n \) was considered to be fixed. In those cases when we obtain decidability it is by proving small-model properties about the length of the sequences that need to be assembled.

We study two specific versions of the problem, arising from how we specify \( \alpha \). We begin with the case where \( \alpha \) is specified as either a tgd or an egd, which we denote as CONSTRAINT READINESS. We then study the case where \( \alpha \) is a boolean CQ \( Q \), denoted as QUERY READINESS.

6.1 Readying Data with Respect to Constraints

In the previous sections we have seen that fundamental problems in our proposed framework can be solved if we restrict ourselves to procedures with safe scope. Unfortunately, as the following proposition shows, this is not the case for the data-readiness problem.
**Proposition 10.** The problem constraint readiness is undecidable, even if \( \Pi \) is a set of procedures with safe scope and \( \Sigma \) contains a single acyclic tgd.

The proof is by reduction from the universal halting problem for Turing machines, along the lines of the proof used in [18] to show that the termination of chase is undecidable. The proof uses \( \Pi \) to simulate each of the constraints being chased in the proof in [18].

On the other hand, the results of Section 5 suggest a way to solve the problem for sets of procedures with safe scope that use full tgds only. Intuitively, it suffices to guess a sequence of procedures, compute the representation of their outcome, and then apply Proposition 8. All that is left to do is to prove a small-model property for the size of the sequence of procedures that we need to guess, as specified in the next result.

**Theorem 3.** The problem constraint readiness is decidable in \( \text{N}^2\text{Exptime} \), for the cases where \( \Pi \) is a set of procedures with safe scope with output constraints comprising full tgds only.

### 6.2 Readying Data with Respect to Queries

We now study data readiness with respect to boolean CQs. Again, it is not enough to restrict our consideration to procedures with safe scope, as we can modify Proposition 10 to obtain undecidability for this case.

**Proposition 11.** The problem query readiness is undecidable, even if \( \Pi \) is a set of procedures with safe scope and \( Q \) is a query of one atom.

Again, we can manage this problem if we only consider procedures with safe scope given by full tgds.

**Theorem 4.** The problem query-readiness is in \( \text{NE} \text{xp} \text{t} \text{ime} \) for the cases where \( \Pi \) is a set of procedures with safe scope with output constraints comprising full tgds only.

In the following section we will extend this result in a significant way, by showing that query readiness continues to be decidable even if we add to \( \Pi \) procedures that alter the schema of instances.

### 7 Procedures over dynamic schemas

So far we have assumed that databases maintain their schemas through the history of procedures applied to them. One could argue that this is not a reasonable assumption, because schemas may and will eventually change along with the needs of the data.
Example 6. In the motivating example in Section 1, we sketched $P_{\text{insur}}$, a procedure that would augment relation $\text{LocVisits}$ with an attribute $\text{insId}$ containing the insurance information of patients, with data drawn from relation $\text{Patients}(\text{pId}, \text{insId})$. For this case, the schema of the outcomes must be different from the schema of the input relation. Thus, to be able to capture this scenario, we need a different notion of outcome.

In this section, we revisit the previously introduced notions, to show that our framework can be modified to include sequences of transformations under dynamic schemas. We will see that, perhaps surprisingly, most of the results of the previous sections still hold under the new, more general definitions.

In this direction of the work, using the named perspective on queries and databases will prove critical, as it allows us to define queries that hold under several schemas (recall Section 2.2). We will then be able to define procedures without a particular schema in mind, requiring only that the conditions and queries therein remain compatible with the input schema.

So how can we redefine procedures to be applicable to more than one schema? Following the same path that we took when defining static outcomes, we now define a dynamic version of the outcome set, wherein we treat schemas as other open propositions. We continue to treat procedures as black boxes, and now permit them to update schemas as well. We thus allow the outcomes to have any schema, as long as they satisfy certain compatibility restrictions that we now introduce.

7.1 Initial Definitions

The first thing we need to do is to extend some of our notation to accommodate the new scenario. Somewhat abusing the notation, we will use $\text{Schema}(I)$ to denote the schema of an instance $I$.

Let $\Sigma$ be a set of structure constraints and data constraints. We say that $I$ satisfies $\Sigma$, and write again $I \models \Sigma$, if (1) $\text{Schema}(I)$ satisfies the structure constraints in $\Sigma$, and (2) $I$ satisfies the data constraints in $\Sigma$. We recall that (2) holds only when $\text{Schema}(I)$ is compatible with all the data constraints in $\Sigma$.

A schema $S'$ extends a schema $S$ if for each relation $R$ such that $S(R)$ is defined, we have $S(R) \subseteq S'(R)$. That is, $S'$ extends $S$ if $S'$ assigns at least the same attributes to all the relations in $S$. An instance $J$ extends an instance $I$ if (1) $\text{Schema}(J)$ extends $\text{Schema}(I)$, and (2) for each relation $R$ in $\text{Schema}(I)$ with assigned attributes $\{A_1, \ldots, A_n\}$ and for each tuple $t$ in $R^I$, there is a tuple $t'$ in $R^J$ such that $t(A_i) = t'(A_i)$ for each $1 \leq i \leq n$. Intuitively, $J$ extends $I$ if the projection of $J$ over the schema of $I$ is contained in $I$.

We now define the dynamic semantics for procedures. The definition is the same as that of Definition 2, except that we now allow instances of different schemas to be in the set of a procedure’s outcomes.

**Definition 6.** Let $I$ be an instance over a schema $S$. An instance $I'$ over schema $S'$ is a possible outcome of applying $P$ to $I$ under the dynamic semantics if the following conditions hold:
1. \( P \) is applicable on \( I \);
2. \( I' \models C_{\text{out}} \);
3. The answers of the query \( Q_{S \setminus \text{Scope}} \) do not change: \( Q_{S \setminus \text{Scope}}(I) = Q_{S \setminus \text{Scope}}(I') \);
4. The answers to each query \( Q \) in \( Q_{\text{pres}} \) over \( I \) are preserved: \( Q(I) \subseteq Q(I') \).

In the definition, we state the schemas of instances \( I \) and \( I' \) explicitly, to reinforce the fact that schemas may change during the application of procedures. However, most of the time the schema can be understood from the instance, so we normally just say that an instance \( I' \) is a possible outcome of \( I \) under the dynamic semantics (even if the schemas of \( I \) and \( I' \) are different).

The set of outcomes for a procedure \( P \) when applied on an instance \( I \) under the dynamic semantics can be thus stated as

\[
dyn-outcomes_P(I) = \{ I' \mid I' \text{ is a possible outcome of applying } P \text{ under the dynamic semantics to } I \},
\]

and we likewise extend the notion of dynamic outcomes to a set of instances (now over possibly different schemas) and for a sequence of procedures, just as we did in the previous sections.

Example 7 (Example 3 continued). Recall the definition of procedure \( P_{\text{migrate}} \) in Example 2. We explained that the instances \( J_1 \) and \( J_2 \) in Figure 1 (b) and (c) belong to the set of outcomes of the instance depicted in Figure 1 (a). Both \( J_1 \) and \( J_2 \) also belong to the set of outcomes under the dynamic semantics. However, this set also contains instances over schemas that extend the schema of \( I \), such as the instance \( J_3 \) in Figure 1 (d). Note that the relation \( \text{LocVisits} \) in \( J_3 \) has an additional attribute \( \text{age} \).

The notion of dynamic semantics allows us to model, for instance, database procedures that add new attributes to relations.

Example 8 (Example 6 continued). Procedure \( P_{\text{insur}} \) from the example in Section 1 is formally described as follows:

\[
\begin{align*}
\text{Scope:} & \quad \text{The scope is the constraint } \text{LocVisits}[\ast]; \\
\text{C}_{\text{in}}: & \quad \text{The precondition is empty;} \\
\text{C}_{\text{out}}: & \quad \text{The postcondition comprises the egd} \quad \text{Patients}(pId : x, \text{insId} : y) \land \text{LocVisits}(pId : x, \text{insId} : y) \rightarrow y = z; \\
\end{align*}
\]

(Note that instances compatible with this egd must each have an attribute \( \text{insId} \) in relation \( \text{LocVisits} \). This constraint also says that the insurance ID of patients in \( \text{LocVisits} \) must correspond to that in relation \( \text{Patients} \).)

\( Q_{\text{pres}} \): We use again the query \( \text{LocVisits}(\text{facility} : x, pId : y, \text{timestp} : z) \); regardless of any newly added attributes, we need to maintain the projection of \( \text{LocVisits} \) onto these three attributes.
7.2 Fundamental Reasoning Tasks

Just as with the static semantics, we begin by studying the problems of applicability and non-emptiness under the dynamic semantics. This is not just a trivial extension from what we had in Section 4. Indeed, the use of dynamic semantics allows for defining procedures for which each instance in the set of outcomes has a schema that is different from the schema of the original instance. (See, e.g., procedure \( P_{\text{insur}} \) of Example 8.)

**Applicability.** We know that applicability is undecidable under reasonable expectations, unless we restrict ourselves to procedures without preconditions. But what if these preconditions were defined using only structure constraints? Such procedures make sense under the dynamic semantics — for instance, a procedure \( P \) may require a certain attribute to be added to the schema before its application. As it turns out, such preconditions can be added with a very low cost to the applicability problem.

**Proposition 12.** Under dynamic semantics, Applicability is in polynomial time for sequences of relational procedures whose preconditions contain only structure constraints.

The proof of this proposition shows that in this case one can construct a minimal schema such that the schema of all instances in the outcomes of sequences of procedures extend the minimal schema.

**Nonemptiness.** Unfortunately, the inclusion of procedures that may alter the schema of instance has an immediate impact on the complexity of nonemptiness. In Section 4 we commented that nonemptiness was decidable for procedures made of full-tgds. Unfortunately, the following negative result shows that nonemptiness is undecidable even in this case, if we also allow procedures whose only goal is to alter the schema of instances.

**Proposition 13.** There exists a sequence \( P_1, P_2, P_3 \) of procedures, with \( P_1 \) and \( P_3 \) having only full tgds and \( P_2 \) having postconditions built using only structure constraints, such that the following problem is undecidable: Given an instance \( I \), is the set \( \text{dyn-outcomes}_{P_1, P_2, P_3}(I) \) nonempty?

**Safe schema alteration.** We define a notion that is analogous to that of safe scope, for the case of procedures that alter the schema of databases. We say that a procedure \( P = (\text{Scope}, C_{\text{in}}, C_{\text{out}}, Q_{\text{pres}}) \) has safe schema-alterations if both the following conditions hold:

- Both \( \text{Scope} \) and \( Q_{\text{pres}} \) are empty; and
- \( C_{\text{out}} \) is a set of structure constraints.

Note that the procedure \( P_{\text{insur}} \) of Example 8 can be represented as two different procedures, one that alters the schema and another that migrates the needed data. The next result delivers on our promise that procedures with safe scope together with procedures with safe schema-alterations form a well-behaved class. For readability, we denote by \( P^{*_{\text{safe,alter}}} \) the class that comprises procedures with safe scope and procedures with safe schema-alterations.
Proposition 14. Given an instance $I$ and a sequence $P_1, \ldots, P_n$ of procedures in $P_{\text{safe, alter}}$, the problem of deciding whether $\text{dyn-outcomes}_{P_1, \ldots, P_n}(I)$ is in polynomial time.

Procedures with safe scope and dynamic semantics: Before turning to more complex reasoning tasks, we observe that the dynamic semantics does not really interfere with reasoning tasks when we deal only with procedures that do not alter the schema. More precisely, let us say that a procedure $P$ does not force alteration of schemas if, for any instance $I$ compatible with $P$ such that $\text{dyn-outcomes}_{P}(I) \neq \emptyset$, the set $\text{dyn-outcomes}_{P}(I)$ contains at least one instance with the same schema as that of $I$. We have the following observation.

Lemma 1. Let $I$ be an instance, $P_1, \ldots, P_n$ a sequence of procedures that do not force alteration of schemas, and $\alpha$ a first-order expression over Schema$(I)$. Then outcomes $P_1, \ldots, P_n(I) \models \alpha$ if and only if $\text{dyn-outcomes}_{P_1, \ldots, P_n}(I) \models \alpha$.

It follows from Lemma 1 that the algorithmic results shown in Sections 5 and 6 continue to hold under the dynamic semantics. Indeed, the challenge now is in reasoning about the outcomes when the mix involves procedures that alter schemas. We proceed to study problems related to query answering, leaving those related to constraints to future work.

7.3 Reasoning About Queries Under the Dynamic Semantics

In this section we address the issue of decidability of reasoning about queries in presence of an instance and a sequence of procedures belonging to the class $P_{\text{safe, alter}}$ (i.e., safe-scope or safe schema-alteration). The main technique we use is the introduction of conditional tables as an approximation of the set of outcomes. To state this result, we recall the notion of conditional tables introduced by Imieliński and Lipski [25].

Let $\mathcal{N}$ be an infinite set of null values that is disjoint from the set of domain values $D$. A naive instance $T$ over schema $S$ assigns a finite relation $R_T \subseteq (D \cup \mathcal{N})^n$ to each relation symbol $R$ in $S$ of arity $n$. Conditional instances extend naive instances by attaching conditions over the tuples. Formally, an element-condition is a positive boolean combination of formulas of the form $x = y$ and $x \neq y$, where $x \in \mathcal{N}$ and $y \in (D \cup \mathcal{N})$. A conditional instance $T$ over schema $S$ assigns to each $n$-ary relation symbol $R$ in $S$ a pair $(R_T, p^R_R)$, where $R_T \subseteq (D \cup \mathcal{N})^n$ and $p^R_R$ assigns an element-condition to each tuple $t \in R_T$. A conditional instance $T$ is positive if none of the element-conditions in its tuples uses inequalities (of the form $x \neq y$).

To define the semantics, let Nulls$(T)$ be the set of all the nulls in any tuple in $T$ or in an element-condition used in $T$. Given a substitution $\nu : \text{Nulls}(T) \rightarrow D$, let $\nu^*$ be the extension of $\nu$ to a substitution $D \cup \text{Nulls}(T) \rightarrow D$ that is the identity on $D$. We say that $\nu$ satisfies an element-condition $\psi$, written $\nu \models \psi$, if for each equality $x = y$ in $\psi$ it is the case that $\nu^*(x) = \nu^*(y)$, and for each inequality $x \neq y$ we have that $\nu^*(x) \neq \nu^*(y)$. Further, we define the set $\nu(R_T)$
as \( \{ \nu^*(t) \mid t \in R^T \text{ and } \nu \models \rho^T_R(t) \} \). Finally, for a conditional instance \( T \), \( \nu(T) \) is the instance that assigns \( \nu(R^T) \) to each relation \( R \) in the schema.

The set of instances represented by \( T \), denoted by \( \text{rep}(T) \), is defined as \( \text{rep}(T) = \{ I \mid \text{there is a substitution } \nu \text{ such that } I \text{ extends } \nu(T) \} \). Note that the instances \( I \) in this definition could have potentially bigger schemas than \( \nu(T) \). In other words, we assume that the set \( \text{rep}(T) \) contains instances over any schema extending the schema of \( T \).

The next result states that conditional instances are good over-approximations for the outcomes of sequences of procedures. More interestingly, these approximations preserve the minimal instances of outcomes. To put this formally, we say that an instance \( J \) in a set \( I \) of instances is minimal if there is no instance \( K \in I, K \neq J \), and such that \( J \) extends \( K \).

**Proposition 15.** Let \( I \) be an instance, and \( P_1, \ldots, P_n \) a sequence of procedures in \( P_{\text{safe,alter}} \) safe, alter. Then either \( \text{dyn-outcomes}_{P_1,\ldots,P_n}(I) = \emptyset \), or one can construct a positive conditional instance \( T \) such that

- \( \text{dyn-outcomes}_{P_1,\ldots,P_n}(I) \subseteq \text{rep}(T) \); and
- If \( J \) is a minimal instance in \( \text{rep}(T) \), then \( J \) is also minimal in \( \text{dyn-outcomes}_{P_1,\ldots,P_n}(I) \).

Further, \( T \) is of double-exponential size with respect to \( P_1, \ldots, P_n \) and \( I \), or exponential if \( n \) is fixed.

We remark that this proposition can be extended to include procedures defined only with egds, at the cost of a much more technical presentation and loosing positiveness of the constructed conditional instance.

**Query answering.** We can use Proposition 15 to derive a decision procedure for the problem of answering conjunctive queries over the outcome set of an instance \( I \) and a sequence \( P_1, \ldots, P_n \) of procedures in \( P_{\text{safe,alter}} \). The procedure computes the conditional table that represents the minimal instances of \( \text{dyn-outcomes}_{P_1,\ldots,P_n}(I) \), and then poses the query over this conditional table. Of course, computing the entire table is not necessary, as we only need the parts that are relevant for answering the query.

**Proposition 16.** Under dynamic semantics, query answering is decidable and in \( \text{NExptime} \) if \( Q \) is a conjunctive query and all procedures involved belong to \( P_{\text{safe,alter}} \). It is in \( \text{NP} \) if the number \( n \) of procedures is considered fixed.

**Query readiness.** We have seen that query readiness can be undecidable even if all the procedures involved are safe scope. To get decidability, we had to restrict ourselves to procedures specified with full tgds only. We are able to obtain an analogous result if we add procedures with safe schema-alterations. The key observation here is that it makes sense to use schema-altering procedures only once, thus we do not lose the small-sequence property of Theorem 4 if we include procedures with safe schema-alterations into the mix.

**Theorem 5.** Under dynamic semantics, query-readiness is in \( \text{N2Exptime} \) when \( \Pi \) is a set of procedures in \( P_{\text{safe,alter}} \) in which all tgds involved are full. It is in \( \text{NExptime} \) if the size of \( \Pi \) is fixed.
8 Conclusions

We have embarked on the task of developing a general framework for data improvement that enables one to determine whether there exists workflows that transform the input data into data that satisfy some desired properties. We believe that our proposal is general enough to cover a wide range of operations over multiple domains and models, possibly including tools from statistics, machine learning, and other data-oriented fields.

In this paper we instantiated the key definitions in a relational setting. We expect that in this setting, our proposed framework will prove its worth by allowing different forms of reasoning about data-preparation workflows. For instance, we have shown how to reason about procedures given by standard relational constraints, which include most data-migration procedures and several kinds of data-quality tasks. In this context, we show that under broad restrictions, the data-readiness problem is decidable, both in the form of constraints and in the form of boolean queries.

It seems promising to continue studying the problem of knowledge-base updates under these classes of procedures. In this respect, we would like to understand the limits of this problem: Can we add more expressivity to procedures and knowledge bases, while still staying in the realm of strong representation systems? For instance, there are numerous forms of description logics and/or datalog variants that have been shown to have good query-answering and reasoning properties (see, e.g., [11] for description logics, and [12] for families of datalog); it might be the case that these properties translate into our setting as well. It also seems promising to pursue the dynamic semantics. In particular, we do not know if there is any reasonable representation system suitable for representing the outcomes of procedures with safe scope under the dynamic semantics.

As a final remark, instantiating our framework in other different scenarios appears to be an exciting direction for future work. The exploration could include, for instance, inclusion of procedures with statistical operations (as in, e.g., [4]), or information extraction from unstructured data [22] or CSV files [33, 2].

References

1. Serge Abiteboul, Richard Hull, and Victor Vianu. Foundations of databases: the logical level. Addison-Wesley Longman Publishing Co., Inc., 1995.
2. Marcelo Arenas, Francisco Maturana, Cristian Riveros, and Domagoj Vrgoč. A framework for annotating csv-like data. Proceedings of the VLDB Endowment, 9(11):876–887, 2016.
3. Marcelo Arenas, Jorge Pérez, and Juan Reutter. Data exchange beyond complete data. Journal of the ACM, 60(4):28, 2013.
4. Vince Barany, Babker ten Cate, Benny Kimelfeld, Dan Olteanu, and Zografoula Vagena. Declarative statistical modeling with datalog. arXiv preprint arXiv:1412.2221, 2014.
5. Daniela Berardi, Diego Calvanese, Giuseppe De Giacomo, Richard Hull, Maurizio Lenzerini, and Massimo Mecella. Modeling data & processes for service specifications in Colombo. In *Proceedings of the Open Interop. Workshop on Enterprise Modelling and Ontologies for Interoperability*, 2005.

6. Daniela Berardi, Diego Calvanese, Giuseppe De Giacomo, Richard Hull, and Massimo Mecella. Automatic composition of web services in Colombo. In *Proceedings of the Thirteenth Italian Symposium on Advanced Database Systems (SEBD)*, pages 8–15, 2005.

7. Daniela Berardi, Diego Calvanese, Giuseppe De Giacomo, Maurizio Lenzerini, and Massimo Mecella. Automatic service composition based on behavioral descriptions. *Int. J. Cooperative Inf. Syst.*, 14(4):333–376, 2005.

8. Moria Bergman, Tova Milo, Slava Novgorodov, and Wang-Chiew Tan. QOCO: A query oriented data cleaning system with oracles. *PVLDB*, 8(12):1900–1911, 2015.

9. Moria Bergman, Tova Milo, Slava Novgorodov, and Wang Chiew Tan. Query-oriented data cleaning with oracles. In *Proceedings of ACM SIGMOD*, pages 1199–1214, 2015.

10. Kamal Bhattacharya, Cagdas Gerede, Richard Hull, Rong Liu, and Jianwen Su. Towards formal analysis of artifact-centric business process models. In *International Conference on Business Process Management*, pages 288–304. Springer, 2007.

11. Meghyn Bienvenu and Magdalena Ortiz. Ontology-mediated query answering with data-tractable description logics. In *Reasoning Web International Summer School*, pages 218–237. Springer, 2015.

12. Andrea Cali, Georg Gottlob, Thomas Lukasiewicz, Bruno Marnette, and Andreas Pieris. Datalog+/-: A family of logical knowledge representation and query languages for new applications. In *Logic in Computer Science (LICS)*, 2010 25th Annual IEEE Symposium on, pages 228–242. IEEE, 2010.

13. Krishnendu Chatterjee, Laurent Doyen, and Moshe Y. Vardi. The complexity of synthesis from probabilistic components. In *Automata, Languages, and Programming - 42nd International Colloquium, ICALP 2015, Kyoto, Japan, July 6-10, 2015, Proceedings, Part II*, pages 108–120, 2015.

14. I.N. Chengalur-Smith and H.L. Pazer. Decision complacency, consensus and consistency in the presence of data quality information. In *Information Quality*, pages 88–101, 1998.

15. Rada Chirkova and Ting Yu. Obtaining information about queries behind views and dependencies. *The Computing Research Repository (CoRR)*, abstract abs/1403.5199, 2014.

16. Alin Deutsch and Tova Milo. *Business Processes: A Database Perspective*. Synthesis Lectures on Data Management. Morgan & Claypool Publishers, 2012.

17. Alin Deutsch, Richard Hull, Fabio Patrizi, and Victor Vianu. Automatic verification of data-centric business processes. In *Proceedings of the 12th International Conference on Database Theory*, pages 252–267. ACM, 2009.

18. Alin Deutsch, Alan Nash, and Jeff Remmel. The chase revisited. In *Proceedings of the twenty-seventh ACM SIGMOD-SIGACT-SIGART symposium on Principles of database systems*, pages 149–158. ACM, 2008.

19. Alin Deutsch, Alan Nash, and Jeff Remmel. The chase revisited (full version). Technical report, University of California, San Diego, 2008.

20. Alin Deutsch and Val Tannen. Optimization properties for classes of conjunctive regular path queries. In *DBPL*, 2001.

21. R. Fagin, P. Kolaitis, R. Miller, and L. Popa. Data exchange: semantics and query answering. *Theoretical Computer Science*, 336:89–124, 2005.
22. Ronald Fagin, Benny Kimelfeld, Frederick Reiss, and Stijn Vansummeren. Document spanners: A formal approach to information extraction. *Journal of the ACM (JACM)*, 62(2):12, 2015.

23. Ronald Fagin, Phokion G Kolaitis, Renée J Miller, and Lucian Popa. Data exchange: semantics and query answering. *Theoretical Computer Science*, 336(1):89–124, 2005.

24. Wenfei Fan and Floris Geerts. *Foundations of Data Quality Management*. Synthesis Lectures on Data Management. Morgan & Claypool Publishers, 2012.

25. Tomasz Imieliński and Witold Lipski Jr. Incomplete information in relational databases. *Journal of the ACM (JACM)*, 31(4):761–791, 1984.

26. B.K. Kahn, D.M. Strong, and R.Y Wang. Information quality benchmarks: Product and service performance. *Comm. ACM*, 45(4w):184–192, 2002.

27. Phokion G Kolaitis, Jonathan Panttaja, and Wang-Chiew Tan. The complexity of data exchange. In *Proceedings of the twenty-fifth ACM SIGMOD-SIGACT-SIGART symposium on Principles of database systems*, pages 30–39, 2006.

28. Pradap Konda, Sanjib Das, Paul Suganthan G. C., AnHai Doan, Adel Ardalan, Jeffrey R. Ballard, Han Li, Fatemah Panahi, Haojun Zhang, Jeffrey F. Naughton, Shishir Prasad, Ganesh Krishnan, Rohit Deep, and Vijay Raghavendra. Magellan: Toward building entity matching management systems. *PVLDB*, 9(12):1197–1208, 2016.

29. Sanjay Krishnan, Jiannan Wang, Michael J. Franklin, Ken Goldberg, Tim Kraska, Tova Milo, and Eugene Wu. SampleClean: Fast and reliable analytics on dirty data. *IEEE Data Eng. Bull.*, 38(3):59–75, 2015.

30. Y.W. Lee, L.L. Pipino, R.Y. Wang, and J.D. Funk. *Journey to Data Quality*. MIT Press, 2009.

31. Y.W. Lee and D.M. Strong. Knowing-why about data processes and data quality. *Journal of Management Information Systems*, 20(3):13–39, 2004.

32. Y.W. Lee, D.M. Strong, B.K. Kahn, and R.Y Wang. AIMQ: a methodology for information quality assessment. *Information & Management*, 40:133–146, 2002.

33. Wim Martens, Frank Neven, and Stijn Vansummeren. Sculpt: A schema language for tabular data on the web. In *Proceedings of the 24th International Conference on World Wide Web*, pages 702–720, ACM, 2015.

34. Werner Nutt, Sergey Paramonov, and Ognjen Savkovic. Implementing query completeness reasoning. In *ACM CIKM*, pages 733–742, 2015.

35. Simon Razniewski, Flip Korn, Werner Nutt, and Divesh Srivastava. Identifying the extent of completeness of query answers over partially complete databases. In *ACM SIGMOD*, pages 561–576, 2015.

36. Yehoshua Sagiv and Mihalis Yannakakis. Equivalences among relational expressions with the union and difference operators. *Journal of the ACM (JACM)*, 27(4):633–655, 1980.

37. Sergei Vorobyov and Andrie Voronkov. Complexity of nonrecursive logic programs with complex values. In *Proceedings of the seventeenth ACM SIGACT-SIGART symposium on Principles of database systems*, pages 244–253. ACM, 1998.

38. R.Y Wang. A product perspective on total data quality management. *Comm. ACM*, 41(2), 1998.

39. R.Y Wang, Y.L. Lee, L.L. Pipino, and D.M. Strong. Manage your information as product: The keystone to quality information. *MIT Sloan Management Review*, 39(4):95–105, 1998.

40. R.Y Wang and D.M. Strong. Beyond accuracy: What data quality means to data consumers. *Journal of Management Information Systems*, 12(4):5–34, 1996.
41. Xubo Zhang and Meral Özsoyoglu. Implication and referential constraints: A new formal reasoning. *IEEE TKDE*, 9, 1997.

42. Zheng Zhang and Alberto O. Mendelzon. Authorization views and conditional query containment. In *Database Theory - ICDT 2005, 10th International Conference, Edinburgh, UK, January 5-7, 2005, Proceedings*, pages 259–273, 2005.
A Proofs and Additional Results

Remark. Since up to section 6 we consider only procedures under static schemas, for readability in most of the proofs of these sections we will use the unnamed assumption on schemas and queries. We can switch back from one to the other by using the order on attributes, as explained in the Preliminaries.

A.1 Proof of proposition 1

The reduction is from the complement of the embedding problem for finite semigroups, shown to be undecidable in [27], and it is itself an adaptation of the proof of Theorem 7.2 in [3]. Note that, since we do not intend to add attributes nor relations in the procedures of this proof, we can drop the named definition of queries, treating CQs now as normal conjunctions of relational atoms.

The embedding problem for finite semigroups problem can be stated as follows. Consider a pair \( (A,g) \), where \( A \) is a finite set and \( g : A \times A \rightarrow A \) is a partial associative function. We say that \( A \) is embeddable in a finite semigroup if there exists \( B = (B,f) \) such that \( A \subseteq B \) and \( f : B \times B \rightarrow B \) is a total associative function. The embedding problem for finite semigroups is to decide whether an arbitrary \( (A,g) \) is embeddable in a finite semigroup.

Consider the schema \( \mathcal{S} = \{ C(\cdot, \cdot), E(\cdot, \cdot), N(\cdot, \cdot), G(\cdot, \cdot, \cdot), F(\cdot), D(\cdot) \} \). The idea of the proof is as follows. We use relation \( G \) to encode binary functions, so that a tuple \((a, b, c)\) in \( G \) intuitively corresponds to saying that \( g(a, b) = c \), for a function \( g \). Using our procedure we shall mandate that the binary function encoded in \( G \) is total and associative. We then encode \( (A, g) \) into our input instance \( I \): the procedure will then try to embed \( A \) into a semigroup whose function is total.

In order to construct the procedures, we first specify the following set \( \Sigma \) of tgds. First we add to \( \Sigma \) a set of dependencies ensuring that all elements in the relation \( G \) are collected into \( D \):

\[
\begin{align*}
G(x, u, v) & \rightarrow D(x) \\
G(u, x, v) & \rightarrow D(x) \\
G(u, v, x) & \rightarrow D(x)
\end{align*}
\]

The next set verifies that \( G \) is total and associative:

\[
\begin{align*}
D(x) \land D(y) & \rightarrow \exists z G(x, y, z) \\
G(x, y, u) \land G(u, z, v) \land G(y, z, w) & \rightarrow G(x, w, v)
\end{align*}
\]

Next we include dependencies that are intended to force relation \( E \) to be an equivalence relation over all elements in the domain of \( G \).

\[
\begin{align*}
D(x) & \rightarrow E(x, x) \\
E(x, y) & \rightarrow E(y, x) \\
E(x, y) \land E(y, z) & \rightarrow E(x, z)
\end{align*}
\]
The next set of dependencies we add $\Sigma$ ensure that $G$ represents a function that is consistent with the equivalence relation $E$.

\[
G(x, y, z) \land E(x, x') \land E(y, y') \land E(z, z') \to G(x', y', z')
\]

(9)

\[
G(x, y, z) \land G(x', y', z') \land E(x, x') \land E(y, y') \to E(z, z')
\]

(10)

The final tgd in $\Sigma$ serves us to collect possible errors when trying to embed $A = (A, g)$. The intuition for this tgd will be made clear once we outline the reduction, but the idea is to state that the relation $F$ now contains everything that is in $R$, as long as a certain property holds on relations $E$, $C$, and $N$.

\[
E(x, y) \land C(u, x) \land C(v, y) \land N(u, v) \land R(w) \to F(w)
\]

(11)

Let then $\Sigma$ consists of tgds (1)-(11). We construct fixed procedures $P_1 = (\text{Scope}^1, C_{\text{in}}^1, C_{\text{out}}^1, Q_{\text{pres}}^1)$ and $P_2 = (\text{Scope}^2, C_{\text{in}}^2, C_{\text{out}}^2, Q_{\text{pres}}^2)$ as follows.

Procedure $P_1$:

**Scope**\(^1\): The scope of $P_1$ consists of relations $G$, $E$, $D$ and $F$, which corresponds to the constraints \{\([G], E, [D], F\)\}.

**$C_{\text{in}}^1$**: There are no preconditions for this procedure.

**$C_{\text{out}}^1$**: The postconditions are the tgds in $\Sigma$.

**$Q_{\text{pres}}^1$**: A single query ensuring that no information is deleted from all of $G$, $E$ and $F$ (and thus that no attributes are added to them): $G(x, y, z) \land E(u, v) \land D(w) \land F(p)$.

Procedure $P_2$:

**Scope**\(^2\): The scope of $P_2$ is empty.

**$C_{\text{in}}^2$**: The precondition for this constraint is $R(x) \to F(x)$.

**$C_{\text{out}}^2$**: There are no postconditions.

**$Q_{\text{pres}}^2$**: There are no preserved queries.

Note that $P_2$ does not really do anything, it is only there to check that $R$ is contained in $F$. We can now state the reduction. On input $A = (A, g)$, where $A = \{a_1, \ldots, a_n\}$, we construct an instance $d_A$ given by the following interpretations:

- $E^{IA}$ contains the pair $(a_i, a_i)$ for each $1 \leq i \leq n$ (that is, for each element of $A$);
- $G^{IA}$ contains the triple $(a_i, a_j, a_k)$ for each $a_i, a_j, a_k \in A$ such that $g(a_i, a_j) = a_k$;
- $D^{IA}$ and $F^{IA}$ are empty, while $R^{IA}$ contains a single element $d\not\in A$;
- $C^{IA}$ contains the pair $(i, a_i)$ for each $1 \leq i \leq n$; and
- $N^{IA}$ contains the pair $(i, j)$ for each $i \neq j$, $1 \leq i \leq n$ and $1 \leq j \leq n$.

Let us now show $A = (A, g)$ is embeddable in a finite semigroup if and only if $\text{outcomes}_P(I)$ contains an instance $I'$ such that $I'$ does not satisfy the precondition $R(x) \to F(x)$ of procedure $P_2$. 
\( \Rightarrow \) Assume that \( A = (A, g) \) is embeddable in a finite semigroup, say the semigroup \( B = (B, f) \), where \( f \) is total. Let \( J \) be the instance such that \( E^J \) is the identity over \( B \), \( D^J = B \) and \( G^J \) contains a pair \((b_1, b_2, b_3)\) if and only if \( f(b_1, b_2) = b_3 \); \( F^J \) is empty and relations \( N, C \) and \( R \) are interpreted as in \( I_A \). It is easy to see that \( J \models \Sigma, Q_{\text{pres}}(I_A) \subseteq Q_{\text{pres}}(J) \), this last because \( A \) was said to be embeddable in \( B \). We have that \( J \) then does belong to \( \text{outcomes}_{P_1}(I) \), but \( J \) does not satisfy the constraint \( R(x) \rightarrow F(x) \).

\( \Leftarrow \) Assume now that there is an instance \( J \in \text{outcomes}_{P_1}(I) \) that does not satisfy \( R(x) \rightarrow F(x) \). Note that, because of the scope of \( P_1 \), the interpretation of \( C, N \) and \( R \) of \( J \) must be just as in \( I \). Thus it must be that the element \( d \) is not in \( F^J \), because it is the only element in \( R^J \). Construct a finite semigroup \( B = (B, f) \) as follows. Let \( B \) consists of one representative of each equivalence class in \( E^J \), with the additional restriction that each \( a_i \) in \( A \) must be picked as its representative. Further, define \( f(b_1, b_2) = b_3 \) if and only if \( G(b_1, b_2, b_3) \) is in \( G \). Note that \( J \) satisfies the tgd\( s \) in \( \Sigma \), in particular \( G \) is associative and \( E \) acts as en equivalence relation over \( G \), which means that \( f \) is indeed associative, total, and well defined. It remains to show that \( A \) can be embedded in \( B \), but since \( G^J \) and \( E^J \) are supersets of \( G^A \) and \( E^A \) (because of the preservation query of \( P_1 \)), all we need to show is that each \( a_i \) is in a separate equivalence relation. But this hold because of tgd \((11)\) in \( \Sigma \): if two elements from \( A \) are in the same equivalence relation then the left hand side of \((11)\) would hold in \( I_A \), which contradicts the fact that \( F^J \) does not contain \( d \).

A.2 Proof of proposition [2]

This proof is a simple adaptation of the reduction we used in the proof of Proposition [1] Indeed, consider again the schema \( S \) from this proof, and the procedure \( P \) given by:

- \( \text{Scope} \): The scope of \( P \) consists of relations \( G, E, D \) and \( F \), which corresponds to the constraints \( G[s], E[s], D[s] \) and \( F[s] \).
- \( C_{\text{in}} \): There are no preconditions for this procedure.
- \( C_{\text{out}} \): The postconditions are the tgd\( s \) in \( \Sigma \) plus the tgd \( F(x) \rightarrow R(x) \).
- \( Q_{\text{pres}} \): This query ensures that no information is deleted from all of \( G, E \) and \( F \): \( G(x, y, z) \land E(u, v) \land D[w] \land F(p) \).

Given a finite semigroup \( A \), we construct now the following instance \( I_A \):

- \( E^A \) contains the pair \((a_i, a_i)\) for each \( 1 \leq i \leq n \) (that is, for each element of \( A \));
- \( G^A \) contains the triple \((a_i, a_j, a_k)\) for each \( a_i, a_j, a_k \in A \) such that \( g(a_i, a_j) = a_k \);
- All of \( D^A, E^A \) and \( R^A \) are empty;
- \( C^A \) contains the pair \((i, a_i)\) for each \( 1 \leq i \leq n \); and
- \( N^A \) contains the pair \((i, j)\) for each \( i \neq j, 1 \leq i \leq n \) and \( 1 \leq j \leq n \).

By a similar argument as the one used in the proof of Proposition [1] one can show that \( \text{outcomes}_{P}(I_A) \) has an instance if and only if \( A \) is embeddable
in a finite semigroup. The intuition is that now we are adding the constraint
\( F(x) \rightarrow R(x) \) as a postcondition, and since \( R \) is not part of the scope of the
procedure the only way to satisfy this restriction is if we do not fire the tgd (11)
of the set \( \Sigma \) constructed in the aforementioned proof. This, in turn, can only
happen if \( A \) is embeddable.

A.3 Proof of proposition 3

This proof is just a slight adaptation of the Proof of Proposition 13. The only
thing needed to be done is to replace the tgd:

\[
D(x) \land D(y) \rightarrow G^{\text{binary}}(x, y)
\]
in that proof for the (non-full) tgd:

\[
D(x) \land D(y) \rightarrow \exists z G^{d\text{binary}}(x, y)
\]
The rest follows just as in the proof of Proposition 13.

A.4 Proof of Proposition 4

Let \( I \) and \( P_1, \ldots, P_n \) be as specified in the statement of the Proposition, assuming
the postconditions of each \( P_i \) correspond to a set \( \Sigma_i \) of tgds. Then chasing \( I \) with
\( \Sigma_1, \Sigma_2, \) etc yields an instance in \( \text{outcomes}_{P_1, \ldots, P_n}(I) \). Indeed, if the chase yields
instances \( I_1, \ldots, I_n \) with \( I_0 = I \) (so that \( I_{i+1} \) is the chase of \( I_i \) with \( \Sigma_{i+1} \)), then
each \( I_{i+1} \) is a possible outcome of applying \( P_{i+1} \) to \( I_i \).

A.5 Proof of Proposition 5

A consequence of the following Theorem 1.

A.6 Proof of Theorem 1

This is a consequence of Theorem 2. Exponential time follows from the fact that
\( \text{RemoveRelations}(\Gamma, \text{Scope}) \) works in \( O(2^{\lvert \Gamma \rvert}) \) and that (since tgds are full) the
maximum size of an instance produced out of chasing is of order \( \lvert I \rvert^S \).

A.7 Proof of Theorem 2

For readability, in this proof we specify the Scopes of procedures using just the
relation names (since they can only be formed with constraints of the form \( R[s] \)),
and we sometimes omit the definition of \( Q_{\text{pres}} \), since for procedures of safe scope
this set depends only on the scope of processes. We also continue using the
unnamed assumption.
We begin with some notation. The premise of a tgd is its left-hand side, and
the conclusion is its right-hand side. The dependency graph \( \Gamma \) of a set of tgds is
a graph whose nodes are the relation names used in the dependencies in \( \Gamma \) and
where there is an edge from a node \( R \) to a node \( S \) if there is a dependency in \( \Gamma \)
with \( R \) in its premise and \( S \) in its consequence. A set \( \Gamma \) of tgds is acyclic if its
dependency graph is acyclic.

Acyclicity plays an important role in this proof, as we show that one essen-
tially needs to keep up an acyclic set of dependencies (even though subse-
quent procedures may introduce cycles). It also allows us to define a procedure
RemoveRelations(\( \Gamma, \text{Scope} \)), for an acyclic set \( \Gamma \) of tgds and a set \( \text{Scope} \) of rela-
tion names. The procedure RemoveRelations(\( \Gamma, \text{Scope} \)) works as follows. Let us
first assume without loss of generality that each dependency in \( \Gamma \) uses different
variables. Let also \( R_1, \ldots, R_n \) be an enumeration of the relations in \( \text{Scope} \) that
are used in \( \Gamma \) and that is consistent with the partial order of the nodes in the
dependency graph of \( \Gamma \). We consider \( R_n \) is the greatest node in this order, i.e.,
a node without a directed path to any of the nodes \( R_1, \ldots, R_{n−1} \).

Then, for each \( i = n, n−1, n−2, \ldots, 1 \):

- Let \( \Omega_i \subseteq \Gamma \) contain all dependencies using \( R_i \) in its premises.
- Initialize the set \( \Omega'_i \) as \( \Omega_i \).
- For each tgd \( \lambda \) in \( \Omega_i \) of the form \( \phi(x) \rightarrow \psi(z) \), for each different atom \( R_i(\tilde{y}) \)
in \( \phi(x) \) and for each dependency \( \sigma \) in \( \Gamma \setminus \Omega_i \) of the form \( \theta(\tilde{u}) \rightarrow \eta(\tilde{v}) \) such
that there is an atom \( R_i(\tilde{w}) \) in \( \eta(\tilde{v}) \).
  - Let \( \Pi \) contain all possible equivalence relations for the variables in \( \tilde{w} \).
    For each equivalence relation \( \pi \in \Pi \), let \( \pi(\tilde{w}) \) denote the renaming of
    the variables in \( \tilde{w} \) where each variable is sent to one representative of
    the equivalence relation. If there is a homomorphism \( h : \tilde{y} \rightarrow \pi(\tilde{w}) \)
from \( R_i(\pi(\tilde{w})) \) to \( R_i(\tilde{y}) \), then
    - Let \( \hat{h} \) be the extension of \( h \) that is the identity on any variable in \( \tilde{x} \) but
      not in \( \tilde{y} \), \( \hat{\pi} \) the extension of \( \pi \) that is the identity over any variable in \( \tilde{v} \)
      not in \( \tilde{w} \), and let \( \phi'(\tilde{x}) \) be the result of removing the atom \( R_i(\tilde{y}) \)
from \( \phi(\tilde{x}) \).
    - Construct the dependency \( \lambda' = \phi'(\hat{h}(\tilde{x})) \land \theta(\hat{\pi}(\tilde{u})) \rightarrow \psi(\hat{h}(\tilde{z})) \).
      Note that this is well defined because each variable in \( \tilde{z} \) must appear in \( \tilde{x} \), and since
      \( R_i \) cannot appear in \( \theta \) we have removed at least one occurrence of \( R_i \).
    - Create a copy of \( \lambda' \) using only fresh variables, and add it to \( \Omega'_i \).
    - Continue until no more dependencies in \( \Omega'_i \) contain \( R_i \) in their premises.
- Define \( \Gamma = \Gamma \setminus \Omega_i \cup \Omega'_i \). Note that we have removed \( R_i \) from the premise
of the dependencies in \( \Gamma \), but \( \Gamma \) remains an acyclic set of full tgds (because
on the \( i \)-th step we never introduce dependencies with a relation \( R_j \) in its
premises that is higher in the order than \( R_i \)).

We now have all the ingredients to prove this theorem. Let \( K = (I, \Gamma, \text{Scope}) \)
be a scoped knowledge base and such that \( \Gamma \) is an acyclic set of full tgds, and

\[ \text{Note that because of acyclicity } \theta \text{ cannot contain atoms } R_j \text{ with } j \geq i \]
Claim. If the $i$-th step of the chase produces tuples $\psi(h(\bar{z}))$ out of a dependency $\lambda = \phi(\bar{x}) \rightarrow \psi(\bar{z})$ and an assignment $h$ so that $chase_{\Gamma}^{-1}(K)$ satisfies $\phi(h(\bar{x}))$ but not $\psi(h(\bar{z}))$, then there is a dependency $\theta(h) \rightarrow \psi(h)$ in $RemoveRelations(\Gamma, \text{Scope}_P)$ and an assignment $f$ such that $K$ satisfies $\theta(f(\bar{u}))$ and where $\psi(f(\bar{v})) = \psi(h(\bar{z}))$.

Proof. For the base case when there is a single chase step, we have that none of the atoms in $\theta$ is in $\text{Scope}_P$, and thus $\lambda$ is in $RemoveRelations(\Gamma, \text{Scope}_P)$ by construction.

Now assume the claim holds for all chase steps earlier than step $k$, and let $\lambda = \phi(\bar{x}) \rightarrow \psi(\bar{z})$ as in the claim. Further, assume $\phi(\bar{x})$ is of the form $S_1(\bar{x}_1) \land \cdots \land S_m(\bar{x}_m)$. Then for each such atom, either $S_j$ is not in $\text{Scope}_P$, or
the atom $S_j(h(\bar{x}_j))$ it was produced earlier in the chase. Let us assume that there is only one such atom (if there are more the proof just follows by repeating the same argument). By induction, such atom comes from a dependency $\theta(u) \rightarrow \eta(v)$ and an assignment $f$ such that $K$ satisfies $\theta(f(u))$ and where there is an atom $S_j(\bar{u})$ in $\eta(\bar{v})$ such that $f(\bar{u}) = h(\bar{x}_j)$.

We note that function $f$ induces an equivalence relation in the variables $\bar{v}$, where two variables $u_1$ and $u_2$ are in the same equivalence relation if $f(u_1) = f(u_2)$. If $\pi$ is the assignment mandated by the equivalence relation, then clearly there is a homomorphism $g$ from $S_j(\bar{x}_j)$ to $S_j(\pi(\bar{w}))$.

Let $\bar{\pi}$ be the extension of $\pi$ that is the identity on all variables in $\bar{u}$ not in $\bar{w}$. Note that since $\pi$ is the relation induced by $f$, we have that $f(\bar{u}) = f(\pi(\bar{u}))$.

Next, let $\hat{g}$ be the extension of $g$ that is the identity on every variable of $\bar{x}$ not in $\bar{x}_j$.

For each $S_j$ is in Scope$_P$ and we have shown $\pi$ and $g$ as in the condition of the procedure, at some point during the application of RemoveRelations, the dependency $\lambda$ was replaced by $\lambda' = \phi'(\hat{g}(\bar{x})) \land \theta(\hat{\pi}(\bar{u})) \rightarrow \psi(\hat{g}(\bar{z}))$, where $\phi'(\hat{g}(\bar{x}))$ is the result of removing $R_j(g(\bar{y}))$ from $\phi(\hat{g}(\bar{x}))$.

Define a homomorphism $h^* : g(\bar{x}) \rightarrow D$ so that $h^*(x) = x$ if $x \not\in \bar{x}$ and $h^*(x) = f(g(x))$ otherwise. Note that $h(\bar{x}) = h^*(g\bar{x})$, since these two only differ in the variables in $\bar{x}_j$ and $f(\bar{w}) = h(\bar{x}_j)$.

Let $h^* : \bar{x} \cup \bar{u} : \rightarrow D$ define the union of homomorphisms $h$ and $f$. Then we have that $K$ must satisfy $\phi(h^*(\hat{g}(\bar{x})) \land \theta(h^*(\hat{\pi}(\bar{u})))$. It satisfies $\phi(h^*(\hat{g}(\bar{x})))$ because $\hat{g}$ is the identity on each variable in $\bar{x}$ not in $\bar{x}_j$, and $f(\hat{g}(x)) = h(x)$ for each $x \in \bar{x}_j$, and it satisfies $\theta(h^*(\hat{\pi}(\bar{u})))$ because we know that $K$ satisfies $\theta(f(\bar{u}))$ and $f(\bar{u}) = f(\pi(\bar{u}))$.

Again, since $f(\bar{w}) = h(\bar{x}_j)$ and $\hat{g}$ is the identity over any variable not in $\bar{x}_j$, we also obtain that $\psi(h^*(\hat{g}(\bar{z})))$ corresponds to $\psi(h(\bar{z}))$. This proofs the claim.

We continue with the proof of fact (b): $N \subseteq N'$. Let us assume otherwise, so that there is a tuple $\bar{a}$ and a relation $R$ so that $\bar{a}$ is in $R$ and not in $R'$. Clearly $\bar{a}$ must not be in $R^K$, since by definition $K \subseteq N'$. Thus, $\bar{a}$ was added to $R$ as a product of the chase. Assume without loss of generality that $\bar{a}$ was the first such tuple added by the chase, product of chasing a dependency $\phi(\bar{x}) \rightarrow \psi(\bar{z})$ and an assignment $h : \bar{x} \rightarrow D$, where $K$ satisfies $\phi(h(\bar{x}))$ but not $\psi(h(\bar{z}))$.

By the Claim above we know that, instead of chasing $\phi(\bar{x}) \rightarrow \psi(\bar{z})$ we could have chased a relation $\theta(u) \rightarrow \psi(v)$ in RemoveRelations($I, \text{Scope}_P$) with the same result. But this last dependency is in $I''$ by construction, and therefore since $N'$ satisfies $I''$, it must be the case that $\bar{a}$ is actually in $R^N$, which contradicts our initial assumption.

Finally, (c): $N$ and $N'$ differ only in relations within $\text{Scope}_P$, follows from that fact that $K$ and $N'$ differ only in relations within $\text{Scope}_P$ and $\bar{K} \subseteq N \subseteq N'$. This proves $N'$ belongs to outcomes$_P(N)$.

**Completeness.** Let $K$, $P$, $\Sigma$ and $K'$ be defined as above, and consider an instance $N'$ in outcomes$_P(\text{rep}(K))$. Then there is an instance $N \in \text{rep}(K)$ such that $N' \in \text{outcomes}_P(N)$. We show that $N'$ belongs also to $\text{rep}(K')$. We need to
prove that (1) \( \text{chase}_a(I) \subseteq N' \), (2) \( R^{N'} = R^\text{chase}_a(I) \) for each \( R \notin \text{Scope}' \), and (3) \( N' \models I' \).

For (1), note that \( N \subseteq N' \) because of the preservation queries in \( P \). Since \( N' \) satisfies, in particular, \( \Sigma \), and \( I \subseteq N \), it must be that \( \text{chase}_a(I) \subseteq N' \).

For (2), we observe that \( N \) and \( N' \) differ only in relations not in \( \text{Scope}' \), and, furthermore, \( I \) and \( N' \) differ only in relations from \( \text{Scope} \). Since \( \text{Scope}' = \text{Scope} \cup \text{Scope}_P \), one could find a tuple in a relation \( R \notin \text{Scope}' \) such that \( N' \) and \( \text{chase}_\Sigma(I) \) differ on \( R \), then either \( N' \) and \( N \) differ on \( R \), or \( N \) and \( I \) differ on \( R \), which we know it is not possible.

For (3), note that \( N \) satisfies \( I \), and therefore it satisfies \( \text{RemoveRelations}(I, \Sigma) \). Now \( N' \) is a superset of \( N \) that satisfies \( \Sigma \). If \( N' \) does not satisfy a dependency \( \lambda \) in \( I' \), then \( \lambda \) must belong to \( \text{RemoveRelations}(I, \Sigma) \) and thus \( N \) satisfies \( \lambda \). All relations in the premise of \( \lambda \) do not belong to \( \text{Scope}_P \), and thus since \( N \) and \( N' \) only differ in relations from \( \text{Scope}_P \), any assignment \( h \) from the premise of \( \lambda \) to \( N' \) is also an assignment to \( N \). Furthermore, since \( N \subseteq N' \), if \( h \) is not an assignment from the consequence of \( \lambda \) to \( N' \) it is also not an assignment from the consequence of \( \lambda \) to \( N \). This contradicts the fact that \( N \) satisfies \( \lambda \).

### A.8 Proof of proposition 6

Recall we omit preservation queries from procedures with safe scope. Fix a number \( i \geq 1 \). Let \( S \) contains unary relation \( R \) and \( n \)-ary relation \( T \), and let \( I \) such that \( R^I = \{0,1\} \) and \( T^I = \emptyset \). Let \( P' \) be the procedure with scope \( R \), no preconditions and postcondition \( \exists x_2 \exists x_3 \exists x_n T(x_1, \ldots, x_n) \rightarrow R(x_1) \). Let \( P_i \) be a procedure with with scope \( T \), no preconditions and postcondition \( R(x_1) \land R(x_2) \land \cdots \land R(x_i) \rightarrow T(x_1, \ldots, x_i) \).

Now note that all instances \( K \) in \( \text{outcomes}_{P, P'} (I) \) must be such that \( K^T \) contains all tuples of length \( i \) that can be formed with \( 0 \)s and \( 1 \)s. Furthermore, since the scope of \( P' \) is \( R \), for every SKB \( (I, \Gamma, \text{Scope}) \) representing \( \text{outcomes}_{P, P'} (I) \) it must be that \( \Gamma \) does not contain tgds with \( R \) in its premises (this follows from the construction of Theorem 2). Then clearly \( J \) must contain all \( 2^i \) tuples.

### A.9 Proof of Proposition 7

Let \( K = (I, \Gamma, \text{Scope}) \) be as in the statement of the Proposition. Let also \( \sigma \) be of the form \( \phi(X) \rightarrow Y = Z \), where each of \( Y \) and \( Z \) is a term in the vector \( X \), and let \( \phi^O(X^O) \) be the restriction of \( \phi \) to only the relations in \( \text{Scope} \), and \( \phi^C(X^C) \) the restriction of \( \phi \) to relations not in \( \text{Scope} \). Consider now an enumeration \( h_1, \ldots, h_\ell \) of all mappings from \( \phi^C(X) \) to \( I \). Next, for each such mapping \( h \), construct an assignment \( g \) that extends \( h \) by assigning all variables not in \( X^C \) to a fresh element. Furthermore, for each such assignment \( g \), construct a set of assignments \( g_1, \ldots, g_n \), where \( g_1 = g \) and where each assignment \( g_j \), with \( 1 < j \leq n \), is a modification of \( g_1 \) that allows some elements in the image of \( X \) to be the same fresh element or to be an element used in \( I \) in \( \text{SKB} \). We choose
n so that all possible such restrictions (up to renaming the null symbols) are included in the set \{ g_1, \ldots, g_n \}.

Let us now assume \{ \tau_1, \ldots, \tau_k \} is the set of all assignments constructed in this way. We construct an instance \( D_i \) for each such assignment: Each \( D_i \) is created by adding to I the set of tuples \( \phi(\tau_i(X)) \). We then chase each \( D_i \) with \( \Gamma \), and check whether the resulting instance \((D_i)^\Gamma\) satisfies the egd \( \sigma \). There are two cases here:

1. There exists an \( i \in [1,k] \) such that \((D_i)^\Gamma \models \sigma\) does not hold. But it is easy to see that \( D_i \) belongs to the set \( \text{rep}(K) \), so we have a counterexample and we conclude that \((I, \Gamma, \text{Scope})\) does not satisfy \( \sigma \).

2. (This is the “small-witness counterexample” property at the center of this proof.) Suppose it is the case that \((D_i)^\Gamma \models \sigma\) for each \( i \in [1,k] \). In this case, we conclude that \((I, \Gamma, \text{Scope})\) satisfies \( \sigma \).

Indeed, assume toward a contradiction that there exists an instance \( D_\ast \) in \((I, \Gamma, \text{Scope})\) such that \( D_\ast \) does not satisfy \( \sigma \). By the fact that \((D_i)^\Gamma \models \sigma\) for each \( i \in [1,k] \), then there cannot exist a homomorphism to \( D_\ast \) from \((D_i)^\Gamma\) for any \( i \in [1,k] \), such that the image of the homomorphism would include one or more violations of \( \sigma \) in \( D_\ast \). The reason for the nonexistence of any such homomorphism is that each \((D_i)^\Gamma\) is “minimal” in terms of satisfying both \( I \) and \( \sigma \), and \( D_\ast \) does not satisfy \( \sigma \) while \((D_i)^\Gamma\) satisfies \( \sigma \) for each \( i \in [1,k] \). Note that all the instances \((D_i)^\Gamma\) taken together cover all the “minimal” instances that satisfy all of \( I \), \( \Gamma \), and \( \sigma \). Thus, to obtain \( D_\ast \), we need to add at least one tuple to some \((D_i)^\Gamma\), and then chase the result (call this result \( D_{\ast\ast} \)) with \( \Gamma \).

By construction of \( D_{\ast\ast} \) and \( D_\ast \), there must be a homomorphism, \( h \), from \( D_{\ast\ast} \) to the part of \( D_\ast \) that has all the tuples in \( \nu(\phi) \) (recall that \( \phi \) is the body of \( \sigma \)) with \( \nu(Y) \neq \nu(Z) \), for some valuation \( \nu \) from \( \phi \) to \( D_\ast \). Thus, it must be possible to extend \( h \) to a homomorphism, \( h' \), from \( D_{\ast\ast} \) to \( D_\ast \), such that the preimage of \( h' \) includes all of \( I \). Take one \( h' \) such that its preimage \( D' \) is exactly \( I \) plus the minimal set (potentially empty) of extra tuples that are needed to cover all of the preimage of \( h \) by the preimage of \( h' \). Then, by construction of the instances \((D_i)^\Gamma\) (by that construction, there must be a homomorphism from the I in \( \text{SKB} \) to \((D_i)^\Gamma\) for each \( i \in [1,k] \)), \( D' \) must be isomorphic to \((D_i)^\Gamma\) for some \( i \in [1,k] \). It follows that there exists a homomorphism from that \((D_i)^\Gamma\) to a part of \( D_\ast \) that contains at least one violation of \( \sigma \). We get the desired contradiction, as the existence of such a homomorphism is impossible by construction of the \((D_i)^\Gamma\) and by our assumption that there exists a ground instance \( D_\ast \) of \( \text{SKB} \) that violates \( \sigma \).

**Membership in coNP.** From the remarks above, to solve the complement of the satisfaction problem it suffices to guess one of the \( D_i \)'s (which are of polynomial size), a mapping \( h \) from \( \phi(X) \) to the chase of \( D_i \) with \( \Gamma \) such that \( h(Z) \neq h(y) \), and the appropriate chase rules (plus their assignments) to take us from \( D_i \) to
the images of h (thus, instead of chasing the entire $D_i$ we just guess the witnesses to cover the image of h).

**Proof of coNP-hardness.** We reduce from the compliment of the 3-colorability problem. Given a graph $G$, let $Q_G$ be the corresponding boolean CQ whose underlying graph is $G$ (using fresh variables), using a binary relation $E$ to specify its edges. Further, let $R$ and $S$ unary relations, and let $I$ be an instance such that $I^R = \{1\}$, $I^S = \{2\}$, $I^K = \{(r,b), (b,r), (b, w), (w,b), (w, r), (r, w)\}$, and define the skb $K$ as $(I, \emptyset, \{E\})$. Consider then the egd $\sigma = Q_G \land R(x) \land S(y) \rightarrow x = y$, where $x$ and $y$ are again fresh variables not used in $Q_G$. It follows that $K \models \sigma$ if and only if $G$ is not 3-colorable.

### A.10 Proof of proposition [8]

**Example 9.** We illustrate via an example the subtleties in the interplay between the closed-world and open-world aspects of our setting. (Recall that we explore a setting that is partially closed world, as we use a particularly simple case of exact materialized views to model relations that are not in the specified scope of a scoped knowledge base. At the same time, our setting is also partially open world, as expressed by the relations that are in scope in the given scoped knowledge base.)

Consider a scoped knowledge base $SKB = (I, \Gamma, Scope)$ over schema $S = \{R(A), T(B)\}$, with $\Gamma = \emptyset$, the relation $T$ being the only relation in $Scope$, and $I$ consisting of four tuples $R(a), R(b), T(a),$ and $T(b)$.

(i) Let us check first whether tgd $\sigma_1 : R(X) \rightarrow T(X)$ holds on $SKB$. Intuitively, $\sigma_1$ should hold on $SKB$. Indeed, the relation $R$ in $I$ is exact (closed world), and thus stays the same (i.e., always is exactly $\{R(a), R(b)\}$) in all the ground instances in $SKB$. At the same time, relation $T$ in $I$ is open world, and thus each ground instance in $SKB$ has an instance of $T$ that is a superset of $\{T(a), T(b)\}$.

To verify formally that the tgd $\sigma_1$ holds on $SKB$, we transform each of the body and head of $\sigma_1$ into two respective CQ queries, $Q_1$ and $Q_2$: $Q_1(X) \leftarrow R(X); Q_2(X) \leftarrow T(X)$.

By Proposition 9, the tgd $\sigma_1$ holds on $SKB$ iff the result of transforming $Q_1$ using the information we have in $SKB$ is contained in $Q_2$.

We begin the transformation of $Q_1$ by conjoining its body with the conjunction of all the facts in $I$, and denote the result by $Q_1'$: $Q_1'(X) \leftarrow R(X), R(a), R(b), T(a), T(b)$.

We now chase $Q_1'$ with a dependency, $\tau$, generated from the materialized view $V(X) \leftarrow R(X)$. (The view $V$ expresses the fact that the relation $R$ in $I$ is exact — closed world — and thus is exactly $\{R(a), R(b)\}$ in all the ground instances in $SKB$.) The dependency $\tau$ is constructed from the definition of the view $V$ and from its answer, which is the relation $\{R(a), R(b)\}$ given in $SKB$: $\tau : R(X) \rightarrow X = a \lor X = b$.

The chase transforms the query $Q_1'$ into a UCQ query $Q_1''$: $Q_1''(a) \leftarrow R(a), R(a), R(b), T(a), T(b)$.
we have that the tgd $Q_1''$ is contained in $Q_2$. Further, by the containment mapping $\mu_2 : \{ X \to b \}$, we have that $Q_1''(2)$ is contained in $Q_2$. We conclude that $Q_1''$ is contained in $Q_2$. Thus, by Proposition ?? we have that the tgd $\sigma_1$ holds on $SKB$.

(ii) Let us now check whether tgd $\sigma_2 : T(X) \rightarrow R(X)$ holds on $SKB$. Intuitively, $\sigma_2$ should not hold on $SKB$. (Recall that the relation $R$ in $I$ is closed world and thus is exactly $\{ R(a), R(b) \}$ in all the ground instances in $SKB$. At the same time, relation $T$ in $I$ is open world, and thus each ground instance in $SKB$ has an instance of $T$ that is a proper superset of $\{ T(a), T(b) \}$, in particular a proper supersets of this set in an infinite number of ground instances of $I$ in $SKB$.)

By the process that is symmetric to that in part (i) of this example, we obtain from $\sigma_2$ two CQ queries, $P_1$ and $P_2$:

$P_1(X) \leftarrow T(X); \quad P_2(X) \leftarrow R(X)$.

By Proposition ??, the tgd $\sigma_2$ holds on $SKB$ iff the result of transforming $P_1$ using the information we have in $SKB$ is contained in $P_2$.

We begin the transformation of $P_1$ by conjoining its body with the conjunction of all the facts in $I$, and denote the result by $P_1'$:

$P_1'(X) \leftarrow T(X), R(a), R(b), T(a), T(b)$.

We now chase $P_1'$ with the dependency, $\tau$, featured in part (i) of this example: $\tau : R(X) \rightarrow X = a \lor X = b$.

The chase keeps the query $P_1'$ intact, as $\tau$ is not applicable. We denote by $P_1''$ the result of thus terminated chase.

$P_1''(X) \leftarrow T(X), R(a), R(b), T(a), T(b)$

There does not exist a containment mapping from $P_2$ to $P_1''$. (Any containment mapping from $P_2$ to $P_1''$ would have to map $X$ in $P_2$ to the head variable of $P_1''$, which would force an invalid mapping from the only subgoal $R(X)$ of $P_2$ to the non-matching subgoal $T(X)$ of $P_1''$.) We prove below that in this case the tgd $\sigma_2$ does not hold on $SKB$.

Let us begin with the general case ($\Pi_2^p$ membership).

Proof. (Proposition ?? first part) Let $\sigma$ be of the form $\phi(\bar{X}, \bar{Y}) \rightarrow \exists \bar{Z} \psi(\bar{X}, \bar{Z})$. Consider two CQ queries $Q(\bar{X}) \leftarrow \phi(\bar{X}, \bar{Y})$ and $P(\bar{X}) \leftarrow \psi(\bar{X}, \bar{Z})$, each constructed from the respective part of the tgd $\sigma$. The proof constructs from $Q(\bar{X})$ a UCQ$^p$ query $Q''(\bar{X})$, such that $Q''$ is equivalent to $Q$ on all ground instances in the scoped knowledge base $SKB$. We then show that $Q''$ is contained in $P$ if and only if the tgd $\sigma$ holds on each instance in $SKB$. As the containment test for UCQ$^p$ queries in CQ queries is decidable in $\Pi_2^p$ (see e.g. ??) the result of the first part follows.

We begin constructing the query $Q''(\bar{X})$ by conjoining $\phi(\bar{X}, \bar{Y})$ with the instance $I$ in $SKB$, treating $I$ as a conjunction of atoms. We then chase the
resulting CQ query $Q'(X)$ with $\Gamma$, after $\Gamma$ has been (i) transformed into a set of dependencies $\Gamma^\#$, and (ii) enhanced with a set $\mathcal{V}^\#$ of dependencies that were introduced in [15] as a straightforward generalization of disjunctive egds [20, 21]. We denote by $\Psi$ the result of transforming $\Gamma$ via (i) and (ii), i.e., $\Psi := \Gamma^\# \cup \mathcal{V}^\#$; as discussed above, we obtain the query $Q'(X)$ by chasing $Q'(X)$ with $\Psi$.

We now provide the details of (i) and (ii) in the construction of $\Psi$, using the exposition in [15].

**Constructing $\Psi$:** The construction of $\Psi$ uses normalized versions of conjunctions of relational atoms (see, e.g., [41]). That is, let $\phi$ be a conjunction of relational atoms. We replace in $\phi$ each duplicate occurrence of a variable or constant with a fresh distinct variable name. As we do each replacement, say of $X$ (or $c$) with $Y$, we add to the conjunction the equality atom $Y = X$ (or $Y = c$). As an illustration, if $\phi = P(X, X) \land S(c, c, X)$, then its normalized version is $\phi^{(\text{norm})} = P(X, Y) \land S(c, Z, W) \land Y = X \land Z = c \land W = X$. By construction, the normalized version of each $\phi$ is unique up to variable renamings. For the normalized version $\phi^{(\text{norm})}$ of a conjunction $\phi$, we will denote by $\mathcal{R}(\phi^{(\text{norm})})$ the conjunction of all the relational atoms in $\phi^{(\text{norm})}$, and will denote by $\mathcal{E}(\phi^{(\text{norm})})$ the conjunction of all the equality atoms in $\phi^{(\text{norm})}$. (If $\phi^{(\text{norm})}$ has no equality atoms, we set $\mathcal{E}(\phi^{(\text{norm})})$ to true.)

A non-egd (negd) is a dependency of the form

$$\sigma : \phi(W) \rightarrow X \neq Y.$$  \hspace{1cm} (12)

Here, $\phi$ is a conjunction of relational atoms, and each of $X$ and $Y$ is an element of the set of variables $W$.

We also use chase with “implication constraints,” see, e.g., [41]. An implication constraint (ic) is a dependency of the form $\tau : \phi(W) \rightarrow \text{false}$, with $\phi(W)$ a conjunction of relational atoms.

Intuitively, to obtain the query $Q'(X)$, we will be performing chase of CQ queries (starting with $Q'(X)$) with the set of dependencies $\Psi$, which includes potentially ics, negds, egds, and tgds. (The chase rules are as defined in [15].)

(i) Dependencies $\Gamma^\#$: We convert each dependency in $\Gamma$ using a conversion rule that follows, and then produce $\Gamma^\#$ as the union of the outputs. The conversion rule for a dependency $\gamma \in \Gamma$ of the form $\gamma : \phi(X, Y) \rightarrow \exists \bar{Z} \psi(\bar{X}, \bar{Z})$ converts $\phi$ into $\mathcal{R}(\phi^{(\text{norm})}) \land \mathcal{E}(\phi^{(\text{norm})})$, and then returns

$$\gamma^{(#)} : \mathcal{R}(\phi^{(\text{norm})}) \rightarrow \exists \bar{Z} \psi(\bar{X}, \bar{Z}) \lor \neg \mathcal{E}(\phi^{(\text{norm})}).$$

(ii) Dependencies $\mathcal{V}^\#$: We use a type of dependencies, as introduced in [15], that collectively enable us to reflect the requirement that in all the ground instances of $SKB$, the contents of all the outside-scope relations are fixed. Let $R_1, \ldots, R_m$ ($m \geq 0$) be the names of all such outside-scope relations in $SKB$. We denote by $V$ the set of $m$ views $V_1, \ldots, V_m$, such that for each $i \in [1, m]$ and for the relation $R_i$, $V_i$ is defined as $V_i(X) \leftarrow R_i(X)$. We now proceed for each $V_i$ as follows:
If, for the instance $I$ in $SKB$, we have $R_i(I) = \emptyset$, we define the implication constraint $\iota_{V_i}$ for $V_i$ as
\[
\iota_{V_i} : R_i(X) \rightarrow false.
\] (13)

Now suppose that the arity $p_i$ of the relation $R_i$ is greater than zero, and that for the instance $I$ in $SKB$, we have $R_i(I) = \{t_1, t_2, \ldots, t_{m_i}\}$, with $m_i \geq 1$. Then we define the generalized negd $\tau_{V_i}$ for $V_i$ as
\[
\tau_{V_i} : R(X) \rightarrow \vee_{j=1}^{m_i} (X = t_j).
\] (14)

Here, $X = [S_1, \ldots, S_{p_i}]$ is the (distinct-variable-only) head vector of the query for $V_i$. For each $j \in [1, m_i]$ and for the ground tuple $t_j = (c_{j1}, \ldots, c_{jp_i}) \in R_i(I)$, we abbreviate by $X = t_j$ the conjunction $\wedge_{l=1}^{p_i} (S_l = c_{jl})$.

The set of dependencies $\psi$ is the union of the implication constraints and generalized negds, one for each relation outside the scope in $SKB$, with the exception that nonempty Boolean relations (if any are present outside the scope in $SKB$) are not represented in $\psi$. (It is shown in [15] that it is not necessary for the correctness of the chase to include such dependencies for nonempty Boolean relations.)

It is shown in [15] that chase of CQ queries with sets of dependencies such as in $\Psi$ terminates and has a unique output (up to variable renaming) that is a UCQ$^\#$ query, provided $\Gamma$ is a weakly acyclic [21] set of egds and tgds. Denote by $Q''(X)$ the output of the chase of the CQ query $Q'(X)$ (as constructed in the beginning of this proof) with the set of dependencies $\Psi = \Gamma^\# \cup \psi$. By construction of $Q''(X)$ (see [15]), we have that for each ground instance $D$ in $SKB$, the queries $Q(X)$ and $Q''(X)$ have on $D$ the same answer set, call it $A_Q(D)$.

Now:

Suppose that we have $Q''(X) \subseteq P(X)$. Then it follows immediately from the definition of tgds and from the reasoning in the previous paragraph that $\sigma$ holds on all ground instances in $SKB$.

Conversely, suppose that $\sigma$ holds on all ground instances $D$ in $SKB$. Then, by definition of $\sigma$, for each such $D$ we have that $Q(D) \subseteq P(D)$.

But we have obtained that the answer $A_Q(D)$ to the query $Q$ on the instance $D$ is also the answer to $Q''(X)$ on $D$. Thus, we have that $Q''(X) \subseteq P(X)$. The latter result is immediate from the following properties of the relationship between $Q$ and $Q''$, by construction of $Q''$ from $Q$:

- On all the instances $D$ that are represented by the given SKB, $Q(D) = Q''(D)$;
- On all the instances $D$ that do not have at least one fact included in $I$ in the given SKB, $Q''(D) = \emptyset$; and
- On each instance $D$ that includes all the facts that are present in $I$ in the given SKB, each valuation from $Q''$ to $D$ is an instance represented by the given SKB.
Next we show \((\text{NP-completeness when the SKB is safe})\).

**Proof.** (Propositions 8–second part) The key ingredient is that, when the SKB is safe, everything produced out of the case belongs to a relation on scope. Thus, we can then proceed with the standard proof for implication of tgds in an instance, where the premise of the tgd is added to \(I\), chased according to \(\Gamma\) so that the conclusion of the tgd can be found in the chase. Since \(\Gamma\) is weakly acyclic, chase terminates and query answering is \(\text{NP-complete (combined complexity)}\) [23].

### A.11 Proof of Proposition 9

The membership in \(\text{Exptime}^{\text{NP}}\) follows from the proof of Proposition 16, as the setting therein strictly generalizes the one in the statement of the Proposition.

For the membership in \(\text{Exptime}\), we can use the following algorithm.

- Compute the skb \(K = (J, \Gamma, \text{Scope})\) representing the set \(\text{outcomes}_{P_1, \ldots, P_n}(I)\).
- We know that \(J\) may be of exponential size, but the amount of data values in \(J\) are the same as in \(I\). Let us denote this number by \(d\).
- Since CQs are preserved under homomorphisms, it suffices to check the satisfaction of \(Q\) over \(J\). In order to do that, we can enumerate the number of homomorphisms \(h\) from \(Q\) to \(J\), which are bounded by \(d^{|Q|}\), and see whether \(h(Q)\) is realised in \(J\).

For the membership in \(\text{Ptime}\), we use the same algorithm as for the \(\text{Exptime}\) case, albeit this time all of \(Q\) and \(P_1, \ldots, P_n\) are fixed. This means that \(J\) is of size polynomial in \(I\), and the number of homomorphisms if also polynomial. This results altogether in a polynomial algorithm.

### A.12 Proof of Proposition 10

The proof reduces the halting problem to \(\text{CONTRAINT READINESS}\) for tgd constraints, encoding the computation of Turing machine on an input word by using a set of relations that describe successive machine configurations and tgds that describe machine transitions. The proof outline here is similar in spirit to the proof outline given in [19, Theorem 1] to show that the problem of deciding whether there exists a terminating chase sequence for a set of tgds is undecidable.

Let \(M = (Q, A, q_0, q_h, \delta)\) be a deterministic Turing machine with a single biinfinite tape, an alphabet \(A\) including a blank symbol that we write as \(b\), and a set of controller states \(Q\) containing an initial state \(q_0\). We assume without loss of generality that \(M\) has a single halting state \(q_h\), distinct from \(q_0\), and that no transitions are defined for this state. Let \(w = a_1, \ldots, a_m\) denote the input word in \(A^*\).

We represent the space-time structure of a computation of \(M\) by a grid of tape cells, in which the top row of cells represents the initial configuration of \(M\), and each successive row beneath the first represents the next machine configuration. Each tape cell in a row is connected by horizontal edges to the cells representing
its left and right neighbors. With some exceptions, every cell in a row is also connected by vertical edges to its correspondents (if any) in the preceding and succeeding rows.

Schema. We represent this grid structure in relations, using a schema $S$ that includes ternary relations $T$ (“tape”) and $H$ (“head”). The relation $T$ describes the tape contents and layout in a machine configuration: $T(x, a, y)$ indicates that cell $x$ contains letter $a$ and lies immediately to the left of cell $y$. The relation $H$ describes the head location and state: $H(x, q, y)$ indicates that the tape head rests on cell $x$ (immediately to the left of cell $y$) and that the machine controller is in state $q$. We can depict the initial configuration of $M$ as follows, with $c_i$ denoting the tape cell numbered $i$, and with $B$ and $E$ denoting special elements, different from any tape symbols, that represent, respectively, the beginning and the end of the used or visited portion of the infinite tape.

\[
\begin{align*}
  c_0 & B c_1 a_1 q_0 a_2 \cdots a_{m-1} c_m a_m c_{m+1} E c_{m+2}
\end{align*}
\]

The schema $S$ also includes two auxiliary binary relations $L$ (“left”) and $R$ (“right”) used to ensure that the tape cells to the left and right of the active head region in each successor step are copies of the tape cells to the left and right in the predecessor step.

To ensure that the tgds within each procedure are acyclic, the schema $S$ includes additional ternary relations $T'$ and $H'$ and binary relations $L'$ and $R'$. These, respectively, have exactly the same interpretation as do $T$, $H$, $L$, and $R$, but serve only as dummies that we use to divide what would otherwise be cyclic tgds in one procedure into matching acyclic sets that appear in separate procedures.

In the remainder of the proof, as in the explanations of $T$ and $H$ above, we use constants to denote the grid cells, states, and tape symbols of $M$. We do not, however, permit tgds to involve constants, and so assume that for each state and symbol constant $c$, the schema $S$ contains a distinct unary relation $C$ that is never in scope and that simulates the use of the constant $c$ in the sense that the interpretation of $C$ is $C = \{c\}$ in the initial instance $I$ and hence in every subsequent instance. For example, an atom of the form $T(x, a, y)$ for some symbol constant $a$ should be read as shorthand for the conjunction $T(x, v, y) \land A(v)$.

Initial instance. The initial instance $I$ represents the initial machine configuration as follows.

- $T^I$ consists of triples $\{(c_0, B, c_1), (c_1, a_1, c_2), \ldots, (c_{m+1}, E, c_{m+2})\}$.
  Here each $c_j$ is a fresh element representing a tape cell.
- $H^I$ consists of the triple $(c_1, q_0, c_2)$, meaning that $M$ starts with the head on cell 1 in the initial state $q_0$.
- $L^I$ and $R^I$ are empty, as are $T'^I$, $H'^I$, $L'^I$, and $R'^I$.

Set of procedures. The set of procedures $Π$ contains one procedure $P_d$ for each transition $d$ in $δ$, plus a procedure $P'_{lr}$ that copies tape cell contents across
configurations, and a procedure $P^{tr}$ that translates the dummy relations back into the primary relations.

We define the translation procedure $P^{tr} = (Scope^{tr}, C^{tr}, Q_{pres})$ so that $Scope^{tr} = \{T[*], H[*], L[*], R[*]\}, C^{tr}$ is empty, $Q_{pres} = \{T(x_1, y_1, z_1), H(x_2, y_2, z_2), L(x_3, y_3), R(x_4, y_4)\}$, and

\[
C^{tr}_{out} = \begin{cases} 
T'(x, y, z) \rightarrow T(x, y, z) \\
H'(x, y, z) \rightarrow H(x, y, z) \\
L'(x, y) \rightarrow L(x, y) \\
R'(x, y) \rightarrow R(x, y).
\end{cases}
\]

Comparison with the definition shows that $P^{tr}$ has safe scope.

For each transition $d = (q, a) \mapsto (q', a', L/R)$ in $\delta$, we define the transition procedure $P^d$ so that $Scope^d = \{T'[*], H'[*], L'[*], R'[*]\}, C^d_{in}$ is empty, $Q_{pres}^d = \{T'(x_1, y_1, z_1), H'(x_2, y_2, z_2), L'(x_3, y_3), R'(x_4, y_4)\}$, and $C^{d}_{out}$ consists of tgd that characterize local transition changes.

1. If $d$ is a right-moving transition, the first tgd in $C^{d}_{out}$ encodes motion that does not extend the used portion of the tape by visiting new cells.

\[
T(x, a, y) \land H(x, q, y) \land T(y, v, z) \rightarrow \\
\exists x' \exists y' \exists z' T'(x', a', y') \land T'(y', v, z') \land \\
H'(y', q', z') \land L'(x, x') \land \neg R'(y, y').
\]

Here variables $x', y'$, and $z'$ name the cells in the successor configuration that correspond to the cells $x$, $y$, and $z$. The symbols $a, a'$, $q$ and $q'$ denote constants, with $a, a' \in A$ and $q, q' \in Q$.

If $d$ is a left-moving transition, the first tgd is defined correspondingly.

\[
T(x, a, y) \land H(x, q, y) \land T(z, v, x) \rightarrow \\
\exists x' \exists y' \exists z' T'(x', a', y') \land T'(z', v, x') \land \\
H'(z', q', x') \land L'(x, x') \land \neg R'(y, y').
\]
2. If \( d \) is a right-moving transition, the second tgd in \( C_d^{\text{out}} \) encodes right moves that extend the used portion of the tape by moving the \( E \) marker right and inserting a blank cell.

\[
T(x, a, y) \land H(x, q, y) \land T(y, E, z) \rightarrow \\
\exists x' \exists y' \exists z' \exists a' T'(x', a', y') \land T'(y', q', z') \land H'(y', q', z') \land L'(x, x') \land R'(z, z').
\]

We include the \( R'(y, y') \) atom in the right-hand side of the tgd for uniformity, though it serves no other purpose in this case, as there are no cells to copy to the right of the cell marked with \( E \) in the prior configuration.

If \( d \) is a left-moving transition, this second kind of tgd is defined correspondingly, this time moving the beginning of tape marker to the left. In this tgd, the \( L(z, z') \) atom is included for uniformity.

\[
T(x, a, y) \land H(x, q, y) \land T(z, B, x) \rightarrow \\
\exists x' \exists y' \exists z' \exists a' T'(x', a', y') \land T'(z', q, x') \land H'(z', q, x') \land L'(z, z') \land R'(y, y').
\]

As sets of such tgds are acyclic, comparison with the definition shows that each \( P_d \) has safe scope.

Finally, we define the left-right copying procedure \( P^{lr} = (\text{Scope}^{lr}, C_{\text{in}}^{lr}, C_{\text{out}}^{lr}, Q_{\text{pres}}^{lr}) \)
so that \( \text{Scope}^{lr} = \{ T'[\ast], L'[\ast], R'[\ast] \} \), \( C_{\text{in}}^{lr} \) is empty, \( Q_{\text{pres}}^{lr} = \{ T'(x_1, y_1, z_1), L'(x_2, y_2), R'(x_3, y_3) \} \), and \( C_{\text{out}}^{lr} \) contains two tgds that simply copy the contents of any cells outside of the active region in one configuration to the corresponding cells in the successor configuration.

The first tgd copies contents of cells to the left of the active region.

\[
T(x, v, y) \land L(y, y') \rightarrow \exists x' T'(x', v, y') \land L'(x, x')
\]
The second tgd copies contents of cells to the right of the active region.

\[ T(x,v,y) \land R(x,x') \rightarrow \exists y' \ T'(x',v,y') \land R'(y,y') \]

Comparison with the definition shows that \( P_{lr} \) has safe scope.

**Undecidability.** Let \( \Sigma \) be the readiness constraint consisting of a single tgd \( t \) that encodes halting of the machine as entry of the machine into the halting state \( q_h \) as the following.

\[ H(x,q_0,y) \rightarrow \exists x' \exists y' \ H(x',q_h,y') \]

Here \( x' \) and \( y' \) denote cells in some successor configuration of the initial configuration, not necessarily immediate successors of \( x \) and \( y \).

This tgd is cyclic, but we explain how to transform it into an acyclic tgd at the end of the proof.

We now show that \( I \) can be readied for \( t \) using \( \Pi \) if and only if \( M \) halts on input \( w \).

**Readable \( \Rightarrow \) halts:** Assume that \( I \) can be readied for \( t \) using \( \Pi \). Let \( P_1, \ldots, P_n \) be a witnessing sequence of procedures, and let \( I_0, \ldots, I_n \) be a sequence of instances such that \( I_0 = I \) and for each \( i > 0 \), \( I_i = chase_i(I_{i-1}) \), where \( chase_i \) denotes chase with respect to the set \( C_{out} \) of tgds in the output constraints of procedure \( P_i \). In particular, \( I_n \) is an instance produced out of chasing dependencies in the output constraints of the procedures in \( \Pi \).

By construction, the initial instance \( I \) characterizes the starting configuration of \( M \) on \( w \), in which the state specification is \( H(c_1,q_0,c_2) \). Also by construction, if a transition procedure applies to a configuration, then \( M \) must have a corresponding transition. Because \( M \) is deterministic, if no transition procedure
applies even after all copying and translation dependencies have been chased, it
must be because the final configuration is one in which $H(c_i, q_h, c_{i+1})$ for some
$i$, meaning that the computation has halted. Therefore $I$ can be readied for $t$
only if some sequence of procedures yields a transition to $q_h$.

(Halts $\Rightarrow$ readable): Assume now that $M$ halts on input $w$. Let $d_1, \ldots, d_n$ be
the sequence of transitions taken by $M$ in moving from the initial configuration
to the final halting configuration, and let $P_i$ denote the transition procedure for
d_i.

We claim that $t$ satisfies each instance in

$$\text{outcomes}_{P_1, p_{tr}, P_2, p_{tr}, \ldots, p_n, p_{tr}}(I).$$

To see this, note that $t$ is satisfied as long as the conjunctive query $\exists x' \exists y' H(x', q_h, y')$
is satisfied. That query, in turn, is satisfied if the chase of $I$ satisfies each of the
$C_{out}$ dependencies of $P_{tr}$, and $P_{di}$ for each $i$. By construction, each of the
transition procedures produces, by chase and in conjunction with the copying and
translation procedures, each successive configuration, so the final transition $d_n$
will require, after translation, that $H$ contains a triple of the form $(c_i, q_h, c_{i+1})$.

We conclude that $I$ can be readied for $t$ using $H$ if and only if $M$ halts on
input $w$. As the halting problem is undecidable, so must also be the constraint
readiness problem.

We note that the claim of Proposition 10 holds even if $\Sigma$ is acyclic. The tgd
t employed in the proof is cyclic, but essentially the same argument would hold
were one to use instead the acyclic tgd

$$T(c_0, B, c_1) \rightarrow \exists x' \exists y' \ H(x', q_h, y'),$$

where here $c_0$ and $c_1$ are the constants so named in the initial instance.

**A.13 Proof of Theorem 3**

It is easy to see that using procedures with safe scope we will never be able
to ready an instance for an egd: if the instance $I$ does not satisfy an egd then
this violation will be carried over no matter what procedures we apply. For this
reason, we focus on tgds only.

Let then $I, \Pi$ and $\sigma$ be as outlined in the statement of the theorem (where
$\sigma$ is a tgd). Let $D$ be the number of different elements in $I$, and $S$ the schema
of $I$.

Further, assume a sequence $P_1, \ldots, P_k$ such that every instance in $\text{outcomes}_{P_1, \ldots, P_k}(I)$
satisfies $\sigma$. By Theorem 1 there is an $K = (J, I, \text{Scope})$ that represents the set
$\text{outcomes}_{P_1, \ldots, P_k}(I)$.

We now show that there is a sequence $P'_1, \ldots, P'_n$ of procedures in $\Pi$ with
the same property, but where now $n$ is bounded exponentially on the size of $I$
and $\Pi$. First, since all tgds involved in all procedures in $\Pi$ are full tgds, the size
of $J$ is bounded by $|D| |S|$.
From Proposition 8, it must be that the instance \( K \) resulting of taking \( J \) together with the frozen body of the premise of \( \sigma \) is such that the consequence of \( \sigma \) holds in \( \text{chase}_f(K) \). The size of \( K \) is bounded by \((|D| + |Q|)|S|\), and thus we can assume that \( \Gamma \) contains only tgds of size bounded by \((|D| + |Q|)|S|\), as any bigger tgd can be equivalent to a tgd of such size when chasing \( K \).

We can enumerate all sets \( \Omega \) containing tgds of size at most \((|D| + |Q|)|S|\), and we know that the number of different such sets is bounded by \(2^{(|D| + |Q|)|S|}\), as any bigger tgd can be equivalent to a tgd of such size when chasing \( K \).

Let \( K_i = (K_i, \Gamma_i, \text{Scope}_i) \) be the SKB representing the set \( \text{outcomes}_{P_1, \ldots, P_\ell}(I) \). As mentioned, we assume without loss of generality that each \( \Gamma_i \) contains tgds of size at most \((|D| + |Q|)|S|\).

If no \( K_i \) is equal, then the sequence \( \ell \) must then be of length at most \(|D||S|\), because each new procedure must at least introduce some data in \( K_i \). Further, if for every maximal sequence \( p, p + 1, p + 2, \ldots, q \) such that \( K_p = K_q \) one cannot find two numbers \( r_1 \) and \( r_2 \) such that \( \Gamma_{r_1} \) is logically equivalent to \( \Gamma_{r_2} \), then \( \ell \) must then be of length at most \(|D||S| \cdot \Pi \cdot 2^{(|D| + |Q|)|S|}\).

On the other hand, if there are \( r_1 \) and \( r_2 \) such that \( \Gamma_{r_1} \) is logically equivalent to \( \Gamma_{r_2} \), we can just prune the sequence from \( r_1 + 1 \) to \( r_2 \).

With the above observations in hand we then outline the \( \text{N2Exptime} \) algorithm:

- Guess a sequence \( P_1, \ldots, P_n \) of procedures. We know it is of length at most doubly-exponential in the size of the input.
- Compute the SKB \( K \) representing \( \text{outcomes}_{P_1, \ldots, P_n}(I) \).
- We need also to guess all appropriate chase steps to show that \( K \models \sigma \), as explained in the proof of proposition 8.

A.14 Proof of Proposition 11

Follows from the proof of 10 simply by using the query \( H(x', q_0, y') \) instead of the tgd employed therein.

A.15 Proof of Theorem 4

We use the same argument as in the proof of Propositions 9 and 10. This time, in addition we need to guess a sequence of procedures that yield the appropriate chase rule.

More precisely, as in the proof of Theorem 3, we can bound the size of the sequence of procedures. In order to do that, assume a sequence \( P_1, \ldots, P_\ell \) of procedures from \( \Pi \) such that every instance in \( \text{outcomes}_{P_1, \ldots, P_\ell}(I) \) satisfies \( Q \). By Theorem 11 there is an \( \mathcal{K} = (J, \Gamma, \text{Scope}) \) that represents the set \( \text{outcomes}_{P_1, \ldots, P_\ell}(I) \). Let also \( K_i = (K_i, \Gamma_i, \text{Scope}_i) \) be the SKB representing the set \( \text{outcomes}_{P_1, \ldots, P_\ell}(I) \).

Note however that, in contrast with the proof of Theorem 3, we do not need to focus on maintaining the sets \( \Gamma_i \) of intermediate SKBs, as we only care about the instances \( K_i \).
We can then construct a corresponding exponential sequence by pruning out all procedures \( P_i \) where \( J_i \) is the same instance as \( J_{i-1} \).

For the \( \text{NE}x\text{ptime} \) algorithm we can then guess this exponential sequence of procedures whose outcome is represented by an SKB of the form \((J, \Gamma', \text{Scope}')\), guess an appropriate homomorphism from \( Q \) to \( J \) and guess the necessary chase steps to produce the image of \( Q \) over \( J \) as in the proof of Propositions 9 and 16.

### A.16 Proof of Proposition 12

Let \( P = (\text{Scope}, \text{C}_{\text{in}}, \text{C}_{\text{out}}, \text{Q}_{\text{pres}}) \). We first show how to construct, for each instance \( I \) over a schema \( S \), the minimal schema \( S_{\text{min}} \) such that all pairs \((J, S')\) that are possible outcomes of applying \( P \) over \((I, S)\) are such that \( S' \) extend \( S_{\text{min}} \).

The algorithm receives a procedure \( P \) and a schema \( S \) and outputs either \( S_{\text{min}} \), if the procedure is applicable, or a failure signal in case there is no schema satisfying the output constraints of the procedure. Along the algorithm we will be assigning numbers to some of the relations in \( S_{\text{min}} \). This is important to be able to decide failure.

**Algorithm \( A(P, S) \) for constructing \( S_{\text{min}} \)**

**Input**: procedure \( P = (\text{Scope}, \text{C}_{\text{in}}, \text{C}_{\text{out}}, \text{Q}_{\text{pres}}) \) and schema \( S \).

**Output**: either failure or a schema \( S_{\text{min}} \).

1. If \( S \) does not satisfy the structural constraints in \( \text{C}_{\text{in}} \) or is not compatible with either \( \text{Q}_{\text{pres}} \) or \( \text{Q}_{S_{\text{min}}} \), output failure. Otherwise, continue.
2. Start with \( S_{\text{min}} = \emptyset \).
3. For each total query \( R \) in \( \text{Q}_{\text{pres}} \), assume that \(|S(R)| = k\). Set \( S_{\text{min}}(R) = S(R) \), and label \( R \) with \( k \).
4. Add to \( S_{\text{min}} \) all relations \( R \) mentioned in an atom \( R[\ast] \) in \( \text{C}_{\text{out}} \) (if they are not already part of \( S_{\text{min}} \)), without associating any attributes to them.
5. In the following instructions we construct a set \( \Gamma(P, S) \) of pairs of relations and attributes. Intuitively, a pair \((R, \{a_1, \ldots, a_n\})\) in \( \Gamma(P, S) \) states that each schema in the output of \( P \) must contain a relation \( R \) with attributes \( a_1, \ldots, a_n \).
   - For each relation \( R \) in \( S \) that is not mentioned in \( \text{Scope} \), add to \( \Gamma(P, S) \) the pair \((R, S(R))\).
   - For each constraint \( R[a_1, \ldots, a_n] \) in \( \text{Scope} \), add the pair \((R, S(R)\setminus\{a_1, \ldots, a_n\})\) to \( \Gamma(P, S) \).
   - For each atom \( R(a_1 : x_1, \ldots, a_n : x_n) \) in \( \text{Q}_{\text{pres}} \), add to \( \Gamma(P, S) \) the pair \((R, \{a_1, \ldots, a_n\})\).
   - For each atom \( R(a_1 : x_1, \ldots, a_n : x_n) \) in a tgd or egd in \( \text{C}_{\text{out}} \), add to \( \Gamma(P, S) \) the pair \((R, \{a_1, \ldots, a_n\})\).
   - For each constraint \( R[a_1, \ldots, a_n] \) in \( \text{C}_{\text{out}} \), add to \( \Gamma(P, S) \) the pair \((R, \{a_1, \ldots, a_n\})\).
6. For each pair \((R, A)\) in \( \Gamma(P, S) \), do the following.
   - If \( R \) is not yet in \( S_{\text{min}} \), add \( R \) to \( S_{\text{min}} \) and set \( S_{\text{min}}(R) = A \);
   - If \( R \) is in \( S_{\text{min}} \), update \( S_{\text{min}}(R) = S_{\text{min}}(R) \cup A \).
7. If $S_{\text{min}}$ contains a relation $R$ labelled with a number $n$ where, $S_{\text{min}}(R) > n$, output failure. Otherwise output $S_{\text{min}}$.

By direct inspection of the algorithm, we can state the following.

**Observation 1** Let $P = (\text{Scope}, C_{\text{in}}, C_{\text{out}}, Q_{\text{pres}})$ be a relational procedure and $S$ a relational schema. Then for each relation $R$ in $S_{\text{min}}$ with attributes $\{a_1, \ldots, a_n\}$, every instance $I$ over $S$ and every pair $(J, S')$ in the outcome of applying $P$ to $(I)$, we have that $S(R)$ is defined, with $\{a_1, \ldots, a_n\} \subseteq S(R)$.

Furthermore, the following lemma specifies, in a sense, the correctness of the algorithm.

**Lemma 2.** Let $P = (\text{Scope}, C_{\text{in}}, C_{\text{out}}, Q_{\text{pres}})$ be a relational procedure and $S$ a relational schema. Then:

i) If $A(P, S)$ outputs failure, either $P$ cannot be applied over any instance $I$ over $S$, or for each instance $I$ over $S$ the set $\text{outcomes}_P(I)$ is empty.

ii) If $A(P, S)$ outputs $S_{\text{min}}$, then the schema of any instance in $\text{outcomes}_P(I)$ extends $S_{\text{min}}$.

**Proof.** For i), if some of the components of $P$ are not compatible with $S$, or $S$ does not satisfy the constraints in $C_{\text{in}}$, then clearly $P$ cannot be applied over any instance $I$ over $S$. Assume then that $S$ satisfies all compatibilities and pre-conditions in $P$, but $A(P, S)$ outputs failure. Then $S_{\text{min}}$ contains a relation $R$ such that $|S_{\text{min}}(R)| = m$, but $R$ is labelled with number $k$, for $k < \ell$. From the algorithm, we this implies that $|S_{\text{min}}(R)| > |S(R)|$, but that there is a query $R$ in $Q_{\text{pres}}$. Clearly, $Q_{\text{pres}}$ cannot be preserved under any outcome, since by Observation 1 we require the schemas of outcomes to assign more attributes to $R$ than those assigned by $S_{\text{min}}$, and thus the cardinality of tuples in the answer of $R$ differs between $I$ and its possible outcomes. Finally, item ii) is a direct consequence of Observation 1.

The algorithm $(A, P)$ runs in polynomial time, and that the total size of $S_{\text{min}}$ (measured as the number of relations and attributes) is at most the size of $S$ and $P$ combined. Thus, to decide the applicability problem for a sequence $P_1, \ldots, P_n$ of procedures, all we need to do is to perform subsequent calls to the algorithm, setting $S_0 = S$ and then using $S_i = A(P_i, S_{i-1})$ as the input for the next procedures. If $A(P_n, S_{n-1})$ outputs a schema, then the answer to the applicability problem is affirmative, otherwise if some call to $A(P_i, S_{i-1})$ outputs failure, the answer is negative.

**A.17 Proof of proposition 13**

The reduction, just as that of Proposition 1 is by reduction from the embedding problem for finite semigroups, and builds up from this proposition. Let us start by defining the procedures $P_1$, $P_2$ and $P_3$. 
For procedure $P_1$ we first build a set $\Gamma_1$ of tgds. This set is similar to the set $\Sigma$ used in Proposition 1, but using three additional dummy relations $G^d, E^d$ and $G^{binary}$.

First we add to $\Gamma_1$ dependencies that collect elements of $G$ into $D$, and that initialize $E$ as a reflexive relation.

\[
\begin{align*}
G(x, u, v) & \rightarrow D(x) \\
G(u, x, v) & \rightarrow D(x) \\
G(u, v, x) & \rightarrow D(x) \\
D(x) & \rightarrow E(x, x)
\end{align*}
\]

Next the dependency that states that $F$ contains everything in $R$ if some conditions about $E$ occur.

\[
E(x, y) \land C(u, x) \land C(v, y) \land N(u, v) \land R(w) \rightarrow F(w) \quad (15)
\]

The dependencies that assured that $E$ was an equivalence relation where acyclic, so we replace the right hand side with a dummy relation.

\[
\begin{align*}
E(x, y) & \rightarrow E^d(y, x) \\
E(x, y) \land E(y, z) & \rightarrow E^d(x, z)
\end{align*}
\]

Next come the dependencies assuring $G$ is a total and associative function, using also dummy relations.

\[
\begin{align*}
D(x) \land D(y) & \rightarrow G^{binary}(x, y) \\
G(x, y, u) \land G(u, z, v) \land G(y, z, w) & \rightarrow G^d(x, w, v)
\end{align*}
\]

Finally, the dependencies that were supposed to ensure that $E$ worked as the equality over function $G$, using again the dummy relations.

\[
\begin{align*}
G(x, y, z) \land E(x, x') \land E(y, y') \land E(z, z') & \rightarrow G^d(x', y', z') \\
G(x, y, z) \land G(x', y', z') \land E(x, x') \land E(y, y') & \rightarrow E^d(z, z')
\end{align*}
\]

We can now define procedure $P_1$:

**Scope:** The scope of $P_1$ consists of relations $G, E, D, F, G^d, E^d$ and $G^{binary}$ which corresponds to the constraints $G[*], E[*], D[*], F[*], E^d[*], G^d[*]$ and $G^{binary[*]}$.

**C_in:** There are no preconditions for this procedure.

**C_out:** The postconditions are the tgds in $\Gamma_1$.

**Q_pres:** This query ensures that no information is deleted from all of $G, E, F, G^d, E^d$ and $G^{binary}$: $G(x, y, z) \land E(u, v) \land D(w) \land F(p) \land G^d(x', y', z') \land E^d(u', v') \land G^{binary}(a, b)$. 

Note that, even though relations $G$ and $E$ are not mentioned in the right hand side of any tgd in $\Gamma_1$, they are part of the scope and thus they could be modified by the procedures $P_1$.

The procedure $P_2$ has no scope, no safety queries, no precondition, and the only postcondition is the presence of a third attribute, say $C$, in $G^{binary}$, by using a structural constraint $G^{binary}[A,B,C]$ (to maintain consistency with our unnamed perspective, we assume that these three attributes are ordered $A < A B < A C$).

To define the final procedure, consider the following set of tgds $\Gamma_3$.

$$
E^{d}(x, y) \rightarrow E(x, y) \\
G^{d}(x, y, z) \rightarrow G(x, y, z) \\
G^{binary}(x, y, z) \rightarrow G(x, y, z) \\
F(x) \rightarrow F^{check}(x)
$$

Then we define procedure $P_3$ as follows.

Scope: The scope of $P_3$ is again empty.

$C_{in}$: There are no preconditions for this procedure.

$C_{out}$: The postconditions are the tgds in $\Gamma_3$.

$Q_{pres}$: There are also no safety queries for this procedure.

Let $S$ be the schema containing relations $G$, $E$, $D$, $F$, $F^{check}$, $G^{d}$, $E^{d}$ and $G^{binary}$ and $R$. The attribute names are of no importance for this proof, except for $G^{binary}$, which associates attributes $A$ and $B$.

Given a finite semigroup $A$, we construct now the following instance $I_A$:

- $E^{IA}$ contains the pair $(a_i, a_i)$ for each $1 \leq i \leq n$ (that is, for each element of $A$);
- $G^{IA}$ contains the triple $(a_i, a_j, a_k)$ for each $a_i, a_j, a_k \in A$ such that $g(a_i, a_j) = a_k$;
- All of $D^{IA}$, $F^{IA}$ and $F^{checkIA}$ are empty;
- $R^{IA}$ has a single element $d$ not used elsewhere in $I_A$
- $C^{IA}$ contains the pair $(i, a_i)$ for each $1 \leq i \leq n$; and
- $N^{IA}$ contains the pair $(i, j)$ for each $i \neq j$, $1 \leq i \leq n$ and $1 \leq j \leq n$.

Let us now show $A = (A,g)$ is embeddable in a finite semigroup if and only if $\text{outcomes}_{P_1, P_2, P_3}(I)$ is nonempty.

($\Rightarrow$) Assume that $A = (A,g)$ is embeddable in a finite semigroup, say the semigroup $B = (B,f)$, where $f$ is total. Let $J$ be the instance over $S$ such that both $E^{dJ}$ and $E^{J}$ are the identity over $B$, $D^{J} = B$, both $G^{dJ}$ and $G^{J}$ contains a pair $(b_1, b_2, b_3)$ if and only if $f(b_1, b_2) = b_3$; $G^{binaryJ}$ is the projection of $G^{J}$ over its two first attributes, $F^{J}$ and $F^{checkJ}$ are empty and relations $N$, $C$ and $R$ are interpreted as in $I_A$. 


It is easy to see that $J$ is in the outcome of applying $P_1$ over $I$. Now, let $S'$ be the extension of $S$ where $G^{\text{binary}}$ has an extra attribute, $C$, and $K$ is an instance over $S'$ that is just like $J$ except that $G^{\text{binary}}_K$ is now the same as $G_J$ (and therefore $G^K$). By definition we obtain that $K$ is a possible outcome of applying $P_2$ over $J$, and therefore $K$ is in $(K_1,P_2,K_3)$ outcomes. Furthermore, one can see that the same instance $K$ is again an outcome of applying $P_3$ over $K$, therefore obtaining that $(K_1,P_2,P_3,K_3)$ outcomes is nonempty.

$(\Leftarrow)$ Assume now that there is an instance $L \in (K_1,P_2,P_3,K_3)$. Then by definition there are instances $J$ and $K$ such that $J$ is in $(K_1,P_1)$, $K$ is in $(K_1,P_2)$, and $L$ is in $(K_1,P_3)$. Let $J^*$ be the restriction of $J$ over the schema $S$. From a simple inspection of $P_1$ we have that $J^*$ satisfies as well the dependencies in $P_1$, so that $J^*$ is in $(K_1,P_1)$. Let now $S'$ be the extension of $S$ that assigns also attribute $C$ to $G^{\text{binary}}$.

Now, since $K$ is the outcome of $P_2$ over $J$ and $P_2$ has no scope, if we define $K^*$ as the restriction of $K$ over $S'$, then clearly $K^*$ must be in the outcome of applying $P_2$ over $J^*$. Note that, by definition of $P_3$ (since its scope is empty), the restriction of $L$ up to the schema of $K$ must be the same instance as $K$, and therefore the restriction $L^*$ of $L$ to $S'$ must be the same instance than $K^*$. Furthermore, since $L$ (and thus $L^*$) satisfies the constraints in $P_3$, and the constraints only mention relations and atoms in $S'$, we have that $K^*$ must be an outcome of applying $P_3$ over $(K^*,S')$.

We now claim that $K^*$ satisfy all tgd (1)-(11) in the proof of Proposition 1. Tgds (1-3) and (6) are immediate from the scopes of procedures, and the satisfaction for all the remaining ones is shown in the same way. For example, to see that $K^*$ satisfies $E(x,y) \rightarrow E(y,x)$, note that $J^*$ already satisfies $E(x,y) \rightarrow E^a(y,x)$. From the fact that the interpretations of $E^a$ and $E$ are the same over $J^*$ and $K^*$ and that $K^*$ satisfies $E^a(x,y) \rightarrow E(x,y)$ we obtain the desired result.

Finally, since $K^*$ satisfies $F(x) \rightarrow F^{\text{check}}(x)$, and the interpretation of $F^{\text{check}}$ over all of $I$, $J^*$ and $K^*$ must be empty, we have that the interpretation of $F$ over $K^*$ is empty as well. Given that $K^*$ satisfies all dependencies in $\Sigma$, it must be the case that the left hand side of the tgd (11) is not true $K^*$, for any possible assignment. By using the same argument as in the proof of Proposition 1 we obtain that $A = (A,y)$ is embeddable in a finite semigroup.

A.18 Proof of proposition 14

Follows from Proposition 13 and Proposition 12. We need to check first whether each procedure in the sequence is applicable. Once we do that, from Proposition 13 we know that the resulting outcome is non-empty.

A.19 Proof of proposition 15

For the proof we assume that all procedures does not use preconditions. We can treat them by first doing an initial check on compatibility that only complicates the proof.
We also specify an alternative set of representatives for conditional instances (which is actually the usual one). The set \( \hat{\text{rep}}(G) \) of representatives of a conditional instance \( G \) is simply \( \hat{\text{rep}}(G) = \{ I \mid \text{there is a substitution } \nu \text{ such that } \nu(T) \subseteq I \} \). That is, \( \hat{\text{rep}}(G) \) only specifies instances over the same schema as \( G \). The following lemma allows us to work with this representation instead; it is immediate from the definition of safe scope procedures.

**Lemma 3.** If \( G \) is a conditional instance, then (1) \( \hat{\text{rep}}(G) \subseteq \text{rep}(G) \), and (2) an instance \( J \) is minimal for \( \text{rep}(G) \) if and only if it is minimal for \( \hat{\text{rep}}(G) \).

Moreover, from the fact that procedures with safe scope are acyclic, we can state Theorem 5.1 in [3] in the following terms:

**Lemma 4 ([3]).** Given a set \( \Sigma \) of tgd's and a positive conditional instance \( G \), one can construct, in exponential time, a positive conditional instance \( G' \) such that (1) \( \hat{\text{rep}}(G') \subseteq \hat{\text{rep}}(G) \) and (2) all minimal models of \( \hat{\text{rep}}(G') \) satisfy \( \Sigma \).

Moreover, by slightly adapting the proof of Proposition 4.6 in [3], we can see that the conditional instance constructed above has even better properties. In order to prove this theorem all that one needs to do is to adapt the notion of solutions for data exchange into a scenario where the target instance may already have some tuples (which will not fire any dependencies because of the safeness of procedures).

**Lemma 5 ([3]).** Let \( P = (\text{Scope}, C_{in}, C_{out}, Q_{pres}) \) be a procedure with safe scope, and let \( G \) be a positive conditional instance. Then one can construct (in exponential time) a positive conditional instance \( G' \) such that, for every minimal instance \( I \) of \( \hat{\text{rep}}(G) \), the set \( \hat{\text{rep}}(G') \) contains all minimal instances in \( \text{outcomes}_{P}(I) \), and for every minimal instance \( J \) in \( \hat{\text{rep}}(G') \) there is a minimal instance \( I \) of \( \text{rep}(G) \) such that \( J \) is minimal in \( \text{outcomes}_{P}(I) \).

Finally, we can show the key result for this proof.

**Lemma 6.** Let \( I \) be a set of instances, and \( G \) a positive conditional table that is minimal for \( I \), and \( P = (\text{Scope}, C_{in}, C_{out}, Q_{pres}) \) a procedure with safe scope. Then either \( \text{outcomes}_{P}(I) = \emptyset \) or one can construct, in exponential time, a positive conditional instance \( G' \) such that

i) \( \text{outcomes}_{P}(I) \subseteq \text{rep}(G') \); and

ii) If \( J \) is a minimal instance in \( \text{rep}(G') \), then \( J \) is also minimal in \( \text{outcomes}_{P}(I) \).

**Proof.** Using the chase procedure mentioned in Lemma 5 we see that the conditional table \( G' \) produced in this lemma satisfies the conditions of this Lemma, for \( \hat{\text{rep}}(G) \).

For i), let \( J \) be an instance in \( \text{outcomes}_{P}(I) \). Then there is an instance \( I \) in \( I \) such that \( J \in \text{outcomes}_{P}(I) \). Let \( I^* \) be a minimal instance in \( I \) such that \( I^* \) extends \( I^* \). By our assumption we know that \( I^* \) belongs to \( \text{rep}(G) \), and since \( I^* \) is minimal it must be the case that \( I^* \) belongs (and is minimal) for \( \hat{\text{rep}}(G) \). Therefore, by Lemma 5 we have that \( \hat{\text{rep}}(G') \) contains all minimal instances for
outcomes$_P(I^*)$. But now notice that for every assignment $\tau$ and tgd $\lambda$ such that $(I^*, \tau)$ satisfies $\lambda$, we have that $(I, \tau)$ satisfy $\lambda$ as well. This means that every instance in the set outcomes$_P(I)$ must extend a minimal instance in outcomes$_P(I^*)$ (if not, then a tgd would not be satisfied due to some assignment that would not be possible to extend). Since every minimal instance in outcomes$_P(I^*)$ is in \(\hat{r}ep(G')\), then by the semantics of conditional tables it must be the case that $J$ belongs to $\hat{r}ep(G')$ as well, and therefore to $rep(G')$.

Item [ii)] follows from the fact that any minimal instance in $rep(G')$ must also be minimal for $\hat{rep}(G')$ and a direct application of Lemma 5.

The next Lemma constructs the desired outcomes for alter schema procedures.

**Lemma 7.** Let $I$ be a set of instances, and $G$ a conditional table that is minimal for $I$, and $P = (\text{Scope}, C_{\text{in}}, C_{\text{out}}, Q_{\text{pres}})$ an alter schema procedure. Then either outcomes$_P(I) = \emptyset$ or one can construct, in polynomial time, a conditional instance $G'$ such that

i) outcomes$_P(I) \subseteq rep(G')$; and
ii) If $J$ is a minimal instance in $rep(G')$, then $J$ is also minimal in outcomes$_P(I)$.

**Proof.** Assume that outcomes$_P(I) \neq \emptyset$ (this can be easily checked in polynomial time). Then one can compute the schema $S_{\text{min}}$ from the proof of Proposition 12. This schema will add some attributes to some relations in the schema of $G$, and possibly some other relations with other sets of attributes. Let Schema($G$) = $S$.

We extend $G$ to a positive conditional table $G'$ over $S_{\text{min}}$ as follows:

1. For every relation $R$ such that $S_{\text{min}}(R) \neq S(R)$, with $n \geq 1$, for tuples from $G'$ by adding to each tuple in $G$ a fresh null value in each of the attributes $A_1, \ldots, A_n$.
2. For every relation $R$ such that $S(R)$ is not defined, but $S_{\text{min}}(R)$ is defined, set $R^{G'} = \emptyset$.

The properties of the lemma now follow from a straightforward check.

The proof of Proposition 15 now follows from successive applications of Lemmas 7 and 6: one just need to compute the appropriate conditional table for each procedure in the sequence $P_1, \ldots, P_n$. That each construction is in exponential size if the number $n$ of procedures is fixed, or doubly-exponential in other case, follows also from these Lemmas, as the size of the conditional table $G'$, for a procedure $P$ and a conditional table $G$, is at most exponential in $|G^{P}|$ (and thus if we have $n$ procedures of size $|P|$ the size is of order $(|G^{P}|)^n$, or $|G^{n|P|})$).

**A.20 Proof of proposition 16**

Let $T$ be a conditional instance, $I$ an instance in $\hat{r}ep(T)$ and $Q$ a boolean conjunctive query. By definition of conditional instances and the fact that CQs are preserved under homomorphisms, we have the following fact.
Observation 2. $Q$ holds in every minimal instance in $\hat{\text{rep}}(T)$ if and only if $Q$ holds in every instance in $\text{rep}(T)$.

Thus, if we want to compute the certain answers for a query $Q$ over a conditional instance $I$, all we need to do is to guess a counterexample: an assignment $\nu$ for $T$ such that the minimal instance $\nu(T)$ does not satisfy the query. We obtain (see e.g. C. Grahne. The Problem of Incomplete Information in Relational Databases. Springer, 1991.)

Observation 3. Computing certain answers of conditional instance is in $\Pi^P_2$.

However, again by construction we can show the following for positive conditional instances:

Lemma 8. Let $T$ be a positive conditional instance, and $N$ the naive instance given by dropping all conditions from $T$. Then $Q$ holds in every minimal instance in $\hat{\text{rep}}(T)$ if and only if $Q$ holds in every instance in $\text{rep}(N)$.

Proof. The if direction follows because an arbitrary assignment for the nulls in $N$ that sends each null to a fresh constant not appearing anywhere (not even in conditions) in $T$ yields an instance in both $\hat{\text{rep}}(T)$ and $\text{rep}(N)$ that is also minimal for $\hat{\text{rep}}(T)$. For the only if direction we show that there is a homomorphism from $N$ to every minimal instance in $\hat{\text{rep}}(T)$. Indeed, let $J$ be a minimal instance in $\hat{\text{rep}}(T)$, built from an assignment $\nu$ for $T$. Then the function mapping each null in $N$ as mandated by $\nu$ is indeed a homomorphism from $N$ to $J$: by construction it could be that $J$ contains more tuples than $\nu(N)$, but not the other way around.

We immediately obtain

Observation 4. Computing certain answers of positive conditional instance is in $\text{NP}$, and for boolean queries $Q$ it suffices to check a homomorphism from $Q$ to $N$, where $N$ is the naive instance resulting of dropping all tuple with conditions in positive conditional instances.

Membership in $\text{NP}$ when $n$ is fixed. We can now outline our algorithm for query answering, given $P_1,\ldots, P_n$, $I$ and $Q$ from the statement of the problem. Let $T$ an instance representing $\text{outcomes}_{P_1,\ldots, P_n}(I)$, and let $N$ the naive instance constructed by dropping tuples with conditions in $T$.

- Guess a homomorphism $h$ from $Q$ to $N$.
- For each atom in $h(Q)$, guess a set rules producing this atom, and for each such rule all homomorphisms needed to fire the rule during a chase. This set is at most exponential size, in $n$ (and polynomial if $n$ is fixed) because each atom in the conditional instance representing $\text{outcomes}_{P_1,\ldots, P_n}(I)$ is produced by a rule in $P_i$, having at most $|P_i|$ atoms from $\text{outcomes}_{P_1,\ldots, P_{i-1}}(I)$. The resulting size of the set is then bounded by $|P|^n$, where $P$ is the size of the biggest procedure in the sequence $P_1,\ldots, P_n$.
- We can then check that by chasing the sequence $P_1,\ldots, P_n$ of procedures one does produce the set of atoms and rules needed to witness $h(Q)$. The check is polynomial in the size of the set of rules producing $h(Q)$.
A.21 Proof of Theorem 5

The key idea for this proof is the fact that, when computing the conditional instances representing the outcome of procedures as dictated by Proposition 15, procedures with safe schema-alteration can only produce nulls the first time they appear in a sequence.

To be more precise, assume a sequence \( P_1, \ldots, P_\ell \) of procedures from \( \Pi \) such that every instance in \( \text{outcomes}_{P_1, \ldots, P_\ell}(I) \) satisfies \( Q \). By Proposition 15, there is a conditional table \( T \) whose minimal instances coincide with the minimal instances in \( \text{outcomes}_{P_1, \ldots, P_\ell}(I) \).

Let also \( T_i \) the conditional instance representing the minimal instances of \( \text{outcomes}_{P_1, \ldots, P_i}(I) \). While \( T_i \) may contain nulls, at most one null can be computed for each procedure with safe-schema alteration in \( \Pi \) and each assignment tuple in \( T_{i-1} \). The first time we apply such a procedure we can create at most \( D|S| \) nulls, where \( D \) is the number of elements in \( I \) and \( |S| \) is the schema of \( T \), and thus the size of the resulting instance is at most \( (D|S|)^{|S|} \). Then the number of nulls created is at most \( D|S|^{|\Pi|} \).

We can then continue the argument in the proof of Theorem 4 except that instead of querying the minimal instance of the SKB we query the naive table resulting out of removing tuples with conditions from \( T \). Since we now have a doubly-exponential number of elements, sequences may be of double exponential size (unless the number of procedures is fixed), from which the \( \mathsf{N2Exptime} \) follows.