### WHEN CAN WE ANSWER QUERIES USING RESULT-BOUNDED DATA INTERFACES?

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ABSTRACT. We consider answering queries on data available through *access methods*, that provide lookup access to the tuples matching a given binding. Such interfaces are common on the Web; further, they often have *bounds* on how many results they can return, e.g., because of pagination or rate limits. We thus study *result-bounded methods*, which may return only a limited number of tuples. We study how to decide if a query is *answerable* using result-bounded methods, i.e., how to compute a *plan* that returns all answers to the query using the methods, assuming that the underlying data satisfies some integrity constraints. We first show how to reduce answerability to a query containment problem with constraints. Second, we show "schema simplification" theorems describing when and how result-bounded services can be used. Finally, we use these theorems to give decidability and complexity results about answerability for common constraint classes.

### 1. INTRODUCTION

Web services expose programmatic interfaces to data. Many of these services can be modeled as an *access method*: given a set of arguments for some attributes of a relation, the method returns all matching tuples for the relation.

**Example 1.1.** Consider a Web service that exposes university employee information. The schema has a relation Prof(id, name, salary) and an access method pr on this relation: the input to pr is the *id* of a professor, and an access to this method returns the *name* and *salary* of the professor. The schema also has a relation Udirectory(*id*, *address*, *phone*), and an access method ud: it has no input and returns the *id*, *address*, and *phone* of all university employees.

Our goal is to answer queries using such services. In the setting of Example 1.1, the user queries are posed on the relations Prof and Udirectory, and we wish to answer them using the methods pr and ud. To do so, we can exploit *integrity constraints* that the data is known to satisfy: for instance, the referential constraint  $\tau$  that says that the *id* of every tuple in Prof is also in Udirectory.



**Example 1.2.** Consider  $Q_1(n) : \exists i \operatorname{Prof}(i, n, 10000)$ , the query that asks for the names of professors with salary 10000. If we assume the integrity constraint  $\tau$ , we can implement  $Q_1$  as the following *plan*: first access ud to get the set of all ids, and then access pr with each id to obtain the salary, filtering the results to return only the names with salary 10000. This plan *reformulates*  $Q_1$  over the access methods: it is equivalent to  $Q_1$  on all instances satisfying  $\tau$ , and it only uses pr and ud to access Prof and Udirectory.

Prior work (e.g., [DLN07, BtCT16]) has formalized this reformulation task as an *an-swerability* problem: given a schema with access methods and integrity constraints, and given a query, determine if we can answer the query using the methods. The query has to be answered in a *complete* way, i.e., without missing any results. This prior work has led to implementations (e.g., [BLT14, BLT15, BLT16]) that can determine how to evaluate a conjunctive query using a collection of Web services, by generating a plan that makes calls to the services.

However, all these works assume that when we access a Web service, we always obtain *all* tuples that match the access. This is not realistic: to avoid wasting resources and bandwidth, virtually all Web services impose a *limit* on how many results they will return. For instance, the ChEBI service (chemical entities of biological interest, see [BLT16]) limits the output of lookup methods to 5000 entries, while IMDb's web interfaces impose a limit of 10000 [IMD17]. With some services, we can request more results beyond the limit, e.g., using pagination or continuation tokens, but there is often a *rate limitation* on how many requests can be made [Fac17, Git17, Twi17], which also limits the total number of obtainable results. Thus, for many Web services, beyond a certain number of results, we cannot assume that all matching tuples are returned. In this work, we introduce *result-bounded* methods to reason on these services.

**Example 1.3.** The ud method in Example 1.1 may have a result bound, e.g., it may return at most 100 entries. If this is the case, then the plan of Example 1.2 is not equivalent to  $Q_1$  as it may miss some result tuples.

Result-bounded methods make it very challenging to reformulate queries. Indeed, they are *nondeterministic*: if the number of results is more than the result bound, then the Web service only returns a subset of results, usually according to unknown criteria. For this reason, it is not even clear whether result-bounded methods can be useful at all to answer queries in a complete way. However, this may be the case:

**Example 1.4.** Consider the schema of Example 1.1 and assume that ud has a result bound of 100 as in Example 1.3. Consider the query  $Q_2 : \exists i \, a \, p$  Udirectory(i, a, p) asking if there is *some* university employee. We can answer  $Q_2$  with a plan that accesses the ud method and returns true if the output is non-empty. It is not a problem that ud may omit some result tuples, because we only want to know if it returns something. This gives a first intuition: result-bounded methods are useful to check for the existence of matching tuples.

Further, result-bounded methods can also help under integrity constraints such as keys or functional dependencies:

**Example 1.5.** Consider the schema of Example 1.1 and the access method  $ud_2$  on Udirectory that takes an *id* as input and returns the *address* and phone number of tuples with this *id*. Assume that  $ud_2$  has a result bound of 1, i.e., returns at most one answer when given an *id*. Further assume the functional dependency  $\phi$ : each employee id has exactly one *address* 

(but possibly many phone numbers). Consider the query  $Q_3$  asking for the address of the employee with id 12345. We can answer  $Q_3$  by calling ud<sub>2</sub> with 12345 and projecting onto the *address* field. Thanks to  $\phi$ , we know that the result will contain the employee's address, even though only one of the phone numbers will be returned. This gives a second intuition: result-bounded methods are useful when there is a functional dependency that guarantees that some projection of the output is complete.

In this paper, we study how and when we can use result-bounded methods to reformulate queries and obtain complete answers, formalizing in particular the intuition of Examples 1.4 and 1.5. We then show decidability and complexity results for the answerability problem. We focus on two common classes of integrity constraints on databases: *inclusion dependencies* (IDs), as in Example 1.4, and *functional dependencies* (FDs), as in Example 1.5. But we also show results for more expressive constraints: see Table 1 for a summary.

The first step of our study (Section 4) is to reduce the answerability problem to *query* containment under constraints. Such a reduction is well-known in the context of reformulating queries over views [NSV10], and of answering queries with access methods without result bounds [BtCLT16]. But the nondeterminism of result-bounded methods means that we cannot apply these results directly. We nevertheless show that this reduction technique can still be applied in the presence of result bounds. This reduction does not suffice to solve the problem, because the resulting query containment problem involves complex cardinality constraints, so it does not immediately lead to decidability results.

Our second step (Section 5) is to show schema simplification results, which explain why some of the result bounds can be ignored for the answerability problem. These results characterize how result-bounded methods are useful: they capture and generalize the examples above. For instance, we show that for constraints consisting of IDs, result-bounded methods are only useful as an existence check as in Example 1.4. We also show that, for FD constraints, result-bounded methods are only useful to access the functionally-determined part of the output, as in Example 1.5. The proofs utilize a technique of blowing up models, i.e., we enlarge them to increase the number of outputs of an access, without violating constraints or changing query answers. The simplest version of this technique is to show limitations on which queries can be answered with result bounds in the presence of constraints in first-order logic without equality (Theorem 7.3). This result has some broad similarity to classical finite model theory results on limitations of first-order logic. We will show that the blowing-up method can yield similar limitations even in the presence of equality.

Third, in Section 6, we use the simplification results to deduce that answerability is decidable for these constraint classes, and show tight complexity bounds: we show NP-completeness for constraints consisting of FDs, and EXPTIME-completeness for IDs. We refine the latter result to show that answerability is NP-complete for *bounded-width* IDs, which export only a constant number of variables. We prove this using ideas of Johnson and Klug [JK84], along with a *linearization* technique, extending ideas introduced in [GMP14]: we show how the constraints used to reason about answerability can be "simulated" with restricted inclusion dependencies, and that analyzing this simulation gives finer complexity bounds.

In Section 7, we study more expressive constraint classes, beyond IDs and FDs. We do so using a weaker form of simplification, called *choice simplification*, which replaces all result bounds by 1: this intuitively implies that the number of results does not matter. We show that it suffices to consider the choice simplification for a huge class of constraints, including all TGDs, and also constraints combining FDs and IDs. In Section 8, we use this technique

Fragment	Simplification	Complexity
IDs	Existence-check (Thm 5.2)	EXPTIME-complete (Thm 6.3)
Bounded-width IDs	Existence-check (see above)	NP-complete (Thm 6.4)
FDs	FD (Thm $5.5$ )	NP-complete (Thm $6.2$ )
FDs and UIDs	Choice $(Thm 7.4)$	NP-hard (see above) and in 2EXPTIME (Thm 8.2)
Equality-free FO	Choice $(Thm 7.3)$	Undecidable (Proposition 9.2)
Frontier-guarded TGDs	Choice (see above)	2EXPTIME-complete (Thm 8.1)

Table 1: Simplifiability and complexity results for monotone answerability

to show that decidability of answerability holds much more broadly: in particular it holds for a wide range of classes where query containment is decidable. We conclude the paper by giving some limits to schema simplification and decidability of answerability (Section 9), followed by conclusions (Section 10). In particular, we explain in the conclusions how our results on answerability extend to the practically relevant problem of *extracting a plan* in the case where one exists.

This article is based on the conference paper [AB18a]. In addition to providing full proofs for the major results of [AB18a], in the appendix to this work we give a number of supplementary results, showing the generality of the methods. We do not include all results claimed in the conference paper. In particular, the conference paper claims results also for the finite variant of the answerability problem with result bounds. While we believe these results hold, the proofs in the submission are flawed, and thus we make no such claims in this work, dealing only with the unrestricted variant.

### 2. Related Work

Our paper relates to a line of work about finding plans to answer queries using access methods. The initial line of work considered finding equivalent "executable rewritings" conjunctive queries where the atoms are ordered in a way compatible with the access patterns. This was studied first without integrity constraints [LC01a, Li03], and then with disjunctive TGD constraints [DLN07]. Later [BtCT16, BtCLT16] formulated the problem of finding a *plan* that answers the query over the access patterns, distinguishing two notions of plans with access methods: one with arbitrary relational operators in middleware and another without the difference operator. They studied the problem of getting plans of both types in the presence of integrity constraints: following [DLN07], they reduced the search for executable rewritings to query containment under constraints. Further, [BtCT16, BtCLT16] also related the reduction to a semantic notion of determinacy, originating from the work of Nash, Segoufin, and Vianu [NSV10] in the context of views. Our paper extends the reduction to query containment in the presence of result bounds, relying heavily on the techniques of [DLN07, NSV10, BtCT16, BtCLT16].

Non-determinism in query languages has been studied in other contexts [AV91, ASV90]. However, the topic of this work, namely, using non-deterministic Web services to implement deterministic queries, has not been studied. Result bounds are reminiscent of *cardinality constraints*, for which the answerability problem has been studied [FGC<sup>+</sup>15]. However, the two are different: whereas cardinality constraints restrict the *underlying data*, result bounds concern the *access methods* to the data, and makes them *non-deterministic*: this has not been studied in the past. In fact, surprisingly, our schema simplification results (in Sections 5

and 7) imply that answerability with result bounds can be decided *without* reasoning about cardinality constraints at all.

To study our new setting with result-bounded methods, we introduce several specific techniques to reduce to a decidable query containment problem, e.g., determinacy notions for non-deterministic services and the technique of "blowing up models". The additional technical tools needed to bound the complexity of our problems revolve around analysis of the chase. While many components of this analysis are specific to the constraints produced by our problem, our work includes a *linearization* method, which we believe is of interest in other settings. Linearization is a technique from [GMP14], which shows that certain entailment problems can be reduced to entailment of queries from linear TGDs. We refine this to show that in certain cases we can reduce to entailments involving a restricted class of linear TGDs, where more specialized bounds [JK84] can be applied.

### 3. Preliminaries

**Data and queries.** We consider a relational signature S that consists of a set of relations with an associated arity (a positive integer) and of a finite set of constants. The positions of a relation R of S are  $1 \ldots n$  where n is the arity of R. An instance of R is a set of n-tuples (finite or infinite), and an instance I of S consists of instances for each relation of S, along with a mapping from the constants of the signature to the active domain Adom(I) of I, i.e., the set of all the values that occur in facts of I. Note that this means that two signature constants can be interpreted by the same element. We can equivalently see I as a set of facts  $R(a_1 \ldots a_n)$  for each tuple  $(a_1 \ldots a_n)$  in the instance of each relation R, along with the mapping of constants. A subinstance I' of I is an instance that contains a subset of the facts of I, and I is then a superinstance of I'.

We will study conjunctive queries (CQs), which are logical expressions of the form  $\exists x_1 \ldots x_k \ (A_1 \land \cdots \land A_m)$ , where the  $A_i$  are relational atoms of the form  $R(t_1 \ldots t_n)$ , with R being a relation of arity n and  $t_1 \ldots t_n$  being either variables from  $x_1 \ldots x_k$  or constants. A CQ is Boolean if it has no free variables. A Boolean CQ Q holds in an instance I exactly when there is a homomorphism of Q to I: a mapping h from the variables and constants of Q to Adom(I) which is the identity on constants and which ensures that, for every atom  $R(x_1 \ldots x_n)$  in Q, the atom  $R(h(x_1) \ldots h(x_n))$  is a fact of I. We let Q(I) be the output of Q on I, defined in the usual way: if Q is Boolean, the output is true if the query holds and false otherwise. A union of conjunctive queries (UCQ) is a disjunction of CQs.

**Integrity constraints.** An *integrity constraint* is a restriction on instances: that is, a function mapping every instance of a given schema to a Boolean. When we say that an instance *satisfies* a constraint, we just mean that the function evaluates to true. As concrete syntax for constraints we use fragments of first-order logic (FO), with the active-domain semantics, and disallowing constants. The active-domain semantics can be enforced syntactically, e.g., by restricting first-order logic formulas to always quantify over elements that appear in some relation. In the few cases in this paper where we talk about FO integrity constraints, we will always mean a constraint in such a restricted fragment. With such a restriction, the truth value of an FO integrity constraint on an instance is well-defined. For most of our results we focus on *tuple-generating dependencies* (TGDs) and *functional dependencies* (FDs), which we now review.

A tuple-generating dependency (TGD) is an FO sentence  $\tau$  of the form:  $\forall \vec{x} \ (\phi(\vec{x}) \rightarrow \exists \vec{y} \ \psi(\vec{x}, \vec{y}))$  where  $\phi$  and  $\psi$  are conjunctions of relational atoms:  $\phi$  is the body of  $\tau$  while  $\psi$  is the head. For brevity, in the sequel, we will omit outermost universal quantifications in TGDs. The exported variables of  $\tau$  are the variables of  $\vec{x}$  which occur in the head. A full TGD is one with no existential quantifiers in the head. A guarded TGD (GTGD) is a TGD where  $\phi$  is of the form  $A(\vec{x}) \wedge \phi'(\vec{x})$  where A is a relational atom (called the guard) containing all free variables of  $\phi'$ , while a frontier-guarded TGD (FGTGD) is one where there is a conjunct A of  $\phi$  containing all the exported free variables. An inclusion dependency (ID) is a GTGD where both  $\phi$  and  $\psi$  consist of a single atom with no repeated variables. The width of an ID is the number of exported variables, and an ID is unary (written UID) if it has width 1. For example,  $R(x, y) \rightarrow \exists z w \ S(z, y, w)$  is a UID.

A functional dependency (FD) is an FO sentence  $\phi$  written as  $\forall \vec{x} \ \vec{y} \ (R(x_1 \dots x_n) \land R(y_1 \dots y_n) \land (\bigwedge_{i \in D} x_i = y_i) \to x_j = y_j)$ , with  $D \subseteq \{1 \dots n\}$  and  $j \in \{1 \dots n\}$ , Intuitively,  $\phi$  asserts that position j is determined by the positions of D, i.e., when two R-facts match on the positions of D, they must match on position j as well. We write  $\phi$  as  $D \to j$  for brevity. The positions in D are the determinant of  $\phi$  and j the determined position of  $\phi$ .

Query and access model. We model a collection of Web services as a service schema Sch, which we simply call a *schema*. It consists of:

- (1) a relational signature  $\mathcal{S}$ ;
- (2) a set of integrity constraints  $\Sigma$  given as FO sentences; and
- (3) a set of access methods (or simply methods).

Each access method mt is associated with a relation R and a subset of positions of R called the *input positions* of mt. The other positions of R are called *output positions* of mt.

In this work, we allow each access method to have an optional result bound. We study two kinds of result bounds. Result upper bounds assert that mt returns at most k matching tuples for some  $k \in \mathbb{N}$ . Result lower bounds assert that, for some  $k \in \mathbb{N}$ , the method mt returns all matching tuples if there are no more than k of them, and otherwise returns at least k of the matching tuples. We call mt a result-bounded method associated to  $k \in \mathbb{N}$  if it has both a result lower bound and a result upper bound for k. We say that mt has no result bound if it has neither a result lower bound nor a result upper bound. In the schemas that we will consider, we will assume that every access method is either result-bounded or has no result bound; but we will quickly show a technical result asserting that it is sufficient to consider result lower bounds.

An access on an instance I is a method mt on a relation R with a binding AccBind for I: the binding is a mapping from the input positions of mt to values in Adom(I). The matching tuples M of the access (mt, AccBind) are the tuples for relation R in I that match AccBind on the input positions of R, and an output of the access is a subset  $J \subseteq M$ . We will sometimes also refer to the matching facts of the access, i.e.,  $R(\vec{t})$  where  $\vec{t}$  is a matching tuple. If the method has no result bound, then there is only one valid output to the access, namely, the output J := M that contains all matching tuples of I. If there is a result bound k on mt, then we define the notion of a valid output to the access as any subset  $J \subseteq M$  such that:

- (i) J has size at most k;
- (ii) for any  $j \leq k$ , if I has  $\geq j$  matching tuples, then J has size  $\geq j$ . Formally, if  $|M| \geq j$  then  $|J| \geq j$ .

If there is a result lower bound of k on mt, then a valid output is any subset  $J \subseteq M$  satisfying point (ii) above, and similarly for a result upper bound.

We give specific names to two kinds of methods. A method is *input-free* if it has no input positions. A method is *Boolean* if all positions are input positions. Note that accessing a Boolean method with a binding AccBind just checks if AccBind is in the relation associated to the method (and result bounds have no effect).

**Plans.** We use *plans* to describe programs that use the access methods, formalizing them using the terminology of [BtCT16, BtCLT16]. In the body of the paper we will deal with *monotone plans*, which are called this way because they define transformations that are monotone as the set of facts in an input instance grows. In the appendix we will extend our study to so-called *RA plans*, which define transformations that are not necessarily monotone. RA plans and their relationship to monotone plans are described in Appendix D.

The monotone relational algebra operators are:

- the product operator (×), taking as input two relation instances of arities m and n and returning a relation instance of arity m + n;
- the union operator  $(\cup)$ , taking as input two relation instances of the same arity m and returning a relation instance of arity m;
- the projection operators  $\pi_A$ , where A is a finite set of positions, taking as input a relation instance of some fixed arity m and returning the instance containing, for each m-tuple  $\bar{t}$  in the input, the |A|-tuple formed from restricting  $\bar{t}$  to positions in A.
- the selection operator  $(\sigma_c)$ , taking as input a relation of some arity m and returning a relation instance of the same arity m, where c is an equality or inequality comparing two positions  $1 \le i \le m$  or comparing a position with a constant.

The semantics of these operators are standard [AHV95]. A monotone relational algebra expression is a term built up by composing these operators. Monotone relational algebra expressions define the same class of queries as positive first-order logic — that is, first-order logic built up from relational atoms and inequalities using the connectives  $\land, \lor$  and existential quantification — under the active-domain semantics.

A monotone plan PL is a sequence of commands that produce temporary tables. There are two types of commands:

- Query middleware commands, of the form T := E, with T a temporary table and E a monotone relational algebra expression over the temporary tables produced by previous commands.
- Access commands, written  $T \Leftarrow_{\mathsf{OutMap}} \mathsf{mt} \Leftarrow_{\mathsf{InMap}} E$ , where E is a monotone relational algebra expression over previously-produced temporary tables,  $\mathsf{InMap}$  is an *input mapping* from the output attributes of E to the input positions of  $\mathsf{mt}$ ,  $\mathsf{mt}$  is a *method* on some relation R,  $\mathsf{OutMap}$  is an *output mapping* from the positions of R to those of T, and T is a temporary table. We often omit the mappings for brevity.

The *output table*  $T_0$  of PL is indicated by a special command Return  $T_0$  at the end, with  $T_0$  being a temporary table.

We must now define the semantics of PL on an instance I. Because of the nondeterminism of result-bounded methods, in this work we will do so relative to an *access* selection for Sch on I, i.e., a function  $\sigma$  mapping each access (mt, AccBind) on I to a set of facts  $J := \sigma(\text{mt}, \text{AccBind})$  that match the access. We say that the access selection is *valid* if it maps every access to a valid output: intuitively, the access selection describes which valid output is chosen when an access to a result-bounded method matches more tuples than the bound. Note that the definition implies that performing the same access twice must return the same result; however, all our results still hold without this assumption (see Appendix A).

For every valid access selection  $\sigma$ , we can now define the semantics of each command of PL for  $\sigma$  by considering them in order. For an access command  $T \leftarrow_{\mathsf{OutMap}} \mathsf{mt} \leftarrow_{\mathsf{InMap}} E$  in PL, we evaluate E to get a collection C of tuples. For each tuple  $\vec{t}$  of C, we use InMap to turn it into a binding AccBind, and we perform the access on  $\mathsf{mt}$  to obtain  $J_{\vec{t}} := \sigma(\mathsf{mt}, \mathsf{AccBind})$ . We then take the union  $\bigcup_{\vec{t} \in C} J_{\vec{t}}$  of all outputs, rename it according to  $\mathsf{OutMap}$ , and write it in T. For a middleware query command T := E, we evaluate E and write the result in T. The *output* of PL on  $\sigma$  is then the set of tuples that are written to the output table  $T_0$ .

The possible outputs of PL on I are the outputs that can be obtained with some valid access selection  $\sigma$ . Intuitively, when we evaluate PL, we can obtain any of these outputs, depending on which valid access selection  $\sigma$  is used.

**Example 3.1.** The plan of Example 1.4 is as follows:

 $T \Leftarrow \mathsf{ud} \Leftarrow \emptyset;$   $T_0 := \pi_{\emptyset} T;$  Return  $T_0;$ 

The first command runs the relational algebra expression  $E = \emptyset$  returning the empty set, giving a trivial binding for ud. The result of accessing ud is stored in a temporary table T. The second command projects T to the empty set of attributes, and the third command returns the result. For every instance I, the plan has only one possible output (no matter the access selection), describing if Udirectory is empty in I. We will say that the plan *answers* the query  $Q_2$  of Example 1.4.

Answerability. Let Sch be a schema consisting of a relational signature, integrity constraints, and access methods, and let Q be a CQ over the relational signature of Sch. A monotone plan PL answers Q under Sch if the following holds: for all instances I satisfying the constraints, PL on I has exactly one possible output, which is the query output Q(I). In other words, this is the standard definition of answerability, requiring that the output of PL on I is equal to Q(I), but we have extended it to our setting of result-bounded methods by requiring that this holds for every valid access selection  $\sigma$ . Of course, PL can have a single possible output (and answer Q) even if some intermediate command of PL has multiple possible outputs.

We say that Q is monotonically answerable under schema Sch if there is a monotone plan that answers it. Monotone answerability generalizes notions of reformulation that have been previously studied. In particular, in the absence of constraints and result bounds, it reduces to the notion of a query having an *executable rewriting with respect to access methods*, studied in work on access-restricted querying [LC01a, Li03]. In the setting where the limited interfaces simply expose views, monotone answerability corresponds to the well-known notion of *UCQ rewriting* with respect to views [LMSS95].

Query containment and chase proofs. We will reduce answerability to the standard problem of query containment under constraints. Query Q is contained in query Q' relative to constraints  $\Sigma$  if, in any instance that satisfies  $\Sigma$ , the tuples returned by Q are a subset of the tuples returned by Q'. We write  $Q \subseteq_{\Sigma} Q'$  to denote this relationship.

In the case where  $\Sigma$  consists of dependencies, query containment under constraints can be solved by the well-known method of searching for a *chase proof* [FKMP05]. We now review this notion. Such a proof starts with an instance called the *canonical database of* Q and denoted CanonDB(Q): it consists of facts for each atom of Q, and its elements are the variables and constants of Q. The proof then proceeds by *firing dependencies*, as we explain next.

A homomorphism  $\tau$  from the body of a dependency  $\delta$  into an instance  $I_0$  is called a trigger for  $\delta$ . A chase step with dependency  $\delta$  and trigger  $\tau$  on  $I_0$  transforms  $I_0$  to a new instance in the following way. If  $\delta$  is a TGD, the result of the chase step on  $\tau$  for  $\delta$  in  $I_0$  is the superinstance  $I_1$  of  $I_0$  obtained by adding new facts corresponding to an extension of  $\tau$  to the head of  $\delta$ , using fresh elements to instantiate the existentially quantified variables of the head: we denote these elements as nulls as well. The remaining elements that occur in these new facts will be said to be exported in the chase step. If  $\delta$  is an FD with  $x_i = x_j$  in the head, then a chase step yields  $I_1$  which is the result of identifying  $\tau(x_i)$  and  $\tau(x_j)$  in  $I_0$ . A chase sequence for  $\Sigma$  is a sequence of chase steps with dependencies of  $\Sigma$ , with the output of each step being the input of the next. We can thus associate each such sequence with a sequence of instances  $I_0, \ldots$ .

We will be particularly interested in sequences that form a chase proof of  $Q \subseteq_{\Sigma} Q'$ , where Q and Q' have the same free variables  $\vec{x}$ . Recall that for a query with free variables, the free variables become elements within the canonical database of the query. A chase proof of  $Q \subseteq_{\Sigma} Q'$  is a chase sequence where we start by the instance  $I_0 = \text{CanonDB}(Q)$ , which has a homomorphism from Q to  $I_0$  sending each free variable of  $\vec{x}$  to itself, and we must finish with an instance which has a homomorphism from Q', sending each free variable of  $\vec{x}$  to itself.

Chase proofs give a sound and complete method for deciding containment under dependencies:

# **Proposition 3.2** [FKMP05]. For any CQs Q and Q' and for any collection of dependencies $\Sigma$ , the containment $Q \subseteq_{\Sigma} Q'$ holds if and only if there is a chase proof that witnesses the containment.

In particular, when  $\Sigma$  is empty, we obtain the usual characterization for the containment  $Q \subseteq Q'$  without constraints: it holds if and only if there is a homomorphism from Q' to Q which is the identity on free variables.

The variant of Proposition 3.2 holds also for chase proofs based on so-called *restricted* chase sequences, which we now define. A trigger  $\tau$  for a dependency  $\delta$  is active in an instance I if it cannot be extended to a homomorphism from the head of  $\delta$  to I. In other words, an active trigger  $\tau$  witnesses the fact that  $\delta$  does not hold in I. A restricted chase sequence is one in which all chase steps have active triggers.

If all restricted chase sequences starting with a given initial instance  $I_0$  are finite, we say that the restricted chase with  $\Sigma$  terminates on that instance. In this case, we define the restricted chase of  $I_0$  with  $\Sigma$  as the result of iteratively applying all active triggers according to some arbitrary order. When  $I_0 = \text{CanonDB}(Q)$  we will talk about the restricted chase of Q.

When the phenomenon above occurs for each finite initial instance  $I_0$ , we say that  $\Sigma$  has terminating chase. If  $\Sigma$  has terminating chase we can decide if  $Q \subseteq_{\Sigma} Q'$  by computing the chase of Q with  $\Sigma$  and then searching for a homomorphism of Q' into the chase.

Even when the chase does not terminate, we define the chase of  $I_0$  with  $\Sigma$  as the infinite fixpoint of applying chase steps following some arbitrary order which is fair, i.e., ensuring that every active trigger will eventually be fired. We similarly define the restricted chase of  $I_0$  with  $\Sigma$  in the same way but with restricted chase steps. We can still use the chase and restricted chase to reason about query containment, even though it is an infinite object that cannot generally be materialized. The result is implicit in [FKMP05]; see [One13] for a more detailed exposition.

**Proposition 3.3.** For any CQs Q and Q' and for any collection of dependencies  $\Sigma$ , the containment  $Q \subseteq_{\Sigma} Q'$  holds if and only if there is a homomorphism from Q' to the chase of  $I_0 = \mathsf{CanonDB}(Q)$  with  $\Sigma$ , with the homomorphism being the identity on free variables. The same holds for the restricted chase.

Certain answer problems and TGD implication problems via the chase. We say that a set of first-order sentences  $\lambda$  entails a first-order sentence  $\rho$ , written  $\lambda \models \rho$ , if every instance satisfying  $\lambda$  also satisfies  $\rho$ . Note that a query containment  $Q \subseteq_{\Sigma} Q'$  for Boolean queries Q and Q' is a special case of an entailment, of the form  $Q \wedge \Sigma \models Q'$ .

We will also study another restricted kind of entailment problem, of the form:

$$\bigwedge_{i \le n} A_i \wedge \Sigma \models Q$$

where  $\Sigma$  is a set consisting of TGDs and FDs, each  $A_i$  is a fact, and Q is a CQ. This is the problem of *certain answers* [FKMP05] under dependencies for CQs, and we will also use it when discussing the implication of some facts from other facts and constraints in Section 6.4. We can consider a modification of the definition of chase proof to solve this problem: this is a chase sequence where we fix the initial instance to be  $\{A_1 \dots A_n\}$ , rather than the canonical database of Q. When  $\Sigma$  only contains TGDs, there are well-known reductions between the query containment problem and the certain answers problem, and in particular the analog of Proposition 3.2 holds for certain answer problems: the entailment holds iff there is a chase proof witnessing it [FKMP05]. Based on these equivalences, we freely use known upper and lower complexity bounds stated on the certain answer problem (e.g., from [CGK08, BLMS11]) and apply them to query containment under constraints.

Another special case of entailment is *entailment of a TGD*  $\tau$  by a set of TGDs  $\Sigma$ . This problem can be reduced to the query containment problem: we take the body of  $\tau$  and see if it is contained in the head of  $\tau$  relative to  $\Sigma$ . Thus chase proofs also give a complete method for deciding these entailments.

Note that the reader familiar with the treatment of chase steps involving FDs will find our discussion a bit simplified relative to standard accounts (e.g., [AHV95]). In other accounts there is the possibility that a chase step "fails", but in our setting — e.g., due to our treatment on constants and the restriction on their use in constraints — we will not need to consider this.

A set S of elements in an instance is *guarded* if there is a fact of the instance that contains all these elements. We call such an element a *guard for* S. We note that if  $\tau$  is a trigger for a guarded TGD  $\delta$ , then the image of  $\tau$  must be guarded.

Equivalent formalisms for monotone plans. Monotone plans have a number of other presentations. For instance, if there is only one access per relation, they are equivalent to *executable UCQs* which just annotate each atom of a UCQ with an access method. The semantics is just to execute the method corresponding to each atom in the order that the atoms are given, accumulating all the bindings. Executable queries were the first formalism to implement queries with access methods [Ull89, LC00, LC01b, NL04b, NL04a]. They were considered only in the case of CQs where there is a single access method, without

result bounds, for each relation symbol. The equivalence with monotone plans is proved in [BtCLT16], and extends easily to the presence of multiple access per methods, and to the presence of result bounds with any of the semantics we consider in this work.

**Example 3.4.** Let us consider the plan mentioned in Example 1.2. In our monotone plan syntax it would be written as

 $T \leftarrow \mathsf{ud} \leftarrow \emptyset;$   $T_0 \leftarrow \mathsf{pr} \leftarrow T;$   $T_1 := \pi_{name} \sigma_{salary=10000} T_0;$  Return  $T_1$ 

As an executable CQ, this would be expressed simply as

Udirectory(*id*), Prof(*id*, name, 10000)

Variations of answerability. So far, we have defined monotone answerability. An alternative notion is RA answerability, defined using RA plans that allow arbitrary relational algebra expressions in commands. We think this notion is less natural for CQs and for the class of constraints that we consider. Indeed, CQs are monotone: if facts are added to an instance, the output of a CQ cannot decrease. Thus the bulk of prior work on implementing CQs over restricted interfaces, both in theory [LMSS95, DLN07, LC01a, Li03, RPAS20b] and in practice [ICDK14, DPT06, RPAS20a], has focused on monotone implementations, often phrased in terms of the executable query syntax mentioned above. In fact, even in the setting of views, it was initially assumed that if a CQ can be answered at all, it must have a monotone plan [SV05, LMSS95]. Clever counterexamples to this fact were only found much later [NSV10]. In the body of the paper, we follow the earlier tradition and we focus exclusively on monotone plans. Nevertheless, many of our results extend to answerability with RA plans (see Appendix D). For instance, we can sometimes show that monotone answerability and RA answerability coincide. We discuss the status of monotone vs relational algebra plans further in Section 10.

### 4. Reducing to Query Containment

We start our study of the monotone answerability problem by reducing it to query containment under constraints, defined in the previous section. We explain in this section how this reduction is done. It extends the approach of [DLN07, BtCT16, BtCLT16] to result bounds, and follows the connection between answerability and determinacy notions of [NSV10, BtCLT16]. To design this reduction, we will need to show that monotone answerability is equivalent to a notion of access monotonic-determinacy, already studied in the literature for access methods without result bounds, which we extend to our setting with result bounds. This characterization (Theorem 4.3) will be used many times in the sequel.

4.1. Access Monotone Determinacy and Equivalence to Monotone Rewritability. The query containment problem corresponding to monotone answerability will capture the idea that if an instance  $I_1$  satisfies a query Q and another instance  $I_2$  has more "accessible data" than  $I_1$ , then  $I_2$  should satisfy Q as well. Here the accessible data means the data that can be retrieved by iteratively performing accesses. The motivation is that if we have a monotone plan and the accessible data increases, then the output of the plan can only increase. We will first define accessible data via the notion of accessible part. We use this to formalize the previous idea as access monotonic-determinacy, and as we claimed we show

that it is equivalent to monotone answerability (Theorem 4.3). Using access monotonicdeterminacy we show that we can simplify the result bounds of arbitrary schemas, and restrict to *result lower bounds* throughout this work. We close the section by showing how to rephrase access monotonic-determinacy with result lower bounds as query containment under constraints.

Accessible parts. We first formalize the notion of "accessible data". Given a schema Sch with methods that may have result lower bounds and also result upper bounds, along with an instance I, an *accessible part* of I is any subinstance obtained by iteratively making accesses until we reach a fixpoint. Formally, we define an accessible part by choosing an access selection  $\sigma$  which is valid for the upper and lower bounds and inductively defining sets of facts AccPart<sub>i</sub>( $\sigma$ , I) and sets of values accessible<sub>i</sub>( $\sigma$ , I) by:

 $\begin{aligned} \mathsf{AccPart}_0(\sigma, I) &:= \emptyset \text{ and } \mathsf{accessible}_0(\sigma, I) := \emptyset \\ \mathsf{AccPart}_{i+1}(\sigma, I) &:= \bigcup_{\substack{\mathsf{mt method}, \\ \mathsf{AccBind binding with values in } \mathsf{accessible}_i(\sigma, I) \\ \mathsf{accessible}_{i+1}(\sigma, I) &:= \mathsf{Adom}(\mathsf{AccPart}_{i+1}(\sigma, I)) \end{aligned}$ 

These equations define by mutual induction the set of values (accessible) that we can retrieve by iterating accesses and the set of facts (AccPart) that we can retrieve using those values.

The accessible part under  $\sigma$ , written AccPart $(\sigma, I)$ , is then defined as  $\bigcup_i \text{AccPart}_i(\sigma, I)$ . As the equations are monotone, this fixpoint is reached after finitely many iterations if I is finite, or as the union of all finite iterations if I is infinite. When there are no result bounds, there is only one valid access selection  $\sigma$ , so only one accessible part: it intuitively corresponds to the data that can be accessed using the methods. In the presence of result bounds, there can be many accessible parts, depending on  $\sigma$ , and thus we refer to "an accessible part of instance I" to mean an accessible part for some selection function.

Access monotonic-determinacy. We now formalize the idea that a query Q is "monotone under accessible parts". Let  $\Sigma$  be the integrity constraints of Sch. We call Q access monotonically-determined in Sch (or AMonDet, for short), if for any two instances  $I_1$ ,  $I_2$ satisfying  $\Sigma$ , if there is an accessible part of  $I_1$  that is a subset of an accessible part of  $I_2$ , then  $Q(I_1) \subseteq Q(I_2)$ . Note that when there are no result bounds, there is a unique accessible part of  $I_1$  and of  $I_2$ , and AMonDet says that when the accessible part grows, then Q grows.

In the sequel, it will be more convenient to use an alternative definition of AMonDet, based on the notion of *access-valid* subinstances. A subinstance  $I_{\text{Accessed}}$  of  $I_1$  is *access-valid* in  $I_1$  for Sch if, for any access (mt, AccBind) performed with a method mt of Sch and with a binding AccBind whose values are in  $I_{\text{Accessed}}$ , there is a set J of matching tuples in  $I_{\text{Accessed}}$ such that J is a valid output to the access (mt, AccBind) in  $I_1$ . In other words, for any access performed on  $I_{\text{Accessed}}$ , we can choose an output in  $I_{\text{Accessed}}$  which is also a valid output to the access in  $I_1$ . We can use this notion to rephrase the definition of AMonDet to talk about a common subinstance of  $I_1$  and  $I_2$  that is access-valid:

**Proposition 4.1.** For any schema Sch with arbitrary constraints  $\Sigma$  and methods that can have result lower bounds and result upper bounds, a CQ Q is AMonDet if and only if the following implication holds: for any two instances  $I_1$ ,  $I_2$  satisfying  $\Sigma$ , if  $I_1$  and  $I_2$  have a common subinstance  $I_{\text{Accessed}}$  that is access-valid in  $I_1$ , then  $Q(I_1) \subseteq Q(I_2)$ . To show this, it suffices to show that the two definitions of "having more accessible data" agree. Proposition 4.1 follows immediately from the following proposition:

**Proposition 4.2.** The following are equivalent:

- (i)  $I_1$  and  $I_2$  have a common subinstance  $I_{\text{Accessed}}$  that is access-valid in  $I_1$ .
- (ii) There are  $A_1 \subseteq A_2$  such that  $A_1$  is an accessible part for  $I_1$  and  $A_2$  is an accessible part for  $I_2$ .

Proof. Suppose  $I_1$  and  $I_2$  have a common subinstance  $I_{\text{Accessed}}$  that is access-valid in  $I_1$ . Since  $I_{\text{Accessed}}$  is access-valid in  $I_1$  there is an access selection  $\sigma_1$  which maps any access performed with values of  $I_{\text{Accessed}}$  to some set of matching tuples in  $I_{\text{Accessed}}$ , with  $\sigma_1$  valid in  $I_1$ . We can extend  $\sigma_1$  to be valid in  $I_1$  by choosing tuples arbitrarily for accesses with bindings not in  $I_{\text{Accessed}}$ . We then extend  $\sigma_1$  to an access selection  $\sigma_2$  which returns a superset of the tuples returned by  $\sigma_1$  for accesses with values of  $I_{\text{Accessed}}$ , and returns an arbitrary set of tuples from  $I_2$  otherwise, such that this output to the access is valid in  $I_2$ . We only need to modify  $\sigma_1$  when the full set of matching tuples in  $I_2$ : in this case we just add enough matching tuples from  $I_2$  to achieve the upper bound, or add all the matching tuples in  $I_2$  if the number is still within the method's upper bound. This ensures that  $\text{AccePart}(\sigma_1, I_1) \subseteq \text{AccPart}(\sigma_2, I_2)$ , so that (i) implies (ii).

Conversely, assuming point (ii), let  $\sigma_1$  and  $\sigma_2$  be the access selections used to define the accessible parts  $A_1$  and  $A_2$ , so that  $\mathsf{AccPart}(\sigma_1, I_1) \subseteq \mathsf{AccPart}(\sigma_2, I_2)$ . Let  $I_{\mathsf{Accessed}} :=$  $\mathsf{AccPart}(\sigma_1, I_1)$ , and let us show that  $I_{\mathsf{Accessed}}$  is a common subinstance of  $I_1$  and  $I_2$  that is access-valid in  $I_1$ . By definition, we know that  $I_{\mathsf{Accessed}}$  is a subinstance of  $I_1$ , and by assumption we have  $I_{\mathsf{Accessed}} \subseteq A_2 \subseteq I_2$ , so indeed  $I_{\mathsf{Accessed}}$  is a common subinstance of  $I_1$  and  $I_2$ . Now, to show that it is access-valid in  $I_1$ , consider any access (mt,  $\mathsf{AccBind}$ ) with values in  $I_{\mathsf{Accessed}}$ . We know that there is i such that  $\mathsf{AccBind}$  is in the domain of  $\mathsf{AccPart}_i(\sigma_1, I_1)$  that is in  $\mathsf{accessible}_i(I_1)$ . So by definition of the fixpoint process and of the access selection  $\sigma_1$ there is a valid output that is a subset of the facts within  $\mathsf{AccPart}_{i+1}(\sigma_1, I_1)$ , hence a subset of the facts within  $I_{\mathsf{Accessed}}$ . Thus,  $I_{\mathsf{Accessed}}$  is access-valid. This shows the converse implication, and concludes the proof.

The alternative definition of AMonDet in Proposition 4.1 is more convenient, because it only deals with a subinstance of  $I_1$  and not with accessible parts. Thus, we will use this characterization of monotone answerability in the rest of this paper. Now, the usefulness of AMonDet is justified by the following result:

**Theorem 4.3.** For any CQ Q and schema Sch containing only constraints in active-domain first-order logic, with access methods that may have result upper and lower bounds, the following are equivalent:

- (1) Q is monotonically answerable w.r.t. Sch.
- (2) Q is AMonDet over Sch.

Without result bounds, this equivalence of monotone answerability and access monotonicdeterminacy is proven in [BtCT16, BtCLT16], using a variant of Craig's interpolation theorem. Theorem 4.3 shows that the equivalence extends to schemas with result bounds.

We now begin the proof of Theorem 4.3, which will use Proposition 4.1. We first prove the "easy direction":

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**Proposition 4.4.** Assume that our schema has arbitrary constraints along with methods that may have both upper and lower bounds. If a CQ Q has a (monotone) plan PL that answers it w.r.t. Sch, then Q is AMonDet over Sch.

Proof. We use the definition of AMonDet given in Proposition 4.1. Assume that there are two instances  $I_1, I_2$  satisfying the constraints of Sch and that there is a common subinstance  $I_{\text{Accessed}}$  that is access-valid in  $I_1$ . Let us show that  $Q(I_1) \subseteq Q(I_2)$ . As  $I_{\text{Accessed}}$  is access-valid, let  $\sigma_1$  be a valid access selection for  $I_{\text{Accessed}}$ : for any access with values in  $I_{\text{Accessed}}$ , the access selection  $\sigma_1$  returns an output which is valid in  $I_{\text{Accessed}}$ . We extend  $\sigma_1$  to a valid access selection for  $I_2$  as in the proof of Proposition 4.1: for accesses in  $I_{\text{Accessed}}$ , the access selection  $\sigma_2$ returns a superset of  $\sigma_1$ , which is possible because  $I_{\text{Accessed}} \subseteq I_2$ , and for other accesses it returns some valid subset of tuples of  $I_2$ .

We argue that for each temporary table of PL, its value when evaluated on  $I_1$  with  $\sigma_1$ , is contained in its value when evaluated on  $I_2$  with  $\sigma_2$ . We prove this by induction on PL. As the plan is monotone, the property is preserved by query middleware commands, so inductively it suffices to look at an access command  $T \leftarrow \mathsf{mt} \leftarrow E$  with  $\mathsf{mt}$  an access method on some relation R. Let  $E_1$  be the value of E when evaluated on  $I_1$  with  $\sigma_1$ , and let  $E_2$  be the value when evaluated on  $I_2$  with  $\sigma_2$ . Then by the monotonicity of the query E and the induction hypothesis, we have  $E_1 \subseteq E_2$ . Now, given a tuple  $\vec{t}$  in  $E_1$ , let  $M_{\vec{t}}^1$  be the set of tuples selected by  $\sigma_1$  for the access with  $\mathsf{mt}$  using  $\vec{t}$  in  $I_1$ . Similarly let  $M_{\vec{t}}^2$  be the set selected by  $\sigma_2$  in  $I_2$ . By construction of  $\sigma_2$ , we have  $M_{\vec{t}}^1 \subseteq M_{\vec{t}}^2$ , and thus  $\bigcup_{\vec{t} \in E_1} M_{\vec{t}}^1 \subseteq \bigcup_{\vec{t} \in E_1} M_{\vec{t}}^2$ , which completes the induction.

Thanks to our induction proof, we know that the output of PL on  $I_1$  with  $\sigma_1$  is a subset of the output of PL on  $I_2$  with  $\sigma_2$ . As we have assumed that PL answers Q on Sch, this means that  $Q(I_1) \subseteq Q(I_2)$ , which is what we wanted to show.

To prove the other direction of Theorem 4.3, we first recall the result that corresponds to Theorem 4.3 in the case without result upper and lower bounds:

**Theorem 4.5** [BtCLT16, BtCT16]. For any CQ Q and schema Sch (with no result bounds) whose constraints  $\Sigma$  are expressible in active-domain first-order logic, the following are equivalent:

(1) Q has a monotone plan that answers it over Sch.

(2) Q is AMonDet over Sch.

The theorem above holds even for more general relational algebra queries, but we will not require this generality in this work. Thus, for schemas without result-bounded methods, the existence of a monotone plan is the same as AMonDet, and both can be expressed as a query containment problem. It is further shown in [BtCT16] that a monotone plan can be extracted from any proof of the query containment for AMonDet. This reduction to query containment is what we will now extend to the setting with result-bounded methods. Specifically, we will lift the above result to the setting with result-bounded methods via a simple construction that allows us to rewrite away the result-bounded methods by expressing them in the constraints: we call this *axiomatizing* the result-bounded methods.

**Replacing result bounds on methods with additional constraints.** Given a schema Sch with constraints and access methods, possibly with result upper and lower bounds, we will define an auxiliary schema AxiomRB(Sch) without result bounds. The schema AxiomRB(Sch) includes the relational signature Sch, and for every method mt with result bound k on relation R we also have a new relation  $R_{mt}$  whose arity agrees with that of R. Informally,  $R_{mt}$  stores the tuples returned by the access selection for mt. The constraints include all the constraints of Sch (on the original relation names). In addition, for every method mt with input positions  $i_1 \dots i_m$  we have the following constraints, which we call axioms:

- An axiom stating that  $R_{mt}$  is a subset of R.
- If mt has a result upper bound of k, we have an axiom stating that for any binding of the input positions,  $R_{mt}$  has at most k distinct matching tuples.
- If mt has a lower bound of k then for each  $1 \le j \le k$  we have a result lower bound axiom stating that, for any values  $c_{i_1} \ldots c_{i_m}$ , if R contains at least j matching tuples (i.e., tuples  $\vec{c}$  that extend  $c_{i_1} \ldots c_{i_m}$ ), then  $R_{\rm mt}$  contains at least j such tuples.

In this schema we adjust the access methods of the original schema, removing any access method mt with a result upper or lower bound over R, and in its place adding an access method with no result bound over  $R_{mt}$ .

Given a query Q over Sch, we can consider it as a query over AxiomRB(Sch) instances by simply ignoring the additional relations.

We claim that, in considering Q over AxiomRB(Sch) rather than Sch, we do not change monotone answerability.

**Proposition 4.6.** Let Sch be a schema with active-domain first order constraints, result upper bounds and result lower bounds. For any CQ Q over Sch, there is a monotone plan that answers Q over Sch iff there is a monotone plan that answers Q over AxiomRB(Sch).

In other words, we can axiomatize result upper and lower bounds, at the cost of including new constraints.

*Proof.* Suppose that there is a monotone plan PL over Sch that answers Q. Let PL' be formed from PL by replacing every access with method mt on relation R with an access to  $R_{mt}$  with the corresponding method. We claim that PL' answers Q over AxiomRB(Sch). Indeed, given an instance I' for AxiomRB(Sch), we can drop the relations  $R_{mt}$  to get an instance I for Q, and use the relations  $R_{mt}$  to define a valid access selection  $\sigma$  for each method of Sch, and we can show that PL evaluated with  $\sigma$  over I gives the same output as PL' over I. Since the former evaluates to Q(I), so must the latter.

Conversely, suppose that there is a monotone plan  $\mathsf{PL}'$  that answers Q over  $\mathsf{AxiomRB}(\mathsf{Sch})$ . Construct  $\mathsf{PL}$  from  $\mathsf{PL}'$  by replacing accesses to  $R_{\mathsf{mt}}$  with accesses to R. We claim that  $\mathsf{PL}$  answers Q over  $\mathsf{Sch}$ . To show this, consider an instance I for  $\mathsf{Sch}$ , and a particular valid access selection  $\sigma$ , and let us show that the evaluation of  $\mathsf{PL}$  on I following  $\sigma$  correctly answers Q. We build an instance I' of  $\mathsf{AxiomRB}(\mathsf{Sch})$  by copying I and interpreting each  $R_{\mathsf{mt}}$  as follows: for each tuple  $\vec{t}$  such that  $R(\vec{t})$  holds in I, project  $\vec{t}$  on the input positions  $i_1 \ldots i_m$  of  $\mathsf{mt}$ , and include all of the outputs of this access according to  $\sigma$  in  $R_{\mathsf{mt}}$ . As the outputs of this access according to  $\sigma$  in  $R_{\mathsf{mt}}$ . As the outputs of the corresponding access on R according to  $\sigma$ . Since  $\mathsf{PL}'$  answers Q, we know that evaluating  $\mathsf{PL}'$  on I' with  $\sigma'$  yields the output Q(I') of Q on I'. Now, the definition of  $\sigma'$  ensures that the accesses made by  $\mathsf{PL}'$  on I' under  $\sigma'$  are exactly the same as those made by  $\mathsf{PL}$  on I under  $\sigma$ , and that the outputs of these accesses are the same. Thus  $\mathsf{PL}$  evaluated on I under  $\sigma$  gives the same result as  $\mathsf{PL}'$  does on I' under  $\sigma'$ , namely, Q(I'). Now, Q only uses the original relations of  $\mathsf{Sch}$ , so the definition of I' clearly implies that Q(I') = Q(I), so indeed the evaluation of PL on I under  $\sigma$  returns Q(I). As this holds for any valid access selection  $\sigma$ , we have shown that PL answers Q over Sch, the desired result.

The equivalence of a schema Sch with result bounds and its variant AxiomRB(Sch) easily extends to AMonDet.

**Proposition 4.7.** For any  $CQ \ Q$  over Sch, Q is AMonDet over AxiomRB(Sch) if and only if Q is AMonDet over Sch.

*Proof.* For the forward direction, assume Q that is AMonDet over AxiomRB(Sch), and let us show that Q is AMonDet over Sch. We use the characterization of AMonDet in terms of access-valid subinstances given in Proposition 4.1. Let  $I_1$  and  $I_2$  be instances satisfying the constraints of Sch, and let  $I_{Accessed}$  be a common subinstance of  $I_1$  and  $I_2$  which is access-valid in  $I_1$  for Sch. Let  $\sigma_1$  be a valid access selection for  $I_{\text{Accessed}}$ . As in the proof of Proposition 4.1, we can extend it to an access selection  $\sigma_2$  for  $I_2$  that ensures that every access with  $\sigma_2$ returns a superset of the tuples obtained with  $\sigma_1$ . We now extend  $I_1$  into an instance  $I'_1$ for AxiomRB(Sch) by interpreting each  $R_{mt}$  as the union of the outputs given by  $\sigma_1$  over every possible access with mt on  $I_{\text{Accessed}}$ , as in the proof of Proposition 4.6. We define  $I'_2$  from  $I_2$  and  $\sigma_2$  in the same way. As the access outputs given by  $\sigma_1$  and  $\sigma_2$  must be valid, we know that  $I'_1$  and  $I'_2$  satisfy the new constraints of AxiomRB(Sch), and clearly they still satisfy the constraints of Sch. Now extend  $I_{\text{Accessed}}$  to  $I'_{\text{Accessed}}$  by adding all  $R_{\text{mt}}$ -facts of  $I'_1$  for all mt. Clearly  $I'_{\text{Accessed}}$  is a subinstance of  $I'_1$ . It is access-valid because  $I_{\text{Accessed}}$  was access-valid. It is a subinstance of  $I'_2$  because  $I_{\text{Accessed}}$  is a subinstance of  $I'_2$  and because the  $R_{\text{mt}}$ -facts in  $I'_1$ also occur in  $I'_2$  by construction of  $\sigma_2$ . Thus, because Q is AMonDet over AxiomRB(Sch), we know that  $Q(I'_1) \subseteq Q(I'_2)$ . Now, as Q only uses the relations in Sch, we have  $Q(I_1) = Q(I'_1)$ and  $Q(I_2) = Q'(I'_2)$ , so we have shown that  $Q(I_1) \subseteq Q(I_2)$ , concluding the forward direction.

Conversely, suppose Q is AMonDet over Sch and consider instances  $I'_1$  and  $I'_2$  for AxiomRB(Sch) with valid access selections  $\sigma'_1$  and  $\sigma'_2$  giving accessible parts  $A'_1 \subseteq A'_2$ . We create an instance  $I_1$  for Sch from  $I'_1$  by dropping the relations  $R_{mt}$ , and similarly create  $I_2$  from  $I'_2$ . Clearly both satisfy the constraints of Sch. We modify  $\sigma'_1$  to obtain an access selection  $\sigma_1$  for  $I_1$ : for every access on  $I_1$  with a method mt, the output is that of the corresponding access with  $\sigma'_1$  on  $R_{mt}$ . We do the same to build  $\sigma_2$  from  $\sigma'_2$ . By the additional axioms of AxiomRB(Sch), it is clear that these access selections are valid. That is, that they return valid outputs to any access. And letting  $A_1$  and  $A_2$  be the corresponding accessible parts of  $I_1$  and  $I_2$ , it is clear that  $A_1 \subseteq A_2$ . Thus, because Q is AMonDet over Sch, we know that  $Q(I_1) \subseteq Q(I_2)$ , and again we have  $Q(I_1) = Q(I'_1)$  and  $Q(I_2) = Q(I'_2)$ . So we have  $Q(I'_1) \subseteq Q(I'_2)$ , which concludes the proof.

Putting together Proposition 4.6, Proposition 4.7 and Theorem 4.5, we have completed the proof of Theorem 4.3.

4.2. Elimination of result upper bounds. The characterization of monotone answerability in terms of AMonDet allows us to prove a key simplification in the analysis of result bounds. Recall that a result bound of k declares both an *upper bound* of k on the number of returned results, and a *lower bound* on them: for all  $j \leq k$ , if there are j matches, then j must be returned. We can show that the upper bound makes no difference for monotone answerability. Formally, for a schema Sch with integrity constraints and access methods, some of which may be result-bounded, we define the schema ElimUB(Sch). It has the same vocabulary, constraints, and access methods as in Sch. For each access method mt in Sch with result bound of k, mt has instead a *result lower bound* of k in ElimUB(Sch), i.e., mt does not impose the upper bound. We can then show:

**Proposition 4.8.** Let Sch be a schema with arbitrary constraints and access methods which may be result-bounded. A CQ Q is monotonically answerable in Sch if and only if it is monotonically answerable in ElimUB(Sch).

*Proof.* We show the result for AMonDet instead of monotone answerability, thanks to Theorem 4.3, and use Proposition 4.1. Consider arbitrary instances  $I_1$  and  $I_2$  that satisfy the constraints, and let us show that any common subinstance  $I_{\text{Accessed}}$  of  $I_1$  and  $I_2$  is access-valid in  $I_1$  for Sch iff it is access-valid in  $I_1$  for ElimUB(Sch): this implies the claimed result.

In the forward direction, if  $I_{\text{Accessed}}$  is access-valid in  $I_1$  for Sch, then clearly it is access-valid in  $I_1$  for ElimUB(Sch), as any output of an access on  $I_{\text{Accessed}}$  which is valid in  $I_1$  for Sch is also valid for ElimUB(Sch).

In the backward direction, assume  $I_{\text{Accessed}}$  is access-valid in  $I_1$  for ElimUB(Sch), and consider an access (mt, AccBind) with values of  $I_{\text{Accessed}}$ . If mt has no result lower bound, then there is only one possible output for the access, and it is also valid for Sch. Likewise, if mt has a result lower bound of k and there are  $\leq k$  matching tuples for the access, then the definition of a result lower bound ensures that there is only one possible output, which is again valid for Sch. Finally, if there are > k matching tuples for the access, we let J be a set of tuples in  $I_{\text{Accessed}}$  which is is a valid output to the access in ElimUB(Sch), and take any subset J' of J with k tuples; it is clearly a valid output to the access for Sch. This establishes the backward direction, concluding the proof.

Thanks to this, in our study of monotone answerability in the rest of the paper, we only consider result lower bounds.

4.3. Reducing to query containment. Now that we have reduced our monotone answerability problem to AMonDet, and eliminated result upper bounds, we explain how to restate AMonDet as a query containment problem, which was our original goal in this section. To do so, we will expand the relational signature. We let accessible be a new unary relation, and for each relation R of the original signature, we introduce two copies  $R_{\text{Accessed}}$  and R'with the same arity as R. Letting  $\Sigma$  be the integrity constraints in the original schema, we let  $\Sigma'$  be formed by replacing every relation R with R'. For any CQ Q, we define Q' from Qin the same way. Intuitively, R and R' represent the interpretations of the relation R in  $I_1$ and  $I_2$ ;  $R_{\text{Accessed}}$  represents the interpretation of R in  $I_{\text{Accessed}}$ ; and accessible represents the active domain of  $I_{\text{Accessed}}$ .

The AMonDet containment for Q and Sch is then the CQ containment  $Q \subseteq_{\Gamma} Q'$  for constraints  $\Gamma$  that we will define shortly. Intuitively,  $\Gamma$  will include the original constraints  $\Sigma$ , and the analogue  $\Sigma'$  of  $\Sigma$  on the relations R', to enforce that  $I_1$  and  $I_2$  both satisfy  $\Sigma$ . Further,  $\Gamma$  will include additional constraints called *accessibility axioms*. These axioms will enforce that  $I_{\text{Accessed}}$  is access-valid in  $I_1$ , i.e., that any access performed with values for  $I_{\text{Accessed}}$ returns a valid output which is in  $I_{\text{Accessed}}$ ; and enforce that  $I_{\text{Accessed}}$  is a common subinstance of  $I_1$  and  $I_2$ .

Formally,  $\Gamma$  includes the original constraints  $\Sigma$ , the constraints  $\Sigma'$  on the relations R', and the following *accessibility axioms*:

• For each method **mt** that is not result-bounded, letting R be the relation accessed by **mt**:

$$\left(\bigwedge_{i} \operatorname{accessible}(x_{i})\right) \land R(\vec{x}, \vec{y}) \to R_{\operatorname{Accessed}}(\vec{x}, \vec{y})$$

where  $\vec{x}$  denotes the input positions of **mt** in *R*.

• For each method mt with a result lower bound of k, letting R be the relation accessed by mt, for all  $j \leq k$ :

$$\left(\bigwedge_{i} \operatorname{accessible}(x_{i})\right) \land \exists^{\geq j} \vec{y} \ R(\vec{x}, \vec{y}) \to \exists^{\geq j} \vec{z} \ R_{\operatorname{Accessed}}(\vec{x}, \vec{z})$$

where  $\vec{x}$  denotes the input positions of **mt** in *R*. Note that we write  $\exists^{\geq j} \vec{y} \phi(\vec{x}, \vec{y})$  for a subformula  $\phi$  to mean that there exist at least j different values of  $\vec{y}$  such that  $\phi(\vec{x}, \vec{y})$  holds.

• For every relation R of the original signature:

$$R_{\text{Accessed}}(\vec{w}) \to R(\vec{w}) \land R'(\vec{w}) \land \bigwedge_{i} \operatorname{accessible}(w_{i}).$$

The AMonDet containment above simply formalizes the definition of AMonDet, via Proposition 4.1. The first two accessibility axioms enforce that  $I_{\text{Accessed}}$  is access-valid in  $I_1$ : for non-result-bounded methods, accesses to a method mt on a relation R return all the results, while for result-bounded methods it respects the lower bounds. The last accessibility axiom enforces that  $I_{\text{Accessed}}$  is a common subinstance of  $I_1$  and  $I_2$  and that accessible includes the active domain of  $I_{\text{Accessed}}$ . Hence, from the definitions and from Theorem 4.3 and Proposition 4.1, we have:

**Proposition 4.9.** Let Q be a CQ, and let Sch be a schema with constraints expressible in active-domain first-order logic and with access methods that may have result upper and lower bounds. Then the following are equivalent:

- Q is monotonically answerable with respect to Sch.
- Q is AMonDet over Sch.
- The AMonDet containment for Q and Sch holds.

Proof. We know by Theorem 4.3 that the first two points are equivalent, and we can further rephrase them using Proposition 4.1: Q is monotonically answerable iff whenever two instances  $I_1, I_2$  satisfying  $\Sigma$  have a common subinstance  $I_{\text{Accessed}}$  which is access-valid in  $I_1$ , then we have  $Q(I_1) \subseteq Q(I_2)$ . Assuming this, let us show that the query containment holds. Fix an instance J satisfying  $\Gamma$ . We let  $I_1$  consist of the facts of J over the relations in the original schema, and  $I_2$  consist of the facts  $R'(\vec{c})$  for each fact  $R(\vec{c})$  of J. Clearly  $I_1$  and  $I_2$ satisfy  $\Sigma$ . We consider the instance  $I_{\text{Accessed}}$  containing facts  $R(\vec{c})$  for all facts  $R_{\text{Accessed}}(\vec{c})$  in J. The last class of axioms for  $\Gamma$  guarantee that this is a common subinstance of  $I_1$  and  $I_2$ , while the first two sets of axioms guarantee that  $I_{\text{Accessed}}$  is access-valid in  $I_1$ . We conclude that  $Q(I_1) \subseteq Q(I_2)$ , and this implies that the containment of Q in Q' holds in J.

In the other direction we assume the query containment holds, and consider  $I_1, I_2$  with the required  $I_{\text{Accessed}}$ . Build an instance J by defining the relations R from  $I_1$ , relations R'from  $I_2$ , and relations  $R_{\text{Accessed}}$  from  $I_{\text{Accessed}}$ . We can verify that J satisfies  $\Gamma$ , and the query containment gives  $Q(J) \subseteq Q'(J)$ . Tracing back through the definitions this tells us that  $Q(I_1) \subseteq Q(I_2)$ .

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Note that, for a schema without result bounds, the accessibility axioms above can all be rewritten as follows (as in [BtCT16, BtCLT16]): for each method mt, letting R be the relation accessed by mt and  $\vec{x}$  be the input positions of mt in R, we simply have the axiom:

$$\left(\bigwedge_{i} \operatorname{accessible}(x_{i})\right) \land R(\vec{x}, \vec{y}) \to R'(\vec{x}, \vec{y}) \land \bigwedge_{i} \operatorname{accessible}(y_{i}).$$

**Example 4.10.** Let us apply the reduction above to the schema of Example 1.1 with the result bound of 100 from Example 1.3. We see that monotone answerability of a CQ Q is equivalent to  $Q \subseteq_{\Gamma} Q'$ , for  $\Gamma$  containing:

- the referential constraint from Udirectory into Prof and from Udirectory' into Prof';
- accessible(i)  $\land$  Prof $(i, n, s) \rightarrow$  Prof<sub>Accessed</sub>(i, n, s);
- the following, for all  $1 \leq j \leq 100$ :  $\exists \vec{y_1} \cdots \vec{y_j} (\bigwedge_{1 \leq p \leq q \leq j} \vec{y_p} \neq \vec{y_q} \land \mathsf{Udirectory}(\vec{y_p})) \rightarrow \vec{y_1} \leq \vec{y_1}$  $\exists \vec{z}_1 \cdots \vec{z}_j (\bigwedge_{1 \le p < q \le j} \ \vec{z}_p \neq \vec{z}_q \land \mathsf{Udirectory}_{\mathsf{Accessed}}(\vec{z}_p));$ •  $\mathsf{Prof}_{\mathsf{Accessed}}(\vec{w}) \to \mathsf{Prof}(\vec{w}) \land \mathsf{Prof}'(\vec{w}) \land \bigwedge_i \mathsf{accessible}(w_i) \text{ and similarly for Udirectory.}$

Note that the constraint in the third item is quite complex; it contains inequalities and also disjunction, since we write  $\vec{y} \neq \vec{z}$  to abbreviate a disjunction  $\bigvee_{i < |\vec{y}|} y_i \neq z_i$ . This makes it challenging to decide if  $Q \subseteq_{\Gamma} Q'$  holds. Hence, our goal in the next section will be to simplify result bounds to avoid such complex constraints.

Bottom line: monotone answerability and query containment. The results in this section have allowed us to reduce the analysis of monotone answerability to a problem concerning containment of queries with integrity constraints. We will rely on this equivalence throughout the remainder of the paper, in that all of our results on expressiveness and complexity will go through transformations and analysis of the corresponding containment for AMonDet. Note that since we allow constants that may be equal to one another in our analysis, it will always be possible to reduce the setting for non-Boolean queries to that for Boolean queries: we simply consider the free variables as constants. With this in mind, we will state all of our results for non-Boolean CQs, but in the proofs will assume the Boolean case, relying on this trivial reduction.

### 5. SIMPLIFYING RESULT BOUNDS WITH IDS AND FDS

The results in Section 4 allow us to reduce the monotone answerability problem to a query containment problem. However, for result bounds greater than 1, the containment problem involves complex cardinality constraints, as illustrated in Example 4.10, and thus we cannot apply standard results or algorithms on query containment under constraints to get decidability "out of the box". There is also little hope to establish the decidability of query containment for the precise constraints that we define. Hence, to address this difficulty, we study how to *simplify* result-bounded schemas, i.e., change or remove the result bounds. We do so in this section, with *simplification* results of the following form: if we can find a plan for a query on a result-bounded schema, then we can find a plan in a *simplification* of the schema, i.e., a schema with simpler result bounds or no result bounds at all.

These simplification results have two benefits. First, they give insight about the use of result bounds, following the examples in the introduction. For instance, our results will show that for most of the common classes of constraints used in databases, the actual numbers in the result bounds never matter for answerability. Secondly, they help us to obtain decidability of the monotone answerability problem.

**Existence-check simplification.** The simplest way to use result-bounded methods is to check if some tuples exist, as in Example 1.4. We will formalize this as the *existence-check simplification*, where we replace result-bounded methods by Boolean methods that can only do such existence checks.

Given a schema Sch with result-bounded methods, its *existence-check simplification*  $Sch^{\dagger}$  is formed as follows:

- The signature of  $\mathsf{Sch}^{\dagger}$  is that of  $\mathsf{Sch}$  plus some new relations: for each result-bounded method mt, letting R be the relation accessed by mt, we add a relation  $R_{\mathsf{mt}}$  whose arity is the number of input positions of mt.
- The integrity constraints of Sch<sup>†</sup> are those of Sch plus, for each result-bounded method mt of Sch, two new ID constraints:

$$\begin{aligned} R(\vec{x}, \vec{y}) &\to R_{\mathsf{mt}}(\vec{x}) \\ R_{\mathsf{mt}}(\vec{x}) &\to \exists \vec{y} \ R(\vec{x}, \vec{y}) \end{aligned}$$

where  $\vec{x}$  denotes the input positions of mt in R.

• The methods of  $\operatorname{Sch}^{\dagger}$  are the methods of  $\operatorname{Sch}$  that have no result bounds, plus one new Boolean method  $\operatorname{mt}^{\dagger}$  on each new relation  $R_{\operatorname{mt}}$ , that has no result bounds either.

**Example 5.1.** Recall the schema Sch of Examples 1.1 and 1.5. It featured a relation Prof(id, name, salary) with an access method **pr** having input *id* to obtain information about a professor; and featured a relation Udirectory(*id*, *address*, *phone*) with an access method  $ud_2$  taking an *id* as input and returning the *address* and phone number of tuples with this *id*. We assumed a result bound of 1 on  $ud_2$ , and assumed the functional dependency  $\phi$ : each employee id has exactly one *address* (but possibly many phone numbers).

The existence-check simplification of Sch has a signature with relations Udirectory, Prof, and a new relation Udirectory<sub>ud<sub>2</sub></sub> of arity 1. It has two access methods without result bounds: the method pr on Prof like in Sch, and a Boolean method  $ud'_2$  on Udirectory<sub>ud<sub>2</sub></sub>. Its constraints are those of Sch, plus the following IDs:

$$\begin{split} \mathsf{U}\mathsf{directory}(i,a,p) &\to \mathsf{U}\mathsf{directory}_{\mathsf{ud}_2}(i) \\ \mathsf{U}\mathsf{directory}_{\mathsf{ud}_2}(i) &\to \exists a\,p \; \mathsf{U}\mathsf{directory}(i,a,p) \end{split}$$

Clearly, every plan that uses the existence-check simplification  $\operatorname{Sch}^{\dagger}$  of a schema  $\operatorname{Sch}$  can be converted into a plan using  $\operatorname{Sch}$ , by replacing the accesses on the Boolean method of  $R_{mt}$  to non-deterministic accesses with mt, and only checking whether the result of these accesses is empty. We want to understand when the converse is true. That is, when a plan on  $\operatorname{Sch}$  can be converted to a plan on  $\operatorname{Sch}^{\dagger}$ . For instance, recalling the plan of Example 1.4 that tests whether Udirectory is empty simply by accessing ud<sub>2</sub>, we could implement it in the existence-check simplification of this schema. More generally, we want to identify schemas Sch for which any CQ having a monotone plan over Sch has a plan on the existence-check simplification Sch<sup>†</sup>. We say that Sch is existence-check simplifiable when this holds: this intuitively means that "result-bounded methods of Sch are only useful for existence checks".

Showing existence-check simplifiability. We first show that this notion of existence-check simplifiability holds for schemas like Example 1.2 whose constraints consist of inclusion dependencies:

**Theorem 5.2.** Let Sch be a schema whose constraints are IDs, and let Q be a CQ that is monotonically answerable in Sch. Then Q is monotonically answerable in the existence-check simplification of Sch.

This existence-check simplifiability result implies in particular that for schemas with IDs, monotone answerability is decidable even with result bounds. This is because the existencecheck simplification of the schema features only IDs and no result bounds, so the query containment problem for AMonDet only features guarded TGDs, which implies decidability. We will show a finer complexity bound in the next section.

To prove Theorem 5.2, we show that if Q is not AMonDet in the existence-check simplification Sch<sup>†</sup> of Sch, then it cannot be AMonDet in Sch. This suffices to prove the contrapositive of the result, because AMonDet is equivalent to monotone answerability (Theorem 4.3). As in all of our results concerning entailment problems like AMonDet, in the proof for simplicity we will assume the query Q is Boolean. The general case is handled by simply considering free variables as additional constants.

Let us show, for a Boolean query Q, that Q not being AMonDet in Sch<sup>†</sup> implies that it is not AMonDet in Sch. To do so, we introduce a general method of *blowing up models* that we will reuse in all subsequent simplifiability results. We assume that AMonDet does not hold in the simplification Sch<sup>†</sup>, and consider a *counterexample to* AMonDet for Sch<sup>†</sup>: two instances  $I_1^{\dagger}, I_2^{\dagger}$  both satisfying the schema constraints, such that  $I_1^{\dagger}$  satisfies Q while  $I_2^{\dagger}$ satisfies  $\neg Q$ , and  $I_1^{\dagger}$  and  $I_2^{\dagger}$  have a common subinstance  $I_{\text{Accessed}}^{\dagger}$  which is access-valid in  $I_1^{\dagger}$ . We use them to build a counterexample to AMonDet for the original schema Sch: we will always do so by adding more facts to  $I_1^{\dagger}$  and  $I_2^{\dagger}$  and then restricting to the relations of Sch. We formalize the sufficiency of such a construction in the following lemma, whose proof is immediate, and which we state in full generality as we will use it in multiple places:

**Lemma 5.3.** Let Sch and Sch<sup>†</sup> be schemas and Q a CQ on the common relations of Sch and Sch<sup>†</sup> such that Q is not AMonDet in Sch<sup>†</sup>. Suppose that for some counterexample  $I_1^{\dagger}, I_2^{\dagger}$ to AMonDet for Q in Sch<sup>†</sup> we can construct instances  $I_1$  and  $I_2$  over Sch, satisfying the constraints of Sch, which have a common subinstance  $I_{\text{Accessed}}$  that is access-valid in  $I_1$  for Sch, such that  $I_2$  has a homomorphism to  $I_2^{\dagger}$ , and such that the restriction of  $I_1^{\dagger}$  to the relations of Sch is a subinstance of  $I_1$ . Then Q is not AMonDet in Sch.

*Proof.* The instances  $I_1$  and  $I_2$  satisfy the constraints of Sch and they have a common subinstance which is access-valid in  $I_1$  for Sch. Recall that, by definition of a counterexample,  $I_1^{\dagger}$  satisfies Q and  $I_2^{\dagger}$  does not. Now, instance  $I_1$  satisfies Q, because  $I_1^{\dagger}$  does and Q only mentions the relations of Sch, and  $I_2$  does not satisfy Q, because it has a homomorphism to  $I_2^{\dagger}$  which does not. Hence,  $I_1, I_2$  is a counterexample showing that Q is not AMonDet in Sch.

Using this lemma, we can now prove Theorem 5.2:

*Proof.* We use the equivalence between AMonDet and monotone plans given by Theorem 4.3, and we prove the contrapositive of the theorem, using Lemma 5.3. Let Sch be the original schema and Sch<sup>†</sup> be the existence-check simplification. Notice that the query Q is indeed

posed on the common relations of Sch and Sch<sup>†</sup>, i.e., it does not involve the  $R_{mt}$  relations added in Sch<sup>†</sup>. To use Lemma 5.3, suppose that we have a counterexample  $(I_1^{\dagger}, I_2^{\dagger})$  to AMonDet for Q and the simplification Sch<sup>†</sup>, i.e., the instances  $I_1^{\dagger}$  and  $I_2^{\dagger}$  satisfy the constraints  $\Sigma^{\dagger}$  of Sch<sup>†</sup>, the instance  $I_1^{\dagger}$  satisfies Q and the instance  $I_2^{\dagger}$  violates Q, and  $I_1^{\dagger}$  and  $I_2^{\dagger}$  have a common subinstance  $I_{\text{Accessed}}^{\dagger}$  that is access-valid in  $I_1^{\dagger}$ . We will show how to "blow up" each instance to  $I_1$  and  $I_2$  which have a common subinstance which is access-valid in  $I_1$ , i.e., we must ensure that each access to a method with a result bound in  $I_1$  returns either no tuples or more tuples than the bound. In the blowup process we will preserve the constraints  $\Sigma^{\dagger}$  and the properties of the  $I_i$  with respect to the CQ Q. Intuitively, the blowup process will consider all accesses that can be performed with the common subinstance  $I_{\text{Accessed}}^{\dagger}$ , and instantiate infinitely many witnesses to serve as answers for these accesses. We will then repair the instances by applying chase steps so that they satisfy the constraints again.

We now explain formally how  $I_1$  and  $I_2$  are formed. The first step is "obliviously chasing with the existence-check constraints": for any existence-check constraint  $\delta$  of the form

$$\forall x_1 \dots x_m \ R_{\mathsf{mt}}(\vec{x}) \to \exists y_1 \dots y_n \ R(\vec{x}, \vec{y})$$

and any homomorphism h of the variables  $x_1 \ldots x_m$  to  $I_{\text{Accessed}}^{\dagger}$ , we extend the mapping by choosing infinitely many fresh witnesses for  $y_1 \ldots y_n$ , naming the  $j^{th}$  value for  $y_i$  in some canonical way depending on  $(h(x_1), \ldots h(x_m), \delta, j, i)$ , and creating the corresponding facts. We use the term "obliviously chasing" to emphasize that the trigger may not be active. We let  $I_{\text{Accessed}}^*$  be  $I_{\text{Accessed}}^{\dagger}$  extended with these facts.

The second step is "chasing with the original constraints". Recall the definition of "the chase" in Section 3. Specifically, we let  $I_{\text{Accessed}}$  be the chase of  $I^*_{\text{Accessed}}$  by  $\Sigma$ .

We now construct  $I_1 := I_1^{\dagger} \cup I_{\text{Accessed}}$  and similarly define  $I_2 := I_2^{\dagger} \cup I_{\text{Accessed}}$ . We also remove all facts from  $I_1, I_2$ , and  $I_{\text{Accessed}}$  where the underlying relation is not in Sch.

We now show correctness. First observe that the restriction of  $I_1^{\dagger}$  to the relations of Sch is a subinstance of  $I_1$ , so that  $I_1$  still satisfies Q. Further, we argue that for all  $p \in \{1, 2\}$ , the instance  $I_p$  satisfies  $\Sigma$ . As  $\Sigma$  consists only of IDs, its triggers consist of single facts, so it suffices to check this on  $I_p^{\dagger}$  and on  $I_{\text{Accessed}}$  separately. For  $I_{\text{Accessed}}$ , we know that it satisfies  $\Sigma$ by definition of the chase. For  $I_p^{\dagger}$ , we know it satisfied  $\Sigma^{\dagger}$  (before the last step of removing the facts not on relations of Sch), so it satisfies  $\Sigma$ .

We must now justify that  $I_2$  has a homomorphism h to  $I_2^{\dagger}$ , which will imply that it still does not satisfy Q. We first define h to be the identity on  $I_2^{\dagger}$ . It then suffices to define h as a homomorphism from  $I_{\text{Accessed}}$  to  $I_2^{\dagger}$  which is the identity on  $I_{\text{Accessed}}^{\dagger}$ , because  $I_{\text{Accessed}} \cap I_2^{\dagger} = I_{\text{Accessed}}^{\dagger}$ . We next define h on  $I_{\text{Accessed}}^* \setminus I_{\text{Accessed}}^{\dagger}$ . Consider a fact  $F = R(\vec{a})$  of  $I_{\text{Accessed}}^* \setminus I_{\text{Accessed}}^{\dagger}$  created by obliviously chasing a trigger on an existence-check constraint  $\delta$  on  $I_{\text{Accessed}}^{\dagger}$ . Let  $F' = S(\vec{b})$ be the fact of  $I_{\text{Accessed}}^{\dagger}$  in the image of the trigger: that is, the fact that matches the body of  $\delta$ . We know that  $\delta$  holds in  $I_2^{\dagger}$  and thus there is some fact  $F'' := R(\vec{c})$  in  $I_2^{\dagger}$  that serves as a witness for this. Writing Arity(R) to denote the arity of R, we define  $h(a_i)$  for each  $1 \leq i \leq \text{Arity}(R)$  as  $h(a_i) := c_i$ . In this way, the image of the fact F under h is F''.

We argue that this is consistent with the stipulation that h is the identity on  $I_{\text{Accessed}}^{\dagger}$ . This is because whenever  $a_i \in \text{Adom}(I_{\text{Accessed}}^{\dagger})$ ,  $a_i$  was not a fresh element when firing the trigger that created F. So  $c_i$  was not fresh either and must have been the same element, i.e.,  $c_i = a_i$ . Further, we claim that all these assignments are consistent across the facts of  $I^*_{\text{Accessed}} \setminus I^{\dagger}_{\text{Accessed}}$  because all elements of  $I^*_{\text{Accessed}} \setminus I^{\dagger}_{\text{Accessed}}$  which do not occur in  $\text{Adom}(I^{\dagger}_{\text{Accessed}})$  occur at exactly one position in one fact of  $I^*_{\text{Accessed}} \setminus I^{\dagger}_{\text{Accessed}}$ .

We now define h on facts of  $I_{\text{Accessed}} \setminus I^*_{\text{Accessed}}$  inductively by extending it on the new elements introduced throughout the chase. Whenever we create a fact  $F = R(\vec{a})$  in  $I_{\text{Accessed}}$ for a trigger  $\tau$  mapping to  $F' = S(\vec{b})$  for an ID  $\delta$  in  $I_{\text{Accessed}}$ , we explain how to extend h to the nulls introduced in F. Consider the fact  $h(F') = S(h(\vec{b}))$  in  $I_2^{\dagger}$ . The body of  $\delta$  also matches this fact, and as  $I_2^{\dagger}$  satisfies  $\Sigma^{\dagger}$  there must be a fact  $F'' = R(\vec{c})$  in  $I_2^{\dagger}$  which extends this match to the head of  $\delta$ , since  $\delta$  holds in  $I_2^{\dagger}$ . For the elements  $a_i$  that are not nulls created when firing  $\tau$ , the image  $h(a_i)$  of  $a_i$  by h is already defined, and more precisely we must have  $h(a_i) = c_i$ , by the same reasoning as when we defined h on  $I^*_{\text{Accessed}} \setminus I^{\dagger}_{\text{Accessed}}$ . Now, for the  $a_i$ 's that are nulls, noting that all of them are distinct, we simply set  $h(a_i) := c_i$ . This ensures that h(F) = F'', so F has a homomorphic image. Hence, performing this process inductively indeed creates a homomorphism.

This concludes the proof of the fact that there is a homomorphism from  $I_2$  to  $I_2^{\dagger}$ .

It remains to justify that the common subinstance  $I_{\text{Accessed}}$  in  $I_1$  and  $I_2$  is access-valid in  $I_1$ . Consider one access in  $I_1$  performed with some method mt of a relation R, with a binding AccBind of values in  $I_{\text{Accessed}}$ , and let us show that we can define a valid output to this access in  $I_{\text{Accessed}}$ . It is clear by definition of  $I_{\text{Accessed}}$  that, if some value of AccBind is not in the domain of  $I_{\text{Accessed}}^{\dagger}$ , it must be a null introduced in the chase to create  $I_{\text{Accessed}}$ , in the first or in the second step. In this case the only possible matching facts in  $I_1$  are the facts containing such a null, i.e., the facts in  $I_{\text{Accessed}} \setminus I_{\text{Accessed}}^{\dagger}$ , so these facts are all in  $I_{\text{Accessed}}$  and there is nothing to show as they can all be returned.

We thus focus on the case when all values of AccBind are in  $I_{\text{Accessed}}^{\dagger}$ . If mt is not a result-bounded access, then we can simply use the fact that  $I_{\text{Accessed}}^{\dagger}$  is access-valid in  $I_1^{\dagger}$  to know that all matching tuples in  $I_1^{\dagger}$  were in  $I_{\text{Accessed}}^{\dagger}$ , so the matching tuples in  $I_1$  must be in  $I_{\text{Accessed}}^{\dagger} \cup (I_1 \setminus I_1^{\dagger})$ , hence in  $I_{\text{Accessed}}$ . If mt is a result-bounded access, then consider the access on mt<sup>†</sup> with the same binding. Either this access returns nothing or it tells us that there is a fact  $R_{\text{mt}}$  containing the values of AccBind. In the first case, as  $I_{\text{Accessed}}^{\dagger}$  is access-valid in  $I_1^{\dagger}$ , we know that  $I_1^{\dagger}$  contains no matching tuple, hence the constraints of Sch<sup>†</sup> imply that  $I_1^{\dagger}$  does not contain any *R*-fact which matches AccBind in the input positions of mt. This means that any matching tuple in  $I_1$  for the access on mt must be in  $I_1 \setminus I_1^{\dagger}$ , so they are in  $I_{\text{Accessed}}$  and we can define a valid output to the access in  $I_{\text{Accessed}}$ . This covers the first case.

In the second case, the  $R_{mt}$ -fact of  $I_1^{\dagger}$  implies by construction that  $I_{Accessed}^*$ , hence  $I_{Accessed}$ , contains infinitely many suitable facts matching the access. Letting k be the result bound of mt, we choose k facts among those, and obtain a valid output to the access with AccBind on mt in  $I_1$ . Hence, we have shown that  $I_{Accessed}$  is access-valid in  $I_1$ .

Hence, we have shown the conditions of Lemma 5.3. Using this lemma, we have completed the proof of Theorem 5.2.  $\hfill \square$ 

**FD** simplification. When our constraints include functional dependencies, we can hope for another kind of simplification, generalizing the idea of Example 1.5: an FD can force the output of a result-bounded method to be deterministic on a projection of the output positions. We will define the FD simplification to formalize this intuition.

Given a set of constraints  $\Sigma$ , a relation R that occurs in  $\Sigma$ , and a subset P of the positions of R, we write  $\mathsf{DetBy}(R, P)$  for the set of positions determined by P, i.e., the set of positions i of R such that  $\Sigma$  implies the FD  $P \to i$ . In particular, we have  $P \subseteq \mathsf{DetBy}(R, P)$ . For any access method  $\mathsf{mt}$ , letting R be the relation that it accesses, we let  $\mathsf{DetBy}(\mathsf{mt})$  denote  $\mathsf{DetBy}(R, P)$  where P is the set of input positions of  $\mathsf{mt}$ . Given a schema Sch with result-bounded methods, we can now define its FD simplification  $\mathsf{Sch}^{\dagger}$  as follows:

- The signature of Sch<sup>†</sup> is that of Sch plus some new relations: for each result-bounded method mt, letting R be the relation accessed by mt, we add a relation  $R_{mt}$  whose arity is |DetBy(mt)|.
- The integrity constraints of  $Sch^{\dagger}$  are those of Sch plus, for each result-bounded method mt of Sch, two new ID constraints:

$$\begin{aligned} R(\vec{x}, \vec{y}, \vec{z}) &\to R_{\mathsf{mt}}(\vec{x}, \vec{y}) \\ R_{\mathsf{mt}}(\vec{x}, \vec{y}) &\to \exists \vec{z} \ R(\vec{x}, \vec{y}, \vec{z}) \end{aligned}$$

where  $\vec{x}$  denotes the input positions of mt and  $\vec{y}$  denotes the other positions of DetBy(mt).

• The methods of  $\mathsf{Sch}^{\dagger}$  are the methods of  $\mathsf{Sch}$  that have no result bounds, plus the following: for each result-bounded method mt on relation R in  $\mathsf{Sch}$ , a method  $\mathsf{mt}^{\dagger}$  on  $R_{\mathsf{mt}}$  that has no result bounds and whose input positions are the positions of  $R_{\mathsf{mt}}$  corresponding to input positions of mt.

Note that the FD simplification is the same as the existence-check simplification when the integrity constraints  $\Sigma$  do not imply any FD. Further observe that, even though the methods of Sch<sup>†</sup> have no result bounds, any access to a new method mt<sup>†</sup> of Sch<sup>†</sup> is guaranteed to return at most one result. This is thanks to the FD on the corresponding relation R, and thanks to the constraints that relate  $R_{mt}$  and R.

**Example 5.4.** Recall the schema Sch of Example 1.5 and the FD  $\phi$  on Udirectory. In the FD simplification of Sch, we add a relation Udirectory<sub>ud2</sub>(*id*, *address*), we replace ud<sub>2</sub> by a method ud<sub>2</sub> on Udirectory<sub>ud2</sub> whose input attribute is *id*, and we add the IDs Udirectory(*i*, *a*, *p*)  $\rightarrow$  Udirectory<sub>ud2</sub>(*i*, *a*) and Udirectory<sub>ud2</sub>(*i*, *a*)  $\rightarrow \exists p$  Udirectory(*i*, *a*, *p*). The method ud'<sub>2</sub> has no result bound, but the IDs above and the FD  $\phi$  ensure that it always returns at most one result.

The point of the FD simplification is that it has no result-bounded methods, so that, like for the existence-check simplification, the query containment problem for the schema of the simplification will not use any complex cardinality constraints. This is in contrast to the query containment problem obtained in Example 4.10.

A schema Sch is *FD simplifiable* if every CQ having a monotone plan over Sch has one over the FD simplification of Sch. As for existence-check, if a schema is FD simplifiable, we can decide monotone answerability by reducing to the same problem in a schema without result bounds.

We use a variant of our "blowup process" to show that schemas with only FD constraints are FD simplifiable:

**Theorem 5.5.** Let Sch be a schema whose constraints are FDs, and let Q be a CQ that is monotonically answerable in Sch. Then Q is monotonically answerable in the FD simplification Sch<sup>†</sup> of Sch.

*Proof.* We will again show the contrapositive of the statement. Assume that we have a counterexample  $I_1^{\dagger}, I_2^{\dagger}$  to AMonDet for Sch<sup>†</sup>, with Q holding in  $I_1^{\dagger}$ , with Q not holding in  $I_2^{\dagger}$ ,

and with  $I_1^{\dagger}$  and  $I_2^{\dagger}$  having a common subinstance  $I_{\text{Accessed}}^{\dagger}$  that is access-valid in  $I_1^{\dagger}$  under Sch<sup>†</sup>. We will upgrade these to  $I_1, I_2, I_{\text{Accessed}}$  having the same property for Sch, by blowing up accesses one after the other. To do so, we initially set  $I_1$  to be the restriction of  $I_1^{\dagger}$  to the relations of Sch, i.e., all relations but the  $R_{\text{mt}}$  relations. We define  $I_2$  from  $I_2^{\dagger}$  and  $I_{\text{Accessed}}$ from  $I_{\text{Accessed}}^{\dagger}$  in the same way. We fix some valid access selection  $\sigma_1$  for  $I_1^{\dagger}$  that always returns tuples from  $I_{\text{Accessed}}^{\dagger}$  when performing accesses with values of  $I_{\text{Accessed}}^{\dagger}$ . We consider all possible accesses in parallel, performing for each access a process described just below.

We consider all the (non-result-bounded) access methods  $\mathsf{mt}^{\dagger}$  introduced in  $\mathsf{Sch}^{\dagger}$  — not including the access methods  $\mathsf{mt}$  of  $\mathsf{Sch}^{\dagger}$  which are simply those without result bounds in  $\mathsf{Sch}$ . Given such an  $\mathsf{mt}^{\dagger}$ , we write  $\mathsf{mt}$  for the corresponding (result-bounded) access method in  $\mathsf{Sch}$ . We call  $\mathsf{mt}^{\dagger}$  (and also  $\mathsf{mt}$ ) non-dangerous if the input positions of  $\mathsf{mt}$  determine all positions of the accessed relation. Equivalently,  $\mathsf{DetBy}(\mathsf{mt})$  contains all positions of R. Or again equivalently,  $R_{\mathsf{mt}}$  and  $R_{\mathsf{mt}}^{\dagger}$  have the same arity. We call  $\mathsf{mt}$  and  $\mathsf{mt}^{\dagger}$  dangerous otherwise. The blowup process we provide for each access will differ depending on whether the method is dangerous or non-dangerous.

First, we handle the non-dangerous methods, and simply copy in  $I_{\text{Accessed}}$  the results of accesses on these methods. Consider every non-dangerous method  $\mathsf{mt}^{\dagger}$  of  $\mathsf{Sch}^{\dagger}$ . We again write  $\mathsf{mt}$  the corresponding method in  $\mathsf{Sch}$  and use R to denote the relation of the access. We consider every possible access ( $\mathsf{mt}^{\dagger}, \mathsf{AccBind}$ ) on  $I_1^{\dagger}$  with values in  $I_{\mathsf{Accessed}}^{\dagger}$  such that one tuple (and, by the FDs, exactly one tuple) is returned. The IDs from  $R_{\mathsf{mt}}$  to R imply there is an R-fact with exactly the same elements in  $I_1^{\dagger}$  and  $I_2^{\dagger}$ . We then add this one fact to  $I_{\mathsf{Accessed}}$ . We do this for all the non-dangerous methods and accesses using these methods.

Second, we blow up the dangerous methods, which is the complicated step of the construction. Consider every dangerous method  $\mathsf{mt}^{\dagger}$  of  $\mathsf{Sch}^{\dagger}$ . Write  $\mathsf{mt}$  for the method in  $\mathsf{Sch}$  corresponding to  $\mathsf{mt}^{\dagger}$  and R for the relation of  $\mathsf{mt}$ . Consider every possible access  $(\mathsf{mt}^{\dagger},\mathsf{AccBind})$  on  $I_1^{\dagger}$  with values in  $I_{\mathsf{Accessed}}^{\dagger}$ . There are two possibilities: either this access returns nothing, or, by the FDs of  $\mathsf{Sch}$  and the constraints introduced in  $\mathsf{Sch}^{\dagger}$ , it returns exactly one tuple, which must be in  $I_{\mathsf{Accessed}}^{\dagger}$  because  $I_{\mathsf{Accessed}}^{\dagger}$  is access-valid in  $I_1^{\dagger}$ .

In the first case, we do nothing. Intuitively, we know that there are no matching tuples in  $I_1^{\dagger}$ . Now, considering the ID constraint in the FD simplification that goes from R to  $R_{\rm mt}$ , we infer that there is no R-fact in  $I_1^{\dagger}$  whose projection to the input positions of mt matches AccBind. Thus we will have no problem building a valid answer to this access.

In the second case, consider the fact  $M'_1$  that was returned, following the access selection  $\sigma_1$  in response to the access  $(\mathsf{mt}^{\dagger}, \mathsf{AccBind})$ . Recall that there is an ID constraint in  $\mathsf{Sch}^{\dagger}$  that goes from  $R_{\mathsf{mt}}$  to R. This constraint allows us to infer from the existence of  $M'_1$  that there must be some witnessing facts in  $I_1^{\dagger}$  and in  $I_2^{\dagger}$ , namely, R-facts whose projection to  $\mathsf{DetBy}(\mathsf{mt})$  matches  $M'_1$ . In this case, we perform a modification that we refer to as blowing up the access. Specifically, let X be the positions of R that are not in  $\mathsf{DetBy}(\mathsf{mt})$ . By our assumption that  $\mathsf{mt}^{\dagger}$  is dangerous, X is nonempty. Construct infinitely many R-facts with all positions in  $\mathsf{DetBy}(\mathsf{mt})$  agreeing with  $M'_1$ , and with all positions in X filled using fresh values that are different from each other and from other values in  $I_1^{\dagger} \cup I_2^{\dagger}$ . We add these duplicate facts to  $I_1$ , to  $I_2$ , and to  $I_{\mathsf{Accessed}}$ .

Performing this process for all accesses in  $I_{\text{Accessed}}^{\dagger}$  on all dangerous access methods that return a tuple, we have finished the definition of  $I_1$ ,  $I_2$ , and  $I_{\text{Accessed}}$ .

Having completed our construction, we now check that the conditions are satisfied. It is clear that the restriction of  $I_1^{\dagger}$  to the relations of Sch is a subset of  $I_1$ . We see that  $I_{\text{Accessed}} \subseteq I_1$  and  $I_{\text{Accessed}} \subseteq I_2$ , because these two last inclusions are true initially and all tuples added to  $I_{Accessed}$  are also added to  $I_1$  and  $I_2$ , or in the case of non-dangerous accesses are already present in  $I_1^{\dagger}$  and  $I_2^{\dagger}$ . Further,  $I_2$  has a homomorphism back to  $I_2^{\dagger}$ : we can define it as the identity on  $I_2^{\dagger}$ , and as mapping the fresh elements of every duplicate tuple of  $I_2 \setminus I_2^{\dagger}$  to a witnessing fact in  $I_2^{\dagger}$ . This only collapses fresh values of  $\mathsf{Adom}(I_2)$  to values of  $\mathsf{Adom}(I_2^{\dagger})$ , and is the identity on constants of  $I_2^{\dagger}$ .

We must justify that  $I_1$  and  $I_2$  still satisfy the FD constraints of Sch. This is true because, whenever we add a set of duplicate facts to  $I_1$  and  $I_2$ , each fact in the set contains fresh values at the positions of the set X, and must match the witnessing facts already present in  $I_1^{\dagger}$  and  $I_2^{\dagger}$  at the other positions. Hence, if adding such a duplicate fact violated an FD, the left-hand-side of the FD could not contain a position in X, as elements at these positions are fresh. So the left-hand-side would be contained in  $\mathsf{DetBy}(\mathsf{mt})$ . Thus the right-hand-side would also be contained in DetBy(mt), because DetBy(mt) is closed under the FDs. We conclude that if adding the new fact violated an FD, then the witnessing facts also did, breaking the assumption that  $I_1^{\dagger}$  and  $I_2^{\dagger}$  satisfied the FDs before. We must now show that  $I_{\text{Accessed}}$  is access-valid in  $I_1$ .

To do so, consider a method mt of Sch and binding AccBind. If AccBind contains values from  $\mathsf{Adom}(I_{\mathsf{Accessed}}) \setminus \mathsf{Adom}(I_{\mathsf{Accessed}}^{\dagger})$ , then we know that these values occur only in tuples from  $I_{\text{Accessed}} \setminus I_{\text{Accessed}}^{\dagger}$ . Thus matching tuples in  $I_1$  are all in  $I_{\text{Accessed}}$  and there is nothing to show. Hence, we focus on the case where AccBind consists of values of  $\mathsf{Adom}(I_{\mathsf{Accessed}}^{\mathsf{T}})$ .

We first focus on the subcase where **mt** is not result-bounded. In this subcase, when performing the same access (mt<sup>†</sup>, AccBind) in  $I_1^{\dagger}$ , the valid access selection  $\sigma_1$  that we fixed returns all matching tuples in  $I_1^{\dagger}$ , and these tuples must be part of  $I_{\text{Accessed}}^{\dagger}$  because  $I_{\text{Accessed}}^{\dagger}$ is access-valid. Considering all matching tuples for the access (mt, AccBind) in the larger structure  $I_1$ , we see they are of two kinds. There are those that were already present in  $I_1^{\dagger}$ , which are in  $I_{\text{Accessed}}^{\dagger}$  because as we explained it is access-valid, so so they are in  $I_{\text{Accessed}}$ . The second kind are those that were added in  $I_1 \setminus I_1^{\dagger}$ , and they were added to  $I_{\text{Accessed}}$  as well. So in both cases all matching tuples in  $I_1$  are in  $I_{\text{Accessed}}$ .

Now, if mt is result-bounded but not dangerous, then performing the access ( $mt^{\dagger}$ , AccBind) on  $R_{\mathsf{mt}}$  in  $I_1^{\dagger}$  either returned a single matching tuple or no tuples. If it returned no matching tuple, then the ID from R to  $R_{mt}$  implies that there was no matching tuple to the access  $(\mathsf{mt}^{\dagger},\mathsf{AccBind})$  in  $I_1^{\dagger}$ , hence there is still none in  $I_1$  except potentially those of  $I_{\mathsf{Accessed}} \setminus I_{\mathsf{Accessed}}^{\dagger}$ . So  $I_{\text{Accessed}}$  can be used to construct a valid response. If there is a matching tuple, then the ID from  $R_{mt}$  to R implies that there is a matching tuple for the access (mt<sup>†</sup>, AccBind) in  $I_1^{\dagger}$ , which we added to  $I_{Accessed}$  at the end of the construction. So the matching tuple is in  $I_{Accessed}$ and it is still a valid response to the access (mt, AccBind) in  $I_1$  (recall that the FDs imply that this single tuple is the only possible matching tuple).

We can thus focus on the case where **mt** is result-bounded and dangerous. In this case, when we considered the access (mt, AccBind) in the blow-up process above for mt, either we blew up the access or we did not. If we did not, then we know that there were no matching tuples in  $I_1^{\dagger}$  for the access, and the ID from R to  $R_{\rm mt}$  implies that  $I_1^{\dagger}$  contains no matching tuple for the access (mt<sup>†</sup>, AccBind), so all matching tuples to the access (mt, AccBind) in  $I_1$ are in  $I_{\text{Accessed}}$ . If we did blow the access up, then we know that  $I_{\text{Accessed}}$  contains infinitely many matching tuples to the access that we can use as a valid response to the access in  $I_1$ . Thus,  $I_{\text{Accessed}}$  is indeed access-valid.

Thus, Lemma 5.3 implies that Q is not AMonDet in Sch, concluding the proof of Theorem 5.5.

# 6. Decidability of Monotone Answerability using Existence check and FD simplification

Thus far we have seen a general way to reduce monotone answerability problems with result bounds to query containment problems (Section 4). We have also seen schema simplification results for both FDs and IDs, which give us insight into how result-bounded methods can be used (Section 5). We now show that for these two classes of constraints, the reduction to containment and simplification results combine to give decidability results, along with tight complexity bounds.

6.1. **Decidability for FDs.** We first consider schemas whose constraints consist of FDs. We start with an analysis of monotone answerability in the case *without result bounds*:

**Proposition 6.1.** We can decide whether a CQ is monotonically answerable with respect to a schema without result bounds whose constraints are FDs. The problem is NP-complete.

*Proof.* The lower bound already holds without result bounds or constraints [Li03], so it suffices to show the upper bound. We know that, by Theorem 4.3 and Proposition 4.9, the problem reduces to the AMonDet query containment problem  $Q \subseteq_{\Gamma} Q'$  for Sch. As Sch has no result bounds, we can define  $\Gamma$  using the rewriting of the accessibility axioms given after Proposition 4.9. The constraints  $\Gamma$  thus consist of FDs and of full TGDs of the form:

 $\Big(\bigwedge_i \operatorname{accessible}(x_i)\Big) \wedge R(\vec{x}, \vec{y}) \to R'(\vec{x}, \vec{y}) \wedge \bigwedge_i \operatorname{accessible}(y_i).$ 

Since this is a query containment problem with FDs and TGDs, by Proposition 3.2 it can be solved by computing the chase. As the TGDs are full, we know that we do not create fresh values when computing the chase. Further, because there are no TGD constraints with primed relations in their body, once accessible does not change, the entire chase process has terminated. Besides, when adding values to accessible we must reach a fixpoint in linearly many chase steps since accessible is unary. Thus the chase with  $\Gamma$  terminates in linearly many steps. Thus, we can decide containment by checking in NP whether Q' holds on the chase result, concluding the proof.

We now return to the situation with result bounds. We know that schemas with FDs are FD simplifiable. From this we get a reduction to query containment with no result bounds, but introducing new axioms. We can show that the additional axioms involving  $R_{mt}$  and R do not harm chase termination, so that AMonDet is decidable; in fact, it is NP-complete, i.e., no harder than CQ evaluation:

**Theorem 6.2.** We can decide whether a CQ is monotonically answerable with respect to a schema with result bounds whose constraints are FDs. The problem is NP-complete.

*Proof.* By Theorem 5.5 it suffices to deal with the FD simplification, meaning that we can reduce to a schema of the following form:

- The signature of Sch<sup>†</sup> is that of Sch plus some new relations: for each result-bounded method mt, letting R be the relation accessed by mt, we add a relation  $R_{mt}$  whose arity is |DetBy(mt)|.
- The integrity constraints of Sch<sup>†</sup> are those of Sch plus, for each result-bounded method mt of Sch, two new ID constraints:

$$R(\vec{x}, \vec{y}, \vec{z}) \to R_{\mathsf{mt}}(\vec{x}, \vec{y})$$
$$R_{\mathsf{mt}}(\vec{x}, \vec{y}) \to \exists \vec{z} \ R(\vec{x}, \vec{y}, \vec{z})$$

where  $\vec{x}$  denotes the input positions of mt and  $\vec{y}$  denotes the other positions of DetBy(mt).

• The methods of  $\mathsf{Sch}^{\dagger}$  are the methods of  $\mathsf{Sch}$  that have no result bounds, plus the following: for each result-bounded method mt on relation R in  $\mathsf{Sch}$ , a method  $\mathsf{mt}^{\dagger}$  on  $R_{\mathsf{mt}}$  that has no result bounds and whose input positions are the positions of  $R_{\mathsf{mt}}$  corresponding to input positions of mt.

By Proposition 4.9, we then reduce AMonDet to query containment. The resulting query containment problem involves two copies of the constraints above, on primed and unprimed copies of the schema, along with accessibility axioms for each access method (including the new methods  $R_{mt}$ ). We can observe a few obvious simplifications of these constraints, when working with the restricted chase:

- The "unprimed method-to-regular constraint",  $R_{mt}(\vec{x}, \vec{y}) \rightarrow \exists \vec{z} \ R(\vec{x}, \vec{y}, \vec{z})$  will never fire, since a fact  $R_{mt}(\vec{a}, \vec{b})$  is always generated by a corresponding fact  $R(\vec{a}, \vec{b}, \vec{c})$ .
- When firing a constraint of the form  $\tau : R'(\vec{x}, \vec{y}, \vec{z}) \to R'_{\mathsf{mt}}(\vec{x}, \vec{y})$  to create a fact  $F_2 = R'_{\mathsf{mt}}(\vec{a}, \vec{b})$  from a fact  $F_1 = R'(\vec{a}, \vec{b}, \vec{c})$ , the fact  $F_2$  will not be a trigger for any rule firing. Indeed, the only rule applicable to a  $R'_{\mathsf{mt}}$ -fact is the reverse constraint  $R'_{\mathsf{mt}}(\vec{x}, \vec{y}) \to \exists \vec{z} R'(\vec{x}, \vec{y}, \vec{z})$ , for which  $F_1$  witnesses that  $F_2$  is not an active trigger. What is more, the  $R'_{\mathsf{mt}}$ -facts created by constraints of the form  $\tau$  cannot help make the query true, as the query does not mention relations of the form  $R'_{\mathsf{mt}}$ . For this reason, we can disregard unprimed method-to-regular constraints without changing the query containment problem.

So the constraints that remain in addition to the FDs are:

- The ID constraints  $R(\vec{x}, \vec{y}, \vec{z}) \rightarrow R_{mt}(\vec{x}, \vec{y})$  where  $\vec{x}$  denotes the input positions of mt and  $\vec{y}$  denotes the other positions of DetBy(mt);
- For every access method mt on a relation S, the accessibility axioms which are of the form  $(\bigwedge_i \operatorname{accessible}(x_i)) \wedge S(\vec{x}) \to S_{\operatorname{Accessed}}(\vec{x})$  and  $S_{\operatorname{Accessed}}(\vec{w}) \to S(\vec{w}) \wedge S'(\vec{w}) \wedge \bigwedge_i \operatorname{accessible}(w_i)$ . Note that S may be one of the original relations, or one of the relations  $R_{\operatorname{mt}}$ , depending on whether mt originally had result bounds or not.
- The ID constraints R'<sub>mt</sub>(x, y) → ∃z R'(x, y, z), where x denotes the input positions of mt and y denotes the other positions of DetBy(mt).

The only non-full TGDs in these constraints are those of the last bullet point: these are the only rules that create new values, and these values will never propagate back to the unprimed relations. Further, whenever a primed fact F is created containing a null using such a rule, the only further chase steps that can apply to F are FDs, and these will only merge elements in F. Thus the chase will terminate in polynomially many steps as in the proof of Proposition 6.1, which establishes the NP upper bound and concludes the proof of Theorem 6.2.

6.2. **Decidability for IDs.** Next we consider schemas whose constraints consist of IDs. As we already mentioned, Theorem 5.2 implies decidability for such schemas. We now give the precise complexity bound:

**Theorem 6.3.** We can decide whether a CQ is monotonically answerable with respect to a schema with result bounds whose constraints are IDs. Further, the problem is EXPTIME-complete.

*Proof.* Hardness already holds without result bounds [BBB13], so we focus on the upper bound. By Theorem 5.2, we can equivalently replace the schema Sch with its existence-check simplification  $Sch^{\dagger}$ , and  $Sch^{\dagger}$  does not have result bounds. Further, it is easy to see that  $Sch^{\dagger}$  consists only of IDs, namely, those of Sch plus the IDs added in the simplification. Note that the resulting query containment problem only involves guarded TGDs, and thus we can conclude that the problem is in 2EXPTIME from [CGLP11]. However, we can do better: [BBB13] showed that the monotone answerability problem for schemas where the constraints are IDs is in EXPTIME, and thus we conclude the proof.

6.3. Complexity for Bounded-Width IDs and Special Properties of the Query Containment for Access Methods. Up until now we have seen a reduction of answerability to query answering. We can see that the query answering problem involves adding auxiliary constraints — the "transfer" axioms that capture properties of an access — and these are of a very special form. Our goal now is to illustrate how the restricted shape of these axioms can be used to get lower complexity bounds, compared to what we can get by appealing to coarser classes like guarded or frontier-guarded TGDs.

We illustrate this in an important case for IDs, those whose *width* — the number of exported variables, i.e., of variables shared between the body and the head — is bounded by a constant. Recall that this includes in particular UIDs, which have width 1. For bounded-width IDs, it was shown by Johnson and Klug [JK84] that query containment under constraints is NP-complete. This result showed that the width parameter plays an important role in lowering the complexity of the containment problem. A natural question is whether the same holds for monotone answerability. We accordingly conclude the section by showing the following, which is new even in the setting without result bounds:

**Theorem 6.4.** It is NP-complete to decide whether a CQ is monotonically answerable with respect to a schema with result bounds whose constraints are bounded-width IDs.

To show this result, we will again use the fact that IDs are existence-check simplifiable (Theorem 5.2). Using Proposition 4.9 we reduce to a query containment problem with guarded TGDs. But this is not enough to get an NP bound. The reason is that the query containment problem includes accessibility axioms, which are not IDs. So we cannot hope to conclude directly using [JK84].

The rest of this section will be devoted to the proof of Theorem 6.4. As mentioned above, this will require a finer-grained analysis of the query containment problem produced from our reduction. In fact, we will note a particular property of these containment problems that can be exploited: they involve constraints that are IDs and GTGDs that are "close to IDs": involving only guards and a fixed set of relations, specifically, the accessible relation. Our results give evidence that looking at other parameters in query answering problems for tame classes of dependencies can yield new insights, despite the wealth of results already present in this area [CGL12, GMP14].

We begin with the case *without result bounds*, and then extend to support result bounds.

**Proving Theorem 6.4 without result bounds.** In the absence of result bounds, recall that the AMonDet query containment problem  $Q \subseteq_{\Gamma} Q'$  can be expressed as follows:  $\Gamma$  contains the bounded-width IDs  $\Sigma$  of the schema, their primed copy  $\Sigma'$ , and for each access method **mt** accessing relation R with input positions  $\vec{x}$  there is an accessibility axiom:

$$\left(\bigwedge_{i} \operatorname{accessible}(x_{i})\right) \land R(\vec{x}, \vec{y}) \to R'(\vec{x}, \vec{y}) \land \bigwedge_{i} \operatorname{accessible}(y_{i})$$

For each method **mt**, we can rewrite the accessibility axiom above by splitting its head, and obtain the following pair of axioms, where the truncated accessibility axioms only create the **accessible** facts (hence the name), and the transfer axioms create the primed facts:

- (Truncated Accessibility):  $(\bigwedge_i \operatorname{accessible}(x_i)) \wedge R(\vec{x}, \vec{y}) \to \bigwedge_i \operatorname{accessible}(y_i)$ .
- (Transfer):  $(\bigwedge_i \operatorname{accessible}(x_i)) \land R(\vec{x}, \vec{y}) \to R'(\vec{x}, \vec{y}).$

We let  $\Delta$  be the set of the truncated accessibility axioms and transfer axioms that we obtain for all the methods mt.

The constraints of  $\Delta$  are TGDs but not IDs. However, we will take advantage of their structure to *linearize*  $\Delta$  together with  $\Sigma$ , i.e., construct a set  $\Sigma^{\text{Lin}}$  of IDs that "simulate" the chase by  $\Sigma$  and  $\Delta$ . To define  $\Sigma^{\text{Lin}}$  formally, we will change the signature. Let S be the signature of the relations used in  $\Sigma$ , not including the special unary relation accessible used in  $\Delta$ ; and let  $w \in \mathbb{N}$  be the constant bound on the width of the IDs in  $\Sigma$ . We expand S to the signature  $S^{\text{Lin}}$  as follows. For each relation R of arity n in S, we consider each subset Pof the positions of R of size at most w. For each such subset P, we add a relation  $R_P$  of arity n to  $S^{\text{Lin}}$ . Intuitively, an  $R_P$ -fact denotes an R-fact where the elements in the positions of P are accessible.

Remember that our goal is to *linearize*  $\Sigma$  and  $\Delta$  to a set of IDs  $\Sigma^{\text{Lin}}$  which emulates the chase by  $\Sigma$  and  $\Delta$ . If we could ensure that  $\Sigma^{\text{Lin}}$  has bounded width, we could then conclude using the result of [JK84]. We will not be able to enforce this, but  $\Sigma^{\text{Lin}}$  will instead satisfy a notion of *bounded semi-width* that we now define.

The basic position graph of a set of TGDs  $\Sigma$  is the directed graph whose nodes are the positions of relations in  $\Sigma$  with an edge from position i of a relation T to position j of a relation U if and only if the following is true: there is a dependency  $\delta \in \Sigma$  whose body contains an atom A using relation T, whose head atom A' uses relation U, and with an exported variable x that occurs at position i of A and at position j of A'.

We say that  $\Sigma^{\text{Lin}}$  has *semi-width* bounded by w if it can be decomposed as  $\Sigma^{\text{Lin}} = \Sigma_1^{\text{Lin}} \cup \Sigma_2^{\text{Lin}}$  where  $\Sigma_1^{\text{Lin}}$  has width bounded by w and the basic position graph of  $\Sigma_2^{\text{Lin}}$  is acyclic. The bound on the semi-width of  $\Sigma^{\text{Lin}}$  then implies an NP bound on query containment, thanks to the following easy generalization of the result of Johnson and Klug [JK84]:

**Proposition 6.5.** For any fixed  $w \in \mathbb{N}$ , there is an NP algorithm for containment under IDs of semi-width at most w.

This is proven by a slight modification of Johnson and Klug's argument, so we defer it to Appendix C. Having defined semi-width, we can now state our linearization result:

**Proposition 6.6.** For any fixed  $w \in \mathbb{N}$ , given a set  $\Sigma$  of IDs of width w and a set  $\Delta$  of truncated accessibility and transfer axioms, and given a set of facts  $I_0$ , we can compute in PTIME a set of IDs  $\Sigma^{\text{Lin}}$  of semi-width w and a set of facts  $I_0^{\text{Lin}}$  satisfying the following:

for any Boolean CQ  $Q^*$  over the primed signature using constants from  $I_0$  and existentially quantified variables,  $Q^*$  is entailed from  $I_0$ ,  $\Sigma$ , and  $\Delta$  iff  $Q^*$  is entailed from  $I_0^{\text{Lin}}$  and  $\Sigma^{\text{Lin}}$ .

The proof of this proposition is our main technical challenge, and it is deferred to Section 6.4. The special form of the constraints is crucial in getting an efficient linearization that leads to linear TGDs of small semi-width.

These two results allow us to decide in NP whether the query containment for AMonDet holds. Indeed, first rewrite  $I_0 := \mathsf{CanonDB}(Q)$ , along with  $\Sigma$  and  $\Delta$  to obtain  $I_0^{\mathsf{Lin}}$  and  $\Sigma^{\mathsf{Lin}}$ , using Proposition 6.6. Then, recalling that  $\Sigma^{\mathsf{Lin}}$  has semi-width w, let  $\Gamma_{\mathsf{Bounded}}$  consist of the primed copy  $\Sigma'$  of the constraints, along with the IDs of  $\Sigma^{\mathsf{Lin}}$  that have width  $\leq w$ ; and let  $\Gamma_{\mathsf{Acyclic}}$  consist of the rules of  $\Sigma^{\mathsf{Lin}}$  that do not have width bounded by w. By assumption, these rules have an acyclic position graph. It is clear that  $\Gamma^{\mathsf{Lin}} := \Gamma_{\mathsf{Bounded}} \cup \Gamma_{\mathsf{Acyclic}}$  also has semi-width w. Now, the following is clear:

## **Claim 6.7.** Let the instance $I_0^{\text{Lin}}$ and constraints $\Gamma^{\text{Lin}}$ be defined from $I_0$ and $\Gamma$ as above. Then Q is AMonDet with respect to Sch if and only if the chase of $I_0^{\text{Lin}}$ by $\Gamma^{\text{Lin}}$ satisfies Q'.

*Proof.* We know that AMonDet is equivalent to the containment  $Q \subseteq_{\Gamma} Q'$  with  $\Gamma = \Sigma \cup \Sigma' \cup \Delta$ . This in turn is equivalent to the existence of a chase proof of Q' starting with  $I_0$  using chase steps from  $\Gamma$ . Thus what we need to show is how to convert such a chase proof to a chase proof of Q' starting from  $I_0^{\text{Lin}}$  using steps of  $\Gamma^{\text{Lin}}$ , and vice versa.

We start with the converse direction. It is easy to see that any chase proof of Q' formed from  $I_0^{\text{Lin}}$  using  $\Gamma^{\text{Lin}}$  can be converted to a chase proof from  $I_0$  using  $\Gamma$ . Indeed, Proposition 6.6 ensures that any Boolean CQ over the primed signature that is derivable in  $I_0^{\text{Lin}}$  using  $\Sigma^{\text{Lin}}$  can be derived in  $I_0$  using  $\Sigma$  and  $\Delta$ . And the Boolean CQs that are derivable using  $\Gamma^{\text{Lin}}$  are those that can be derived by first applying chase steps using  $\Sigma^{\text{Lin}}$  to produce some set S of primed facts, and then applying chase steps involving constraints of  $\Sigma'$  to the facts of S. By converting S to a Boolean CQ we see that we can derive a homomorphic image of S using  $\Sigma$  and  $\Delta$ . Thus all Boolean CQs that can be obtained from  $I_0^{\text{Lin}}$  using  $\Gamma^{\text{Lin}}$  can also be obtained using  $\Sigma$ ,  $\Delta$ , and  $\Sigma'$ .

For the forward direction we consider a chase proof of Q' formed from  $I_0$  using  $\Gamma$ : that is, using  $\Sigma$ ,  $\Sigma'$ , and  $\Delta$ . We will show how to obtain a chase proof of Q' from  $I_0^{\text{Lin}}$  using steps of  $\Gamma^{\text{Lin}}$ . We observe that in our input chase proof we can assume that we first fire rules of  $\Sigma \cup \Delta$  to get a set S of primed facts, and then fire rules of  $\Sigma'$  to get I' containing all the facts of the chase proof. Now, from Proposition 6.6 we know that a homomorphic image  $S^{\text{Lin}}$ of the facts of S can all be derived from  $I_0^{\text{Lin}}$  using  $\Gamma^{\text{Lin}}$ . As  $\Gamma^{\text{Lin}}$  contains  $\Sigma'$ , we can also derive a homomorphic image of the facts of I' from  $S^{\text{Lin}}$ , and thus derive homomorphic images of the facts in the chase proof of Q'. This justifies that Q' is also entailed by  $I_0^{\text{Lin}}$ and  $\Gamma^{\text{Lin}}$ , concluding the proof.

Claim 6.7 implies that to solve the AMonDet problem, it suffices determine whether the set of primed facts corresponding to Q' can be derived from  $I_0^{\text{Lin}}$  by applying chase steps with  $\Gamma^{\text{Lin}}$ . This in turn can be determined using Proposition 6.5. This concludes the proof of Theorem 6.4 in the case without result bounds.

**Proving Theorem 6.4 with result bounds.** We now conclude the proof of Theorem 6.4 by handling the case with result bounds. This will require only slight changes to the prior argument. By Theorem 5.2, for any schema Sch whose constraints  $\Sigma$  are IDs, we can reduce the monotone answerability problem to the same problem for the existence-check

simplification  $\mathsf{Sch}^{\dagger}$  with no result bounds, by replacing each result-bounded method  $\mathsf{mt}$ on a relation R with a non-result-bounded access method  $\mathsf{mt}^{\dagger}$  on a new relation  $R_{\mathsf{mt}}$ , and expanding  $\Sigma$  to a larger set of constraints  $\Sigma^{\dagger}$ , adding new constraints that capture the semantics of the "existence-check views"  $R_{mt}$ :

- (Relation-to-view):  $R(\vec{x}, \vec{y}) \to R_{mt}(\vec{x});$
- (View-to-relation):  $R_{\mathsf{mt}}(\vec{x}) \to \exists \vec{y} \ R(\vec{x}, \vec{y}).$

Note that these IDs do not have bounded width, hence we cannot simply reduce to the case without result bounds that we have just proved. We will explain how to adapt the proof to handle these IDs, namely, linearizing using Proposition 6.6 to IDs of bounded semi-width.

Let us consider the query containment problem for the monotone answerability problem of  $\Sigma^{\dagger}$ . This problem is of the form  $Q \subseteq_{\Gamma} Q'$ , where  $\Gamma$  contains  $\Sigma^{\dagger}$ , its copy  $(\Sigma^{\dagger})'$ , and the accessibility axioms. These axioms can again be rephrased. For each access method mt on a relation R, letting  $\vec{x}$  denote the input positions of mt, we have the following two axioms:

- (Truncated Accessibility): (∧<sub>i</sub> accessible(x<sub>i</sub>)) ∧ R(x, y) → ∧<sub>i</sub> accessible(y<sub>i</sub>);
  (Transfer): (∧<sub>i</sub> accessible(x<sub>i</sub>)) ∧ R(x, y) → R'(x, y).

In the above two items the relation R can be any of the relations of  $\Sigma^{\dagger}$ , including relations of the original signature and relations of the form  $R_{\rm mt}$ . For relations in the original schema. mt is an access method of Sch that did not have a result bound. For the new relations, mt is a method of the form  $mt^{\dagger}$  introduced in the existence-check simplification  $Sch^{\dagger}$  for a result-bounded method of Sch, so  $mt^{\dagger}$  has no output positions: this means that, in this case, the (Truncated Accessibility) axiom is vacuous and the (Transfer) axiom further simplifies to:

(Simpler Transfer): 
$$\left(\bigwedge_{i} \operatorname{accessible}(x_{i})\right) \wedge R_{\mathsf{mt}}(\vec{x}) \to R'_{\mathsf{mt}}(\vec{x}).$$

We first observe that in  $\Gamma$  we do not need to include the view-to-relation constraints of  $\Sigma^{\dagger}$ : facts over  $R_{\rm mt}$  can only be formed from the corresponding R-fact with the relation-to-view constraint, so triggers of the view-to-relation constraints will never be active in the chase, and we know that we can decide  $Q \subseteq_{\Gamma} Q'$  by looking at restricted chase sequences — i.e., where non-active triggers are never fired — hence removing view-to-relation constraints makes no difference. Similarly, we do not need to include the relation-to-view constraints of  $(\Sigma^{\dagger})'$ . These rules could fire to produce a new  $R'_{mt}$ -fact, but such a fact could only trigger the corresponding view-to-relation constraint of  $(\Sigma^{\dagger})'$ , resulting in a state of the chase that has a homomorphism to the one before the firing of the relation-to-view constraint. Thus such firings can not lead to new matches. Thus,  $\Gamma$  consists now of  $\Sigma$ , of  $\Sigma'$ , of (Truncated Accessibility) and (Transfer) axioms for each method mt having no result bound in Sch, and for each method mt with a result bound in Sch we have a relation-to-view constraint from Rto  $R_{\rm mt}$  that comes from  $\Sigma^{\dagger}$ , a view-to-relation constraint from  $R'_{\rm mt}$  to R' that comes from  $(\Sigma^{\dagger})'$ , and a (Simpler Transfer) axiom.

We next note that we can normalize chase proofs with  $\Gamma$  so that the relation-to-view constraints are applied only prior to (Simpler Transfer). Thus, for each result-bounded method mt of Sch, we can merge the relation-to-view rule from R to  $R_{\rm mt}$ , the (Simpler Transfer) axiom from  $R_{\rm mt}$  to  $R'_{\rm mt}$ , and the view-to-relation rules from  $R'_{\rm mt}$  to R', into an axiom of the following form, where  $\vec{x}$  denotes the input positions of mt:

(Result-bounded Fact Transfer) 
$$\left(\bigwedge_{i} \operatorname{accessible}(x_{i}) \wedge R(\vec{x}, \vec{y})\right) \to \exists \vec{z} \ R'(\vec{x}, \vec{z}).$$

To summarize, the resulting axioms consist of:

- The original constraints  $\Sigma$  of the schema;
- Their primed copy  $\Sigma'$ ;
- The (Truncated Accessibility) and (Transfer) axioms for each access method without result bounds;
- The (Result-bounded Fact Transfer) axioms for access methods with result bounds.

In other words, the only difference with the setting without result bounds is the last bullet point corresponding to (Result-bounded Fact Transfer).

We will now need an extension of the linearization result, Proposition 6.6, to handle these additional constraints:

**Proposition 6.8.** For any fixed  $w \in \mathbb{N}$ , given a set  $\Sigma$  of IDs of width w and a set  $\Delta$  of truncated accessibility, transfer, and Result-bounded fact transfer axioms, and given a set of facts  $I_0$ , we can compute in PTIME a set of IDs  $\Sigma^{\text{Lin}}$  of semi-width w and a set of facts  $I_0^{\text{Lin}}$  satisfying the following: for any Boolean  $CQ Q^*$  over the primed signature using constants from  $I_0$  and existentially quantified variables,  $Q^*$  is entailed from  $I_0$ ,  $\Sigma$ , and  $\Delta$  iff  $Q^*$  is entailed from  $I_0^{\text{Lin}}$  and  $\Sigma^{\text{Lin}}$ .

The proof of this will be a variation of the argument for Proposition 6.6. It will be explained at the end of Section 6.4.

Thus we follow the same route as before: linearization, noting that the special form of our constraints results in linear constraints of bounded semi-width. This completes the proof of Theorem 6.4 in the case with result bounds.

6.4. Proof of the Linearization Results (Proposition 6.6 and 6.8). We now turn to the missing element in the proof of Theorem 6.4, which are our linearization results, Proposition 6.6 and its analog for result-bounded methods, Proposition 6.8.

We first give the intuition on how our linearization works. In the tree-like chase for guarded TGDs, we have steps that create new nodes, and also *propagation steps*, that replicate facts across tree nodes. An intermediate goal will be to show that for guarded TGDs we can get a similar chase where we do not need to propagate across tree nodes. This will be the *shortcut chase*, defined later, where we only grow the tree and fire full rules at a given node, with no propagation. Note that the point of the shortcut chase is not to actually perform or construct it, but to reason about it. Once we have defined the shortcut chase and shown it is complete, it will be easy to perform linearization. The shortcut chase will make use of full GTGDs that we derive from our original set of GTGDs. The saturation process that creates these GTGDs will be a first step.

First we will review the notion of tree-structured chase proof that is well-known for guarded TGDs [CGL12], and show that we can further enforce the *downward-free* property, where facts only propagate back from a child to its ancestors in the tree. This is a step towards simplifying propagation in the chase. Second we will need to define a more general notion of *truncated accessibility axioms*, and give a PTIME algorithm for generating the ones that are small enough: this will give us the full GTGDs that we will need. Finally we present shortcut chase proofs, where these dependencies are fired in an even more specific order, and show that this definition of the chase is still complete. Lastly we use these tools to prove Proposition 6.6.

**Tree-like chase proofs and the downward-free property.** As a step towards our linearization result, we now present a general result about chase proofs with *single-headed GTGDs*, i.e., GTGDs having a single atom in the head. This will be applicable in particular to our analysis of the chase with IDs and candidate truncated accessibility axioms.

For any chase sequence  $I_0 \ldots I_n$  using single-headed GTGDs, we can associate a *tree-like* chase sequence, i.e., a sequence  $T_0 \ldots T_{n'}$  of chase trees. A chase tree  $T_i$  in such a sequence consists of a tree structure with a function FactsOf<sub>i</sub> that maps each node of  $T_i$  to a collection of facts. Each  $T_i$  is associated to the instance formed by unioning all the facts in its nodes, i.e., the union of FactsOf<sub>i</sub>(v) across all nodes v. Further, if v is not the root, there is a fact F in FactsOf<sub>i</sub>(v), the *birth fact of* v, which serves as a guard for the elements in the facts of FactsOf<sub>i</sub>(v). This fact F for the node v will never change throughout the sequence, so we denote it by BirthFact(v).

In a tree-like chase sequence  $T_0 
dots T_{k'}$ , consecutive chase trees will be linked by two kinds of steps. First, there will be *chase steps*, which add a fact to the tree, possibly in a new node. If  $T_{i+1}$  is produced from  $T_i$  by a chase step, this will correspond to a valid chase step for the two corresponding instances. Second, a step from  $T_i$  to  $T_{i+1}$  can be a *propagation step*, which does not change the underlying instance, but just copies facts from one node to another, i.e., it modifies FactsOf while maintaining the other components. Both steps are described in detail below.

For the case of *chase steps*, when we perform a chase step to transform  $T_i$  to  $T_{i+1}$ , we will always require it to be *tree-friendly*, i.e., we require that the image of the trigger lies in FactsOf<sub>i</sub>(v) for some node v. When a chase step fires a trigger for a GTGD  $\tau$  to create a fact F, we choose one such node v in which the image lies. If  $\tau$  is not full, then we extend the sequence to  $T_{i+1}$  by adding to  $T_i$  a new node v' as a child of v, setting BirthFact(v') := F, and setting FactsOf<sub>i+1</sub>(v') to be F along with any facts in v that are guarded by F — these facts are *forward propagated* from v' to v. If  $\tau$  is full, then we extend the sequence by defining  $T_{i+1} := T_i$  but changing the function FactsOf<sub>i+1</sub>. We set FactsOf<sub>i+1</sub>(v) to be FactsOf<sub>i</sub>(v)  $\cup$  {F} to create the new fact.

For the case of propagation steps, such a step can only take place if the preceding step was a chase step with a full GTGD  $\tau$ . Letting  $F = R(\vec{c})$  be the newly created fact, we consider the set  $B_{\vec{c}}$  of all nodes that contain a guard for  $\vec{c}$ . Our process ensures that  $B_{\vec{c}}$  will form a connected subtree of the chase tree  $T_i$ , and it contains the node v in which the chase step was performed. We choose a subset B' of  $B_{\vec{c}}$ , and propagate the new fact to all these nodes: for every node  $v' \in B'$ , we add F to FactsOf<sub>i+1</sub>(v').

Note that, unlike forward propagation, propagation steps allow us to propagate a fact upwards (from descendants to ancestors) as well as downwards (from descendant to ancestor). Further, it is optional, i.e., we can choose not to propagate.

It is clear that every tree-like chase sequence  $T_0 
dots T_{n'}$  induces a chase sequence in the usual sense of instances  $I_0 
dots I_n$ : propagation steps in the  $T_i$  do not result in any change to the instance, thus n may be less than n'. We say that such a sequence is a *tree-like chase* proof of some entailment if the resulting sequence  $I_0 
dots I_n$  is, and in addition  $T_0$  consists of only a single node with  $\mathsf{FactsOf}_0(r) = I_0$ . Note that any chase proof with single-headed GTGDs can be made into a tree-like chase proof: we can always choose to propagate facts everywhere they are guarded, and then the restriction to tree-friendly chase steps is without loss of generality.

An example is given in Figure 1, and explained in more detail in Example 6.9 just below. Note that as the chase proceeds, we only add nodes to the chase tree and add facts to existing nodes. In other words, given a tree node v associated to some instance  $I_i$  in a chase proof, v will exist at each later stage  $I_j$ , but may have additional facts.

We will be particularly interested in the case of proofs with IDs and candidate derived truncated accessibility axioms. In this case the full TGDs include the full IDs, as well as the candidate derived truncated accessibility axioms, which generate new accessibility facts.

**Example 6.9.** We use an example from [Kap19]. We consider the initial instance  $I_0 = \{R(c,d)\}$  and a set of single-headed GTGDs  $\Sigma$ 

$$\begin{split} R(x_1, x_2) &\to \exists y \, S(x_1, y), & R(x_1, x_2) \to \exists y \, T(x_1, x_2, y) \\ T(x_1, x_2, x_3) &\to \exists y \, U(x_1, x_2, y), & U(x_1, x_2, x_3) \to P(x_2), \\ T(x_1, x_2, x_3) \wedge P(x_2) \to M(x_1), & S(x_1, x_2) \wedge M(x_1) \to \exists y \, N(x_1, y), \end{split}$$

the sequence

$$I_0 = \{R(c,d)\}, I_1 = I_0 \cup \{S(c,d_1)\}, I_2 = I_1 \cup \{T(c,d,d_2)\}, I_3 = I_2 \cup \{U(c,d,d_3)\}, I_4 = I_3 \cup \{P(d)\}, I_5 = I_4 \cup \{M(c)\}, I_6 = I_5 \cup \{N(c,d_4)\}$$

is a chase sequence for  $I_0$  and  $\Sigma$ . A corresponding tree-like chase sequence  $T_0, \ldots, T_8$  is depicted in Figure 1.



Figure 1: Tree-like chase for Example 6.9.

The representation is the following. When we have performed a chase step with a non-full GTGD (e.g., from  $T_0$  to  $T_1$ ), the new created node is represented in red, and the node containing the image of the trigger (its parent node) has a blue border. When such a step performs forward propagation of facts (e.g., from  $T_7$  to  $T_8$ ), the forward propagated fact are written in blue in the parent node, and in red in the newly created node. When we have performed a chase step with a full GTGD (e.g., from  $T_3$  to  $T_4$ ), the node containing

the image of the trigger again has a blue border, and the new fact (created in the same node) is in red. When we have performed a propagation step (e.g., from  $T_4$  to  $T_5$ ), the fact being propagated is written in blue in the node from where we propagate it — namely, the node where it was created in the previous step by a full chase step, and is written in red in the nodes where it is propagated. Note that, in these examples, propagation steps always propagate new facts everywhere they are guarded.

Our linearization result will rely on the fact that chase proofs can be normalized to ensure that the propagation of facts in propagation steps only happens in the "upwards" direction, that is, towards the root of the tree. Note that this does not affect the propagation of facts to child nodes when firing a chase step with a non-full GTGD.

**Definition 6.10** (Downward-free chase sequence). We say that a tree-like chase sequence  $T_0 \ldots T_n$  with single-headed GTGDs is *downward* -free if propagation steps always propagate a fact F to ancestors of the node where it is created. A downward-free chase proof of an entailment is just a downward-free chase sequence that is a chase proof.

**Example 6.11.** We continue with Example 6.9, taken from [Kap19]. The chase depicted in Figure 1 is not downward-free. Indeed, the propagation step from  $T_6$  to  $T_7$  propagates the fact M(c) to the left child of the rood, which is not an ancestor of the node where it was created. However, if we do not propagate it to this node, we can no longer perform the chase step from  $T_7$  to  $T_8$  to create  $N(c, d_4)$ .

Instead, we can redo steps in the chase to make it downward-free. We design a tree-like chase sequence  $T'_0, \ldots, T_{10'}$ , with  $T_i = T'_i$  for all  $0 \le i \le 6$ . We depict  $T'_5 = T_5$ ,  $T'_6 = T_6$ , and  $T'_7, \ldots, T'_{10}$  in Figure 2.



Figure 2: Modification of the chase from Figure 1 to obtain a downward-free chase.
One can think of downward-free chase sequences as a chase version which is more similar to the chase with linear TGDs, because it is never useful to propagate facts when chasing with such TGDs — further chase steps cannot use the propagated fact to fire a rule. Another advantage of downward-free proofs is that if we follow the evolution of a subtree of some node v within a proof, what we see happening in that subtree is a self-contained proof of all facts derived in the subtree, using only the initial facts of v. Indeed, the chase steps performed afterwards outside of the subtree will never modify the contents of the subtree.

**Proposition 6.12.** Let  $T_0 
dots T_j$  be a downward-free chase proof. Assume that, in moving to  $T_i$ , we perform a chase step that creates a node v. Let  $T'_i 
dots T'_m$  be the tree-like chase sequence obtained from  $T_i 
dots T_j$  by restricting to the subtree rooted at v in  $T_i 
dots T_j$ , eliminating duplicate consecutive chase trees. Then  $T'_i 
dots T'_m$  is a downward-free chase proof of the facts of  $T'_m$  from the facts  $\mathsf{FactsOf}_i(v)$  of v in  $T_i$ .

*Proof.* Note that  $T'_i$  consists of a single node containing the facts of v in  $T_i$ . By the definition of the downward-free chase, the triggers in all chase steps within  $T_i \ldots T_j$  used only facts that were generated within the subtree of v earlier in the same sequence in a node in the subtree of v. Thus, by an immediate induction on m - i, all these steps can also be triggered in  $T'_i \ldots T'_m$ . So  $T'_i \ldots T'_m$  is indeed a chase sequence proving the required facts, and it is downward-free because the original sequence was.

This is a variation of Corollary 3.1.5 of [Kap19]. Similar statements appear in our earlier work [AB18b].

We now show the key claim that we can always restrict to downward-free chase sequences:

**Theorem 6.13.** For every tree-like chase sequence using single-headed GTGDs  $T_0 \ldots T_n$ , there is a downward-free tree-like chase sequence  $T_0 = \overline{T_0}, \ldots, \overline{T_m}$  such that there is a homomorphism h from the instance of  $T_n$  to the instance of  $\overline{T_m}$  with h(c) = c for any values c in the domain of the instance of  $T_0$ .

In particular, if we have a chase proof of a UCQ Q from an instance  $I_0$  using GTGDs  $\Sigma$ , then we have downward-free proof of Q, starting from  $T_0$  consisting of a single node containing  $I_0$ , applying chase steps via  $\Sigma$ . The proof is based on the idea in Figure 2. It is inspired by the conference version of this paper, and by Proposition 3.1.6 in [Kap19]. It is presented in Appendix B. Note that, in this downward-free chase, we may need to fire triggers that are not active.

We emphasize that the downward-free chase is never used as an algorithm to get better complexity bounds directly. We will only use it to justify steps in our linearization process.

Generalized truncated accessibility axioms and saturation. Having presented the downward-free chase, we return to the proof of our first linearization result (Proposition 6.6). Recall that this result applies to constraints formed of IDs  $\Sigma$  of width w and a set  $\Delta$  of truncated accessibility and transfer axioms. Recall that a transfer axiom is of the form:

$$\left(\bigwedge_{i} \operatorname{accessible}(x_{i})\right) \land R(\vec{x}, \vec{y}) \to R'(\vec{x}, \vec{y})$$

In the first step towards linearization, we will perform a construction that enlarges the truncated accessibility axioms to certain TGDs that have a similar shape, which we call *candidate derived truncated accessibility axioms.* By this we mean any TGD of the following form:

$$\Big(\bigwedge_{i\in P} \operatorname{accessible}(x_i)\Big) \land R(\vec{x}) \to \operatorname{accessible}(x_j)$$

where R is a relation and P is a subset of the positions of R. Notice that the axioms of the form (Truncated Accessibility) defined earlier can indeed be rewritten to be of this form: the only difference from their original form is that we have rewritten them further to ensure that the head always contains a single accessibility fact.

Intuitively, such an axiom tells us that, when a subset of the elements of an R-fact are accessible, then another element of the fact becomes accessible (by performing an access). We will start by considering what we call the *original truncated accessibility axioms*: these are simply the (Truncated Accessibility) axioms in the set  $\Delta$ , which are in the form above, i.e., with a single **accessible** fact in the head. For these axioms, the set P is the set of input positions of some method **mt** on R. We will also study candidate derived truncated accessibility axioms that are not necessarily given in  $\Delta$ , but which are semantically *entailed* by the original truncated accessibility axioms in  $\Delta$  and by the constraints in  $\Sigma$ . By entailment, we always mean the semantic notion discussed in Section 3, i.e., entailments witnessed by a chase proof starting with facts in the body of the dependency, concluding with an instance having a suitable homomorphism from the head of the dependency. The candidate derived truncated accessibility axioms that are entailed are simply called the *derived truncated accessibility axioms*.

There can be exponentially many derived truncated accessibility axioms, but we will not need to compute all of them: it will suffice to compute those of small *breadth*. Formally, the *breadth* of a candidate derived truncated accessibility axiom is the size of P. Note that the number of possible candidate derived truncated accessibility axioms of breadth b is at most  $r \cdot a^{b+1}$ , where r is the number of relations in the signature and a is the maximal arity of a relation. We show that we can efficiently compute the derived truncated accessibility axioms of a given breadth, by introducing a *truncated accessibility axiom saturation algorithm*.

The algorithm iteratively builds up a set O of triples  $(R, \bar{p}, j)$  with  $\bar{p}$  a set of positions of R of size at most w and j a position of R. Each such triple represents the following candidate derived truncated accessibility axiom of breadth  $\leq w$ :

$$\left(\bigwedge_{i\in\bar{p}}\operatorname{accessible}(x_i)\right)\wedge R(\vec{x})\to\operatorname{accessible}(x_j).$$

The first step of the algorithm is to set  $O := \{(R, \bar{p}, j) \mid j \in \bar{p}\}$ , representing trivial axioms. The algorithm then repeats the steps below:

• (ID): If we have an ID  $\forall \vec{x} \ R(\vec{x}) \to \exists \vec{y} \ S(\vec{z})$ , where  $x_{j_1}, \ldots, x_{j_{m'}}, x_j$  (with  $m' + 1 \leq w$ ) are exported variables that appear respectively in positions  $k_1 \ldots k_{m'}, k$  within the head atom  $S(\vec{z})$ , and if we have  $(S, \{k_1 \ldots k_{m'}\}, k) \in O$ , then we add the tuple  $(R, \{j_1 \ldots j_{m'}\}, j)$  to O.

The intuition for the (ID) step is that derived truncated accessibility axioms that hold on the target relation S can be "propagated upwards" to R, i.e., if an accessible fact is created using the S-fact, then the same creation can happen using the R-fact.

• (Transitivity): If there exists a relation R, a set of positions  $\bar{p}$  of R, and a set of positions  $\{t_1 \dots t_m\}$  of R with  $m \leq w$  such that we have  $(R, \bar{p}, t_i) \in O$  for all  $1 \leq i \leq m$ , and we have  $(R, \bar{r}, t') \in O$  with  $\bar{r} \subseteq \bar{p} \cup \{t_1 \dots t_m\}$ , then we add  $(R, \bar{p}, t')$  to O.

The intuition for (Transitivity) is that we add triples that result from the natural entailment relation on triples, provided that the number of intermediate values that are projected away is not more than w.

• (Access): If we have a method mt on R with input positions  $j_1 \dots j_m$  and a set  $\bar{p}$  of at most w positions such that  $(R, \bar{p}, j_i) \in O$  for all  $1 \leq i \leq m$ , then we add  $(R, \bar{p}, j)$  to O for all j between 1 and the arity of R.

To understand (Access), notice that we cannot add triples corresponding to all access methods, since the number of inputs to an access method might be above the breadth bound. Thus (Access) is actually a special kind of transitivity calculation that adds triples of low breadth that can result from composing derived truncated accessibility axioms with an access method.

We continue the algorithm until we reach a fixpoint.

Note that the maximal number of triples produced is  $r \cdot a^{w+1}$ , with r the number of relations in the schema and a the maximal arity of a relation. Thus a fixpoint must be reached in this number of steps. Thus, for fixed w, it is clear that the algorithm runs in polynomial time in  $\Sigma$  and in the set of access methods.

We will show that this algorithm correctly computes all derived truncated accessibility axioms satisfying the breadth bound:

**Proposition 6.14.** For any fixed  $w \in \mathbb{N}$ , given as input a set of IDs of width w and a set of access methods, the truncated accessibility saturation algorithm computes all derived truncated accessibility axioms of breadth at most w.

Our proof of Proposition 6.14 is where we use the downward-free chase defined earlier.

*Proof.* For one direction, it is straightforward to see that all rules obtained by this process are in fact derived truncated accessibility axioms. Conversely, we claim that, for all derived truncated accessibility axioms of breadth  $\leq w$ 

accessible $(x_{s_1}) \land \ldots \land$  accessible $(x_{s_l}) \land R(\vec{x}) \rightarrow$  accessible $(x_i)$ ,

the corresponding triple  $(R, \{s_1 \dots s_l\}, i)$  is added to O. We write  $\bar{p} = \{s_1 \dots s_l\}$ ; note that  $|\bar{p}| \leq w$ .

Remember that, by the completeness of the chase (see Section 3) this semantic entailment is always witnessed by a chase proof, and remember by Theorem 6.13 that we can assume without loss of generality that it is a downward-free tree-like chase proof. We prove the claim by induction on the length of a downward-free tree-like chase proof of the fact  $\operatorname{accessible}(c_i)$ from  $I_0 = \{R(\vec{c})\} \cup \{\operatorname{accessible}(c_j) \mid j \in \bar{p}\}$ . Here  $I_0$  is the canonical database of the left-hand side of the implication, where we have used  $\vec{c}$  for the variables to emphasize that they are being treated as elements of the canonical database.

If the proof is trivial, i.e., the fact  $\operatorname{accessible}(c_i)$  is one of the  $\operatorname{accessible}(c_{s_j})$ , then clearly  $(R, \bar{p}, i) \in O$  by the initialization of O. If it is non-trivial then some accessibility axiom provided the final firing to produce  $\operatorname{accessible}(c_i)$ , and we can fix a guard atom F and accessibility facts  $F_1 \ldots F_l$  that were hypotheses of the chase step. If F is the fact  $R(\vec{c})$ , then each  $F_j$  is of the form  $\operatorname{accessible}(c_{t_j})$  for some index  $t_j$  and by induction we have  $(R, \bar{p}, t_j) \in O$  for each i. Now by (Access) we deduce that  $(R, \bar{p}, i) \in O$ .

Otherwise, the guard F is the birth fact of some non-root tree node v. Consider the child v' of the root node which is an ancestor of v; potentially v' = v. Let  $S(\vec{d})$  be the birth fact of v'; we know that v' was created by firing an ID  $\delta$  on the root node. Let  $\bar{q}$  be the subset of positions  $j \in \{1, \ldots, |\vec{d}|\}$  for which the fact accessible $(d_j)$  was propagated from

the root node when v' was created. This propagation witnesses that, in the ID  $\delta$ , each position in  $\bar{q}$  in the head atom contains an exported variable, i.e., a variable that also occurs in the body: we call this an *exported head position*. We denote by  $\bar{r}$  the corresponding set of *exported body positions*, i.e., the positions in the body atom of  $\delta$  contains an exported variable. By definition  $|\bar{r}| = |\bar{q}|$ , and further  $|\bar{q}| \leq w$ . For each  $j \in \bar{q}$ , letting j' be the index of  $\bar{r}$  such that  $c_{j'} = d_j$ , we know that the chase up to the creation of v' provided a strictly shorter downward-free tree-like chase proof of  $\operatorname{accessible}(c_{j'})$  from  $I_0$ . Thus, by the induction hypothesis, we have  $(R, \bar{p}, j') \in O$  for each  $j' \in \bar{r}$ .

As v and the root node both contain the value  $c_i$ , the fact  $S(\vec{d})$  must also contain this value. Let i' be an index such that  $d_{i'} = c_i$ . By the downward-free property and Proposition 6.12, we know that the chase within the subtree of v' provides a proof of accessible $(d_{i'})$ from  $S(\vec{d})$  conjoined with accessible $(d_j)$  for  $j \in \bar{q}$ . Again, this is a strictly shorter downwardfree tree-like chase proof, so by induction hypothesis we have that  $(S, \bar{q}, i') \in O$ . We know that the positions of  $\bar{q}$  are exported head positions of  $\delta$ , and we know that i' is also an exported head position head position because  $c_i$  appears in v. Thus, we know by the (ID) axiom that  $(R, \bar{r}, i) \in O$ . Now, putting this together with the conclusion of the previous paragraph, we conclude using the (Transitivity) axiom that  $(R, \bar{p}, i) \in O$ .

Thus we have shown that we can compute in PTIME the implication closure of truncated accessibility axioms of bounded breadth under bounded-width IDs.

**Shortcut chase and completeness.** We know from Theorem 6.13 that for any set of single-headed GTGDs we can do a downward-free chase, where propagation of facts is restricted to be descendant-to-ancestor. We used this in the context of the GTGDs generated from answerability problems with bounded-depth IDs, to justify a saturation algorithm in which certain derived TGDs are added. With this in place, we are now ready to simplify the chase process further, arriving at a tree-like chase process that does *no propagation at all*: the chase only grows the tree structure and adds facts within a node of the tree. Instead of applying chase steps with truncated accessibility axioms, which would have required propagation to ancestors, we will show that we can create the same facts by firing derived axioms of small breadth in a "greedy fashion". To connect this to our final goal of linearization, we note that in doing a tree-like chase with linear TGDs, we do not need to propagate facts at all, since no rule bodies care about multiple facts. Thus a tree-like chase without propagation is bringing us closer to our goal of a chase with linear TGDs.

Recall that  $\Sigma$  consists of IDs of width w and that we have a set  $\Delta$  of truncated accessibility axioms (and transfer axioms, which we do not consider at this stage). Remember that we can use Proposition 6.14 on  $\Sigma$  and  $\Delta$  to compute in PTIME the set of all derived truncated accessibility axioms of breadth at most w, which we denote by  $\Delta^+$ .

A shortcut chase proof on an initial instance  $I_0$  with  $\Sigma$  and  $\Delta$  will be a variation of the notion of tree-like chase proof defined earlier, but specific to IDs and derived truncated accessibility axioms. A shortcut chase proof will alternate between two kinds of steps:

• *ID-steps*, where we fire an ID on a trigger  $\tau$  to generate a fact F: we put F in a new node n which is a child of the node n' containing the fact of  $\tau$ ; and we copy in n all facts of the form accessible(c) that held in n' about any element c that was exported when firing  $\tau$ .



Figure 3: A chase proof (top), and a corresponding shortcut chase proof (bottom) with saturation steps indicated

• Breadth-bounded saturation steps, where we consider a newly-created node n and apply all derived truncated accessibility axioms of breadth at most w on that node, i.e., those of  $\Delta^+$ , until we reach a fixpoint and there are no more violations of these axioms on n.

We continue this process until a fixpoint is reached. Any stage in the proof is thus associated with a tree structure, as in tree-like chase proofs. Each node in the tree corresponds to the application of an ID, which created the *birth fact* for the node; and each node may additionally contain accessibility facts in addition to the birth fact. The name "shortcut" intuitively indicates that we shortcut certain derivations that could have been performed by moving up and down in the chase tree: instead, we apply a derived truncated accessibility axiom. Figure 3 illustrates the notion.

We show that this process correctly generates everything that the usual chase would generate:

**Lemma 6.15.** Let  $\Sigma$  be a set of IDs of width w and  $\Delta$  a set of truncated accessibility axioms. Let  $I_0$  be a set of facts, and I be produced from  $I_0$  as the final instance in a chase proof using  $\Sigma$  and  $\Delta$ . Let  $\Delta^+$  be, as above, the set of derived truncated accessibility axioms of breadth at most w. Lastly, let  $I_0^+$  be the set of facts entailed by  $I_0$  and  $\Delta^+$ .

breadth at most w. Lastly, let  $I_0^+$  be the set of facts entailed by  $I_0$  and  $\Delta^+$ . Then there is  $I^{SC}$  produced by a shortcut chase proof based on  $\Sigma$  and  $\Delta$ , from initial instance  $I_0^+$ , and a homomorphism from I to  $I^{SC}$  which is the identity on  $I_0$ .

To prove this lemma, we start with an observation about the closure properties of shortcut chase proofs.

**Lemma 6.16.** Let  $I_0^+$  be an initial instance closed under  $\Delta^+$ , and suppose that a shortcut chase proof on  $I_0^+$  with  $\Sigma$  and  $\Delta$  has a breadth-bounded saturation step on node n producing a fact accessible(a). Then a is not in  $\operatorname{Adom}(I_0^+)$ , and n was created by the ID-step where a is generated.

*Proof.* Let  $I^-$  be the instance just before the breadth-bounded saturation step generating accessible(a). First, notice that the breadth-bounded saturation step in question must apply to a node which is not the root, as  $I_0^+$  is closed under  $\Delta^+$  so no new accessible facts can be created at the root node. Thus, it applies to a node  $n_1$  created at an ID-step. Let  $\tau$  be the ID that we fired in this step,  $n_0$  be the node on which we fired  $\tau$ . Let E be the birth fact of  $n_0$ , recalling that this is the sole fact over a relation other than accessible holding in the node. Let F be the birth fact of the node  $n_1$ . It suffices to show that E does not contain the element a, as a will then have been introduced in the ID-step that creates node  $n_1$ , in particular it is not in  $Adom(I_0^+)$  because  $n_1$  is not the root node.

To show this that E does not contain a, let us assume by contradiction that it does. Let R be the relation of E,  $\bar{p}$  be the positions of E containing the elements which occur in F and for which the relation accessible holds in  $I^-$ . Let j be the position of a in E. By considering the subtree rooted at the node  $n_0$ , which contains E, we see that a shortcut chase proof starting with the fact E and with the elements at positions  $\bar{p}$  being accessible would also derive that the element at position j is accessible: it would do so with an ID-step firing  $\tau$  to create a child node, and doing the same breadth-bounded saturation step on that node as the one that creates accessible(a) in  $I^-$ . Reusing the triple notation from the saturation algorithm, this implies that  $(R, \bar{p}, j)$  is a derived truncated accessibility axiom. But then this axiom should have been fired in the breadth-bounded saturation step just after the node  $n_0$  was created, contradicting the assumption that accessible(a) is created at node  $n_1$ . Hence, the fact E cannot contain a, which concludes the proof.

We now are ready to finish the proof of Lemma 6.15, which shows completeness of the shortcut chase:

Proof. The instance I is produced from  $I_0$  as the final instance  $I_f$  of a chase proof  $I_1 \ldots I_f$ using  $\Sigma$  and  $\Delta$ . We can extend this sequence to an infinite one  $I_1 \ldots I_f \ldots$  in which every trigger of  $\Sigma \cup \Delta$  in some instance is eventually fired. Thus letting  $I_{\infty}$  denote the union of these instances, we have  $I_{\infty}$  satisfies  $\Sigma \cup \Delta$  and  $I_0$  embeds as a subinstance of  $I_{\infty}$ . Likewise, we can continue the shortcut chase process indefinitely, letting  $I_{\infty}^{SC}$  be the resulting facts. It suffices to show that  $I_{\infty}^{SC}$  satisfies the constraints of  $\Sigma$  and  $\Delta$ . Indeed, by universality of the chase [FKMP05], we would then know that there is a homomorphism from  $I_{\infty}$  into  $I_{\infty}^{SC}$  that is the identity on  $I_0$ . The same function clearly serves as a homomorphism from I into  $I_{\infty}^{SC}$ , as required by the lemma.

It is clear, thanks to the ID-steps, that  $I_{\infty}^{SC}$  satisfies the constraints of  $\Sigma$ . We claim that  $I_{\infty}^{SC}$  also satisfies the constraints of  $\Delta$ . Assume by contradiction that there is an active trigger in  $I_{\infty}^{SC}$  for an axiom of  $\Delta$ , with facts  $(\bigwedge \operatorname{accessible}(c_{m_j})) \wedge R(\vec{c})$ , whose firing would have produced fact  $\operatorname{accessible}(c_i)$ . Consider the node *n* where  $R(\vec{c})$  occurs in the shortcut chase proof.

We first observe that n cannot be the root node corresponding to  $I_0^+$ . Indeed, let us assume that it is. Then, the facts  $\operatorname{accessible}(c_{m_j})$  used in the firing are facts about elements of  $I_0^+$ , and Lemma 6.16 implies that they cannot have been generated in a breadth-bounded saturation step. So they must already be in  $I_0^+$ . But  $I_0^+$  then contains all the facts required to fire the active trigger, contradicting the fact that  $I_0^+$  is closed under the axioms of  $\Delta$ . Thus, n is not the root node.

Now, if the node n is not the root, then consider each fact  $\operatorname{accessible}(c_{m_j})$  in the trigger of the firing. Let us show that n contains all these facts. If  $\operatorname{accessible}(c_{m_j})$  is a fact of  $I_0^+$ , then

it has been propagated from the root node to n, so it is in n. Otherwise,  $\operatorname{accessible}(c_{m_j})$  was created by firing some breath-bounded saturation step. By Lemma 6.16, the node  $n_j$  where this step was fired is the node where  $c_{m_j}$  is generated. Now, as the node n contains  $c_{m_j}$ , it must be a descendant of the node  $n_j$  where  $c_{m_j}$  is generated. Now, as the fact  $\operatorname{accessible}(c_{m_j})$  was created in  $n_j$ , it must have been propagated downwards until we created node n, so it must also be in n. Hence, in all cases, the node n contained all the facts required to fire the active trigger, so the trigger should have been fired at the breadth-bounded saturation step at n. This again yields a contradiction.

We conclude that in fact there cannot be an active trigger in  $I_{\infty}^{SC}$ , so  $I_{\infty}^{SC}$  satisfies the constraints of  $\Delta$ , concluding the proof.

Concluding the proof of Proposition 6.6. Recall that our goal in Proposition 6.6 is to simulate the chase with bounded-width IDs  $\Sigma$  and truncated accessibility and transfer axioms  $\Delta$ . We will now present our definition of the set of IDs  $\Sigma^{\text{Lin}}$  that will do so. Thanks to what precedes (Lemma 6.15), we know that it suffices to simulate the shortcut chase, and conversely it is obvious that the shortcut chase is sound in the sense that any shortcut chase step could be replaced in a derivation of a CQ by a sequence of ordinary chase steps.

We let  $\Delta^+$  be the set of derived truncated accessibility axioms of breadth  $\leq w$  calculated using the truncated accessibility saturation algorithm on  $\Sigma$  and  $\Delta$ , including the axioms already present in  $\Delta$ . To define the linearized axioms, we first need some notation. For a relation R, a subset P of the positions of R, and a position j of R, we will say that Ptransfers j if  $\Delta^+$  contains the following derived truncated accessibility axiom:

$$\left(\bigwedge_{i\in P} \operatorname{accessible}(x_i)\right) \wedge R(\vec{x}) \to \operatorname{accessible}(x_j).$$

Reusing the triple notation from the saturation algorithm, this axiom corresponds to the triple (R, P, j).

We now define  $\Sigma^{\text{Lin}}$ . Recall that it is defined over the signature  $\mathcal{S}^{\text{Lin}}$  where we added a relation  $R_P$  for every relation R and subset P of positions of size at most w, intuitively standing for an R-fact where the elements at position P are accessible. The rules of  $\Sigma^{\text{Lin}}$  are:

• (Lifted Transfer): Consider each relation R, and subset P of positions of R of size at most w. Let P' be the set of positions transferred by P. If P' contains the set of input positions of some access method on R, then we add the full ID:

$$R_P(\vec{x}) \to R'(\vec{x}).$$

• (Lift): Consider each ID  $\delta$  of  $\Sigma$ ,

$$R(\vec{u}) \to \exists \vec{z} \ S(\vec{z}, \vec{u}).$$

For every subset P of positions of R of size at most w, we let P' be the set of positions transferred by P. We let P'' be the intersection of P' with the positions of R that carry an exported variable in the atom  $R(\vec{u})$  within the body of  $\delta$ . Finally, we let P''' be the subset of the exported positions in the head of  $\delta$  that corresponds to P''. Then we add the dependency:

$$R_P(\vec{u}) \to \exists \vec{z} \; S_{P'''}(\vec{z}, \vec{u}).$$

We also need to define the instance  $I_0^{\text{Lin}}$  from  $I_0$ , to account for the effect of  $\Sigma$  and  $\Delta$  when we start the chase. We recall that S denotes the signature of the schema, the constraints of  $\Sigma$  are expressed on S, and the constraints  $\Sigma'$  are expressed on a primed

copy S' of S. Lastly, recall that  $\Delta$  consists of truncated accessibility axioms and transfer axioms that are expressed on S, S', and the unary relation accessible. Given a CQ Q, let  $I_0 := \mathsf{CanonDB}(Q)$  be its canonical database, and let  $I_0^{\mathsf{Lin}}$  be formed by adding atoms to  $I_0$ as follows.

- Apply all of the truncated accessibility axioms of  $\Delta^+$  to  $I_0$  to obtain  $I_0^+$ .
- Initialize  $I_0^{\text{Lin}} := I_0^+$ . Now, consider every relation R of the signature  $\mathcal{S}$ , and every fact  $R(a_1 \ldots a_n)$  of  $I'_0$ . Let P be the set of the  $i \in \{1 \ldots n\}$  such that  $\operatorname{accessible}(a_i)$  holds in  $I_0^+$ . For every  $P' \subseteq P$  of size at most w, add to  $I_0^{\text{Lin}}$  the fact  $R_{P'}(a_1 \ldots a_n)$ . Further, if  $\operatorname{accessible}(a_i)$  holds for each  $1 \leq i \leq n$ , then add the fact  $R'(a_1 \ldots a_n)$  to  $I_0^{\text{Lin}}$ .

It is now easy to see that  $\Sigma^{\text{Lin}}$  and  $I_0^{\text{Lin}}$  satisfy the required conditions: for every Boolean CQ over the primed facts I derived using a chase proof from  $I_0$  with  $\Sigma$  and  $\Delta$ , we can derive the same CQ from  $I_0^{\text{Lin}}$  via a chase proof with  $\Sigma^{\text{Lin}}$ . Indeed, applying chase steps with the (Lift) rules creates a tree of facts that corresponds to a shortcut chase proof, up to an  $I_0$ -preserving isomorphism: when we create an  $R_P$ -fact, the P subscript denotes exactly the set of positions of the new facts that contain exported elements that are accessible. Further, the full (Lifted Transfer) rules create a primed copy of these facts exactly when they can be transferred by applying some method. As for the converse direction, it is clear that applying chase steps with  $\Sigma^{\text{Lin}}$  on  $I_0^{\text{Lin}}$  only generates primed facts that correspond to what would be generated by the shortcut chase, so that whenever we derive a Boolean CQ over the primed facts then we generate a match of the same CQ, up to an  $I_0$ -preserving isomorphism, in the shortcut chase. This justifies that the CQ is also entailed from  $I_0$  by applying chase steps with  $\Sigma$  and  $\Delta$ , first to create the facts of  $I_0^{\text{Lin}}$ , and then to derive the CQ. The only thing left to do is to notice that  $\Sigma^{\text{Lin}}$  has bounded semi-width, but this is

The only thing left to do is to notice that  $\Sigma^{\text{Lin}}$  has bounded semi-width, but this is because the rules (Lift) have bounded width and the rules (Lifted Transfer) clearly have an acyclic position graph. This concludes the proof of Proposition 6.6.

# Handling Result-bounded Fact Transfer axioms and the proof of Proposition 6.8. Recall that to prove Theorem 6.4 in the case *with* result bounds, we need only to prove the corresponding linearization result, Proposition 6.8, which extends Proposition 6.6.

In the presence of result bounds, the reduction to query containment additionally created axioms called (Result-bounded Fact Transfer), of the following form:

$$\left(\bigwedge_{i} \operatorname{accessible}(x_{i})\right) \wedge R(\vec{x}, \vec{y}) \to \exists \vec{z} \ R'(\vec{x}, \vec{z}).$$

We can extend the proof of Proposition 6.6 to prove Proposition 6.8. Our result on restricting to downward-free chase proofs, Theorem 6.13, can be used as-is, because it is stated for single-headed GTGDs. The truncated accessibility saturation algorithm proved in Proposition 6.14 can also be used as-is, as it only considers the truncated accessibility axioms. We can then define the shortcut chase as before, and its completeness result Lemma 6.15, again because this only considers IDs and truncated accessibility axioms. Now, we only change the last step of the proof of Proposition 6.6 and change our definition of the IDs  $\Sigma^{\text{Lin}}$  by adding the following rules to our rewriting:

• (Lifted Result-bounded Fact Transfer): For each relation R and subset P of positions of R of size at most w containing all input positions of some access method **mt** on R with a result bound, we add the ID:

$$R_P(\vec{x}, \vec{y}) \to \exists \vec{z} \ R'(\vec{x}, \vec{z})$$

where  $\vec{x}$  denotes the input positions of mt.

It is clear that adding these axioms, and using them when defining  $I_0^+$  from  $I_0$  in the definition of  $I_0^{\text{Lin}}$  above, ensures that the same primed facts are generated as in the shortcut chase, and the resulting axioms still have bounded semi-width: the (Lifted Result-bounded Fact Transfer) axioms are grouped in the acyclic part together with the (Lifted Transfer) axioms, and they still have an acyclic position graph. Hence, this establishes Proposition 6.8, which was all we needed to conclude the proof of Theorem 6.4 in the case with result bounds.

## 7. Schema simplification for expressive constraints

We have presented in Section 5 the two kinds of simplifications anticipated in the introduction: existence-check simplification (using result-bounded methods to check for the existence of tuples, as in Example 1.4); and FD simplification (using them to retrieve functionally determined information, as in Example 1.5). A natural question is then to understand whether these simplifications capture all the ways in which result-bounded methods can be useful, for integrity constraints expressed in more general constraint languages. It turns out that this is not the case when we move even slightly beyond IDs:

**Example 7.1.** Consider a schema Sch with TGD constraints  $T(y) \wedge S(x) \rightarrow T(x)$  and  $T(y) \rightarrow \exists x \ S(x)$ . We have an input-free access method  $\mathsf{mt}_S$  on S with result bound 1 and a Boolean access method  $\mathsf{mt}_T$  on T. Consider the query  $Q = \exists y \ T(y)$ . Note that the constraints imply that Q is equivalent to  $\exists x \ T(x) \wedge S(x)$ .

The following monotone plan answers Q:

 $T_1 \leftarrow \mathsf{mt}_S \leftarrow \emptyset; \qquad T_2 \leftarrow \mathsf{mt}_T \leftarrow T_1; \qquad T_3 \coloneqq \pi_{\emptyset} T_2; \qquad \mathsf{Return} \ T_3;$ 

That is, we access S and return true if the result is in T.

On the other hand, consider the existence-check simplification  $\mathsf{Sch}^{\dagger}$  of  $\mathsf{Sch}$ . It has an existence-check method on S, but we can only test if S is non-empty, giving no indication whether Q holds. So Q is not answerable in  $\mathsf{Sch}^{\dagger}$ . The same holds for the FD simplification of  $\mathsf{Sch}$ , because  $\mathsf{Sch}$  implies no FDs, so the FD simplification and existence-check simplification are the same.

Thus, existence-check simplification and FD simplification no longer suffice for more expressive constraints. In this section, we introduce a new notion of simplification, called *choice simplification*. We will show that it allows us to simplify schemas with very general constraint classes, in particular TGDs as in Example 7.1. In the next section, we will combine this simplification with our query containment reduction (Proposition 4.9) to show decidability of monotone answerability for much more expressive constraints. Intuitively, choice simplification changes the *value* of all result bounds, replacing them by one; this means that the number of tuples returned by result-bounded methods is not important, provided that we obtain at least one if some exist. We formalize the definition in this section, and show choice simplifiability for two constraint classes: equality-free first-order logic (which includes in particular TGDs), and UIDs and FDs. We study the decidability and complexity consequences of these results in the next section. **Choice simplification.** Given a schema Sch with result-bounded methods, its *choice* simplification Sch<sup>†</sup> is defined by keeping the relations and constraints of Sch, but changing every result-bounded method to have bound 1. That is, every result-bounded method of Sch<sup>†</sup> returns  $\emptyset$  if there are no matching tuples for the access, and otherwise selects and returns one matching tuple. We call Sch *choice simplifiable* if any CQ having a monotone plan over Sch has one over Sch<sup>†</sup>. This implies that the value of the result bounds never matters.

Choice simplifiability is weaker than existence-check or FD simplifiability, in the sense that existence-check simplifiability or FD simplifiability imply choice simplifiability. Still, choice simplifiability has a dramatic impact on the resulting query containment problem:

**Example 7.2.** Recall the schema Sch in Example 1.1 and its naïve axiomatization in Example 4.10. As Sch is choice simplifiable, we can axiomatize its choice simplification instead, and the problematic axiom in the third bullet item becomes a simple ID:  $\mathsf{Udirectory}(\vec{y}) \rightarrow \exists \vec{z} \; \mathsf{Udirectory}_{\mathsf{Accessed}}(\vec{z}).$ 

**Showing choice simplifiability.** We now give a result showing that choice simplification holds for a huge class of constraints: all first-order constraints that do not involve equality. This result implies, for instance, that choice simplification holds for integrity constraints expressed as TGDs:

**Theorem 7.3.** Let Sch be a schema with constraints in equality-free first-order logic (e.g., TGDs), and let Q be a CQ that is monotonically answerable in Sch. Then Q is monotonically answerable in the choice simplification of Sch.

*Proof.* We will again use the equivalence between monotone answerability and AMonDet, and use the "blowing-up" construction of Lemma 5.3. Note that, this time, the schema of Sch and Sch<sup>†</sup> is the same, so we simply need to show that  $I_1^{\dagger}$  is a subinstance of  $I_1$  for each  $p \in \{1, 2\}$ .

Consider a counterexample  $I_1^{\dagger}$ ,  $I_2^{\dagger}$  to AMonDet for Q in the choice simplification: we know that  $I_1^{\dagger}$  satisfies Q, that  $I_2^{\dagger}$  violates Q, that  $I_1^{\dagger}$  and  $I_2^{\dagger}$  satisfy the equality-free first order constraints of Sch, and that  $I_1^{\dagger}$  and  $I_2^{\dagger}$  have a common subinstance  $I_{\text{Accessed}}^{\dagger}$  which is access-valid in  $I_1^{\dagger}$  in the choice simplification of Sch. We will expand them to  $I_1$  and  $I_2$  that have a common subinstance which is access-valid in  $I_1$  for Sch.

For each element a in the domain of  $I_1^{\dagger}$ , introduce infinitely many fresh elements  $a^j$ for  $j \in \mathbb{N}_{>0}$ , and identify  $a^0 := a$ . Now, define  $I_1 := \text{Blowup}(I_1^{\dagger})$ , where  $\text{Blowup}(I_1^{\dagger})$  is the instance with facts  $\{R(a_1^{i_1} \dots a_n^{i_n}) \mid R(\vec{a}) \in I_1^{\dagger}, \vec{i} \in \mathbb{N}^n\}$ . Define  $I_2$  from  $I_2^{\dagger}$  in the same way; it clearly has a homomorphism to  $I_2^{\dagger}$ .

We will now show correctness of this construction. We claim that  $I_1^{\dagger}$  and  $I_1$  agree on all equality-free first-order constraints, which we show using a variant of the standard Ehrenfeucht-Fraïssé game without equality [CDJ96]. In this game there are pebbles on both structures. The play proceeds by Spoiler placing a new pebble on some element in one structure, and Duplicator must respond by placing a pebble with the same name in the other structure. Duplicator loses if the mapping given by the pebbles does not preserve all relations of the signature. If Duplicator has a strategy that never loses, then one can show by induction that the two structures agree on all equality-free first-order sentences.

Duplicator's strategy will maintain the following invariants:

(1) if a pebble is on some element  $a^j \in I_1$ , then the corresponding pebble in  $I_1^{\dagger}$  is on a;

(2) if a pebble is on some element a in  $I_1^{\dagger}$ , then the corresponding pebble in  $I_1$  is on some element  $a^j$  for  $j \in \mathbb{N}$ .

These invariants will guarantee that the strategy is winning. Duplicator's response to a move by Spoiler in  $I_1$  is determined by the strategy above. In response to a move by Spoiler placing a pebble on an element b in  $I_1^{\dagger}$ , Duplicator places the corresponding pebble on  $b^0$  in  $I_1$ .

Clearly the same claim can be shown for  $I_2^{\dagger}$  and  $I_2$ . In particular this shows that  $I_1^{\dagger}$  still satisfies Q and  $I_2^{\dagger}$  still violates Q.

All that remains is to construct the common subinstance. Let  $I_{\text{Accessed}} := \text{Blowup}(I_{\text{Accessed}}^{\dagger})$ . As  $I_{\text{Accessed}}^{\dagger}$  is a common subinstance of  $I_1^{\dagger}$  and  $I_2^{\dagger}$ , clearly  $I_{\text{Accessed}}$  is a common subinstance of  $I_1$  and  $I_2$ . To see why  $I_{\text{Accessed}}$  is access-valid in  $I_1^{\dagger}$ , given an input tuple in  $I_{\text{Accessed}}$ , let  $\vec{t}$  be the corresponding tuple in  $I_{\text{Accessed}}^{\dagger}$ . If  $\vec{t}$  has no matching tuples in  $I_1^{\dagger}$ , then clearly the same is true in  $I_1$ . If  $\vec{t}$  has at least one matching tuple  $\vec{u}$  in  $I_1^{\dagger}$ , then such a tuple exists in  $I_{\text{Accessed}}^{\dagger}$ because it is access-valid in  $I_1^{\dagger}$ , and hence sufficiently many copies exist in  $I_{\text{Accessed}}$  to satisfy the original result bounds, so that we can find a valid output for the access in  $I_{\text{Accessed}}$ . Hence  $I_{\text{Accessed}}$  is access-valid in  $I_1$ , which completes the proof.

**Choice simplifiability with UIDs and FDs.** The previous result does not cover FDs. However, we can also show a choice simplifiability result for FDs, and also add UIDs, i.e., IDs that only export a single element:

**Theorem 7.4.** Let Sch be a schema whose constraints are UIDs and arbitrary FDs, and Q be a CQ that is monotonically answerable in Sch. Then Q is monotonically answerable in the choice simplification of Sch.

Our high-level strategy to prove Theorem 7.4 is to use a "progressive" variant of the process of Lemma 5.3, a variant where we "correct" one access at a time. Remember that Lemma 5.3 said that, if a counterexample to AMonDet in Sch<sup>†</sup> can be expanded to a counterexample in Sch, then Q being AMonDet in Sch implies the same in Sch<sup>†</sup>. The next lemma makes a weaker hypothesis: it assumes that for any counterexample in Sch<sup>†</sup>, for any choice of access (mt, AccBind), we can expand to a counterexample in Sch<sup>†</sup> in which we have corrected this access, i.e., there is an output to (mt, AccBind) which is valid for Sch. We must ensure that correcting an access does not break the accesses that we previously corrected: specifically, we must ensure that every access that previously had a valid output for Sch still has such an output after we expand. Let us formally define the process:

**Definition 7.5.** Let Sch be a schema and Sch<sup>†</sup> be its choice simplification, and let  $\Sigma$  be a set of constraints.

Consider two instances  $I_1^{\dagger}, I_2^{\dagger}$  that satisfy  $\Sigma$ , and a common subinstance  $I_{\text{Accessed}}^{\dagger}$  which is access-valid in  $I_1^{\dagger}$  for Sch<sup>†</sup>. Let (mt, AccBind) be an access in  $I_{\text{Accessed}}^{\dagger}$ 

A single-access blowup of  $I_1^{\dagger}$ ,  $I_2^{\dagger}$  and  $I_{\text{Accessed}}^{\dagger}$  for (mt, AccBind) is a pair of instances  $I_1, I_2$ that satisfy  $\Sigma$ , such that  $I_1$  is a superinstance of  $I_1^{\dagger}$ ,  $I_2$  has a homomorphism to  $I_2^{\dagger}$ ,  $I_1$  and  $I_2$  have a common subinstance  $I_{\text{Accessed}}$  which is access-valid in  $I_1$  for Sch<sup>†</sup>, and we have:

(1)  $I_{\text{Accessed}}$  is a superinstance of  $I_{\text{Accessed}}^{\dagger}$ ;

(2) there is an output to the access mt, AccBind in  $I_{\text{Accessed}}$  which is valid in  $I_1$  for Sch;

- (3) for any access in  $I_{\text{Accessed}}^{\dagger}$  having an output in  $I_{\text{Accessed}}^{\dagger}$  which is valid for Sch in  $I_{1}^{\dagger}$ , there is an output to this access in  $I_{\text{Accessed}}$  which is valid for Sch in  $I_{1}$ ;
- (4) for any access in  $I_{\text{Accessed}}$  which is not an access in  $I_{\text{Accessed}}^{\dagger}$ , there is an output in  $I_{\text{Accessed}}$  which is valid for Sch in  $I_1$ .

We will now state a lemma making an assumption that we can repair the counterexample from  $\mathsf{Sch}^{\dagger}$  to  $\mathsf{Sch}$  by working one access at a time, using single-access blow-ups as above. We show that this is sufficient to reach the same conclusion as with Lemma 5.3:

**Lemma 7.6.** Let Sch be a schema, Sch<sup>†</sup> be its choice simplification, and  $\Sigma$  be a set of constraints.

Assume that, for any CQ Q which is not AMonDet in Sch<sup>†</sup>, for any counterexample  $I_1^{\dagger}, I_2^{\dagger}$  of AMonDet for Q and Sch<sup>†</sup> with a common subinstance  $I_{\text{Accessed}}^{\dagger}$  which is access-valid in  $I_1^{\dagger}$  for Sch<sup>†</sup>, for any access mt, AccBind in  $I_{\text{Accessed}}^{\dagger}$ , we can construct a single-access blowup of  $I_1^{\dagger}, I_2^{\dagger}$  and  $I_{\text{Accessed}}^{\dagger}$  for (mt, AccBind).

Then any CQ which is AMonDet in Sch is also AMonDet in Sch<sup>†</sup>.

*Proof.* As in some of our prior arguments, we will prove the contrapositive. Let Q be a query which is not AMonDet in Sch<sup>†</sup>, and let  $I_1^{\dagger}, I_2^{\dagger}$  be a counterexample, with  $I_{\text{Accessed}}^{\dagger}$  the common subinstance of  $I_1^{\dagger}$  and  $I_2^{\dagger}$  which is access-valid in  $I_1^{\dagger}$  for Sch<sup>†</sup>.

Enumerate the accesses in  $I_{\text{Accessed}}^{\dagger}$  as a sequence  $(\text{mt}^1, \text{AccBind}^1), \ldots, (\text{mt}^n, \text{AccBind}^n), \ldots$ : by the definition of  $I_{\text{Accessed}}^{\dagger}$ , all of them have an output in  $I_{\text{Accessed}}^{\dagger}$  which is valid in  $I_1^{\dagger}$  for Sch<sup>†</sup>, but initially we do not assume that any of these outputs are valid for Sch as well. We then build an infinite sequence  $(I_1^{\dagger}, I_2^{\dagger}) = (I_1^1, I_2^1), \ldots, (I_1^n, I_2^n), \ldots$  with the corresponding common subinstances  $I_{\text{Accessed}}^{\dagger} = I_{\text{Accessed}}^1, \ldots, I_{\text{Accessed}}^n, \ldots, with each <math>I_{\text{Accessed}}^i$  being a common subinstance of  $I_1^i$  and  $I_2^i$  which is access-valid in  $I_1^i$ , by performing the single-access blowup in succession to  $(\text{mt}^1, \text{AccBind}^1), \ldots, (\text{mt}^n, \text{AccBind}^n), \ldots$ . In particular, note that whenever  $(\text{mt}^i, \text{AccBind}^i)$  already has an output in  $I_{\text{Accessed}}^i$  which is valid in  $I_1^i$  for Sch, then we can simply take  $I_1^{i+1}, I_2^{i+1}, I_{\text{Accessed}}^{i+1}$  to be respectively equal to  $I_1^i, I_2^i, I_{\text{Accessed}}^i$ , without even having to rely on the hypothesis of the lemma.

It is now obvious by induction that, for all  $i \in \mathbb{N}$ ,  $I_1^i$  and  $I_2^i$  satisfy the constraints  $\Sigma$ , we have  $I_1 \subseteq I_1^i$  so  $I_1^i$  satisfies Q, we have that  $I_2^i$  has a homomorphism to  $I_2$  so  $I_2^i$  does not satisfy Q, and  $I_{\text{Accessed}}^i$  is a common subinstance of  $I_1^i$  and  $I_2^i$  which is access-valid in  $I_1^i$  for Sch<sup>†</sup>, where the accesses  $(\mathsf{mt}^1, \mathsf{AccBind}^1), \ldots, (\mathsf{mt}^i, \mathsf{AccBind}^i)$  additionally have an output in  $I_{\text{Accessed}}^i$  which is valid in  $I_1^i$  for Sch, and where all the accesses in  $I_{\text{Accessed}}^i$  which are not accesses of  $I_{\text{Accessed}}$  also have an output in  $I_{\text{Accessed}}^i$  which is valid in  $I_1^i$  for Sch. Hence, considering the infinite result  $(I_1^\infty, I_2^\infty), I_{\text{Accessed}}^\infty$  of this process, we know that all accesses in  $I_{\text{Accessed}}^\infty$  have an output in  $I_{\text{Accessed}}^\infty$  which is valid in  $I_1^\infty$  for Sch. Thus  $I_{\text{Accessed}}^\infty$  is actually a common subinstance of  $I_1^\infty$  and  $I_2^\infty$ , and  $I_{\text{Accessed}}^\infty$  is access-valid in  $I_1^\infty$  for Sch. So  $I_1^\infty, I_2^\infty$  is a counterexample to AMonDet of Q in Sch, which concludes the proof.

Thanks to Lemma 7.6, we can now prove Theorem 7.4 by arguing that we can correct each individual access. The rest of the section is devoted to this argument.

*Proof of Theorem 7.4.* Let Sch be the schema, let  $Sch^{\dagger}$  be its choice simplification, and let  $\Sigma$  be the set of constraints.

We explain how we perform the single-access blowup, to fulfil the requirements of Lemma 7.6. Let Q be a CQ and assume that it is not AMonDet in Sch<sup>†</sup>, and let  $I_1^{\dagger}, I_2^{\dagger}$ ,

be a counterexample to AMonDet, with  $I_{\text{Accessed}}^{\dagger}$  being a common subinstance of  $I_1^{\dagger}$  and  $I_2^{\dagger}$ which is access-valid in  $I_1^{\dagger}$  for Sch<sup> $\dagger$ </sup>. Let (mt, AccBind) be an access on some relation R in  $I_{\text{Accessed}}^{\dagger}$ : we know that there is an output to the access in  $I_{\text{Accessed}}^{\dagger}$  which is valid for  $\mathsf{Sch}^{\dagger}$ in  $I_1^{\dagger}$ , but this output is not necessarily valid for Sch, i.e., the output may be returning only one tuple whereas the result bound in the original schema is higher. Our goal is to build a superinstance  $I_1$  of  $I_1^{\dagger}$  and  $I_2$  of  $I_2^{\dagger}$  such that  $I_2$  homomorphically maps to  $I_2^{\dagger}$ . We want both  $I_1$  and  $I_2$  to satisfy  $\Sigma$ , and want  $I_1$  and  $I_2$  to have a common subinstance  $I_{\text{Accessed}}$  which is access-valid in  $I_1$ , where AccBind now has an output which is valid for Sch (i.e., not only for the choice simplification), all new accesses (the ones using new elements) also have an output which is valid for Sch, and no other accesses are affected. At a high level, we will do the same blow-up as in the proof of Theorem 5.5, except that we will need to chase afterwards to make the UIDs true. Even before this chasing phase, the presentation of the blow-up is also a bit different relative to the proof of Theorem 5.5, for two main reasons. First, we are working with the choice simplification in the present proof, so there are no new relations  $R_{mt}$ . Second, we are blowing up one access after another in the present proof, so we will not discuss "dangerous" and "non-dangerous" methods, instead we will focus on the single access (mt, AccBind) that we are blowing up.

First observe that, if there are no matching tuples in  $I_1^{\uparrow}$  for the access (mt, AccBind), then the empty set is already an output in  $I_{\text{Accessed}}^{\dagger}$  to the access which is valid in  $I_1^{\dagger}$  for Sch so there is nothing to do, i.e., we can just take  $I_1 := I_1^{\dagger}$ ,  $I_2 := I_2^{\dagger}$ , and  $I_{\text{Accessed}} := I_{\text{Accessed}}^{\dagger}$ . Further, note that if there is only one matching tuple in  $I_1^{\dagger}$  for the access, as  $I_{\text{Accessed}}^{\dagger}$  is access-valid for the choice simplification, then this tuple is necessarily in  $I_{\text{Accessed}}^{\dagger}$  also, so again there is nothing to do. Hence, it suffices to study the case where there is strictly more than one matching tuple in  $I_1^{\dagger}$  for the access (mt, AccBind); as  $I_{\text{Accessed}}^{\dagger}$  is access-valid for Sch<sup>†</sup>, then it contains at least one of these tuples, say  $\vec{t}_1$ , and as  $I_{\text{Accessed}}^{\dagger} \subseteq I_2^{\dagger}$ , then  $I_2^{\dagger}$  also contains  $\vec{t}_1$ . Let  $\vec{t}_2$  be a second matching tuple in  $I_1^{\dagger}$  which is different from  $\vec{t}_1$ . Let C be the non-empty set of positions of R where  $\vec{t}_1$  and  $\vec{t}_2$  disagree. Note that, since  $I_1^{\dagger}$  satisfies the constraints, the constraints cannot imply an FD from the complement of C to a position  $j \in C$ , as otherwise  $\vec{t}_1$  and  $\vec{t}_2$  would witness that  $I_1^{\dagger}$  violates this FD. Note also that C cannot include input positions of mt. In fact, in the terminology of the proof of Theorem 5.5, C witnesses that mt is dangerous.

We form an infinite collection of facts  $R(\vec{o}_i)$  where  $\vec{o}_i$  is constructed from  $\vec{t}_1$  by replacing the values at positions in C by fresh values. In particular we choose values distinct from those in other positions in R and in other  $\vec{o}_j$ 's. Let  $N := \{R(\vec{o}_1), \ldots, R(\vec{o}_n), \ldots\}$ . We claim that  $I_1^{\dagger} \cup N$  does not violate any FD implied by the schema. The argument is similar to that of the proof of Theorem 5.5. Let us proceed by contradiction and assume that there is a violation of a FD  $\phi$ . The violation  $F_1, F_2$  must involve some new fact  $R(\vec{o}_i)$ , as  $I_1^{\dagger}$  on its own satisfies the constraints. We know that the left-hand-side of  $\phi$  cannot include a position of C, as all elements in the new facts  $R(\vec{o}_i)$  at these positions are fresh. Hence, the left-hand-side of  $\phi$  is included in the complement of C, but recall that we argued above that then the right-hand-side of  $\phi$  cannot be in C. Hence, both the left-hand-side and right-hand-side of  $\phi$ are in the complement of C. But on this set of positions the facts of the violation  $F_1$  and  $F_2$ agree with the existing fact  $\vec{t}_1$  and  $\vec{t}_2$  of  $I_1^{\dagger}$ , a contradiction. So we know that  $I_1^{\dagger} \cup N$  does not violate the FDs. The same argument shows that  $I_2^{\dagger} \cup N$  does not violate the FDs.



Figure 4: Illustration of the blow-up process of Theorem 7.4, where relation R has an access on its first position, we blow up on the access to R with value a, and there is (among other dependencies) an ID  $R(x, y) \to \exists z \ S(y, z)$ 

So far, the argument was essentially the same as in the proof of Theorem 5.5, but now we explain the additional chasing phase. This is analogous to the chasing done in the proof of Theorem 5.2, but we define it differently to avoid introducing FD violations. Formally, let W be the infinite fixpoint of applying restricted chase steps to N with the UIDs, but ignoring triggers whose exported element occurs in  $\vec{t_1}$ . The process is illustrated in Figure 4. We have argued that  $I_1^{\dagger} \cup N$  and  $I_2^{\dagger} \cup N$  satisfy the FDs. We want to show that both the UIDs and FDs hold in  $I_1^{\dagger} \cup W$  and  $I_2^{\dagger} \cup W$ . The key argument to use for this is that every element which is both in the domain of  $I_1^{\dagger}$  and N and which occurs at a certain position (R, i)in N must also occur at position (R, i) in  $I_1^{\dagger}$ , and likewise for  $I_2^{\dagger}$ , namely:

Claim 7.7. Let  $\Sigma_{\text{ID}}$  be a set of UIDs and let  $\Sigma_{\text{FD}}$  be a set of FDs. Let I and N be instances, and let  $\mathcal{J} := \text{Adom}(I) \cap \text{Adom}(N)$ . Assume that I satisfies  $\Sigma_{\text{FD}} \cup \Sigma_{\text{ID}}$ , that  $I \cup N$  satisfies  $\Sigma_{\text{FD}}$ , and that whenever  $a \in \mathcal{J}$  occurs at a position (R, i) in N, then it also occurs at (R, i)in I. Let W denote the restricted chase of N by  $\Sigma_{\text{ID}}$  where we do not fire any triggers which map the exported variable to an element of  $\mathcal{J}$ . Then  $I \cup W$  satisfies  $\Sigma_{\text{ID}} \cup \Sigma_{\text{FD}}$ .

*Proof.* Let us first notice that we have  $\mathsf{Adom}(W) \cap \mathsf{Adom}(I) = \mathcal{J}$ . Indeed, it is a superset of  $\mathsf{Adom}(N) \cap \mathsf{Adom}(I)$  so contains  $\mathcal{J}$ , and all new domain elements in W are fresh by definition of the chase. What is more, we also notice that the facts of  $W \setminus N$  never contain elements of  $\mathsf{Adom}(I)$ . This is because all triggers fired when constructing W must have exported elements not in  $\mathcal{J}$ , hence not in  $\mathsf{Adom}(I)$  by what precedes.

Now, we show that  $I \cup W$  satisfies  $\Sigma_{\text{ID}}$ . Consider a trigger  $\tau$  for a UID  $\delta$  and let us show that it is not active. The range of  $\tau$  is either in I or in W. In the first case, as I satisfies  $\Sigma_{\text{ID}}$ , the trigger  $\tau$  for  $\delta$  cannot be active. So consider the second case and assume  $\tau$  were not active. Then it must map the exported variable to an element of  $\mathcal{J}$ , i.e., it is a trigger which we did not fire in W. Let  $R(\vec{a})$  be the fact of W in the image of  $\tau$ . This fact must be a fact of N, because as we argued the facts of  $W \setminus N$  do not contain elements of  $\mathcal{J}$ . Let  $a_i$ be the image of the exported variable in  $\vec{a}$ , with  $a_i \in \mathcal{J}$ . Hence,  $a_i$  occurs at position (R, i)in N, so by our assumption on N it also occurs at position (R, i) in I. Let  $R(\vec{b})$  be a fact of I such that  $b_i = a_i$ . As I satisfies  $\Sigma_{\text{ID}}$ , for the match of the body of  $\delta$  to  $R(\vec{b})$  there is a corresponding fact F in I extending the match to the head of  $\delta$ . But F also serves as a witness in  $I \cup W$  for the match of the body of  $\delta$ , so  $\tau$  is not active, a contradiction. Hence, we have shown satisfaction of  $\Sigma_{\text{ID}}$ .

We now show that  $I \cup W$  satisfies  $\Sigma_{\text{FD}}$ . We begin by arguing that W satisfies  $\Sigma_{\text{FD}}$ . This is because N satisfies  $\Sigma_{\text{FD}}$ . Now, every time the chase adds a fact F to W, all elements of Fare fresh except one (the exported element), and that element did not occur at the position at which it occurs in F, since otherwise the other fact where it did occur would witness that the trigger fired was not active. Thus, F cannot be part of an FD violation. Hence, by induction, W satisfies  $\Sigma_{\text{FD}}$ . Now, assume by way of contradiction that there is an FD violation  $\{F, F'\}$  in  $I \cup W$ . As I and W satisfy  $\Sigma_{\text{FD}}$  in isolation, it must be the case that one fact of the violation is in I and one is in W: without loss of generality, assume that we have  $F \in I$  and  $F' \in W$ . We cannot have F' in N because we know that  $I \cup N$  satisfies  $\Sigma_{\text{FD}}$ , so we must have  $F' \in N \setminus W$ . But as we argued, facts in  $N \setminus W$  do not contain elements of Adom(I), so F and F' cannot constitute an FD violation as they are on disjoint elements. This establishes that  $I \cup W$  satisfies  $\Sigma_{\text{FD}}$  and concludes the proof.

We return to the proof of Theorem 7.4. Recall that W is the result of applying restricted chase steps to N with the UIDs without firing triggers whose exported element occurs in  $\vec{t_1}$ . Construct  $I_1 := I_1^{\dagger} \cup W$ ,  $I_2 := I_2^{\dagger} \cup W$ , and  $I_{\text{Accessed}} := I_{\text{Accessed}}^{\dagger} \cup W$ . By Claim 7.7, we know that  $I_1$  and  $I_2$  satisfy the constraints.

Let us then conclude our proof of Theorem 7.4 via the process of Lemma 7.6. We show the first conditions on  $I_1$ ,  $I_2$ , and  $I_{\text{Accessed}}^{\dagger}$  stated in Definition 7.5:

- We clearly have  $I_1^{\dagger} \subseteq I_1$ .
- We have just shown that  $I_1$  and  $I_2$  satisfy the constraints.
- We now argue that I<sub>2</sub> has a homomorphism to I<sub>2</sub><sup>†</sup>. This argument is reminiscent of the proof of Theorem 5.2. We first define the homomorphism from I<sub>2</sub><sup>†</sup> ∪ N to I<sub>2</sub><sup>†</sup> by mapping I<sub>2</sub><sup>†</sup> to itself, and mapping the fresh elements of N so that the facts of N are mapped to R(t<sub>1</sub>). This is possible because each fresh element in N occurs at only one position. It is clear that this is a homomorphism. We then extend this homomorphism inductively on each fact created in W in the following way. Whenever a fact S(b) is created by firing an active trigger R(a) for a UID R(x) → S(y) where x<sub>p</sub> = y<sub>q</sub> is the exported variable (so we have a<sub>p</sub> = b<sub>q</sub>), consider the fact R(h(a)) of I<sub>2</sub><sup>†</sup> (with h defined on a by induction hypothesis). As I<sub>2</sub><sup>†</sup> satisfies Σ, we can find a fact S(c) with c<sub>q</sub> = h(a<sub>p</sub>), so we can define h(b) to be c, and this is consistent with the existing image of a<sub>p</sub>.
- Clearly  $I_{\text{Accessed}}$  is a common subinstance of  $I_1$  and  $I_2$  by construction. We now show that  $I_{\text{Accessed}}$  is access-valid for  $I_1$  and  $\text{Sch}^{\dagger}$ . Let (mt', AccBind') be an access in  $I_{\text{Accessed}}$ . We first consider the case when the range of the binding AccBind' includes an element of  $\text{Adom}(I_{\text{Accessed}}) \setminus \text{Adom}(I_{\text{Accessed}}^{\dagger})$ , namely, an element of  $\text{Adom}(W) \setminus \text{Adom}(I_1^{\dagger})$ . In this case, all matching facts must be facts of W. Thus, if mt' has no result bound then all matching facts to be returned are in  $I_{\text{Accessed}}$ , and if mt' is result-bounded then any choice of a tuple from  $W \subseteq I_{\text{Accessed}}$  (or no tuples, if this set is empty) is an output to the access which is valid for the choice simplification  $\text{Sch}^{\dagger}$ . The second case is when AccBind' only involves elements of  $\text{Adom}(I_{\text{Accessed}}^{\dagger})$ . Then (mt', AccBind') is actually an access on  $I_{\text{Accessed}}^{\dagger}$ . As  $I_{\text{Accessed}}^{\dagger}$ is access-valid in  $I_1^{\dagger}$ , let U be a (possibly empty) output to the access from  $I_{\text{Accessed}}^{\dagger}$  which is valid in  $I_1^{\dagger}$  for  $\text{Sch}^{\dagger}$ . Some tuples of W, say U', may also be matching tuples to the access (mt', AccBind') in  $I_1$ . Now, if mt' has no result bound, then all matching facts to be returned are in  $U \cup U'$  and hence in  $I_{\text{Accessed}}^{\dagger}$ . And if mt' is result-bounded, then any choice

of a tuple in  $U \cup U'$  (or no tuple, if  $U \cup U'$  is empty) gives an output to the access which is in  $I_{\text{Accessed}}$  and is valid for  $\mathsf{Sch}^{\dagger}$ . Hence, it is indeed the case that  $I_{\text{Accessed}}$  is access-valid for  $I_1$  and  $\mathsf{Sch}^{\dagger}$ .

We now show the four additional conditions of Definition 7.5:

- (1) It is clear by definition that  $I_{\text{Accessed}} \supseteq I_{\text{Accessed}}^{\dagger}$ .
- (2) We must show that the access (mt, AccBind) is valid for Sch in  $I_{\text{Accessed}}$ . Indeed, there are now infinitely many matching tuples in  $I_{\text{Accessed}}$ , namely, those of N. Thus this access is valid for Sch in  $I_1^{\dagger}$ : we can choose as many tuples as the value of the bound to obtain an output which is valid in  $I_1^{\dagger}$ .
- (3) We must verify that, for any access  $(\mathsf{mt}', \mathsf{AccBind}')$  of  $I_{\mathsf{Accessed}}^{\dagger}$  that has an output which is valid in  $I_1^{\dagger}$  for Sch, we can construct such an output in  $I_{\mathsf{Accessed}}$  which is valid in  $I_1$ for Sch. The argument is the same as in the second case of the fourth bullet point above: from the valid output to the access  $(\mathsf{mt}', \mathsf{AccBind}')$  in  $I_1^{\dagger}$  for Sch, we construct a valid output to  $(\mathsf{mt}', \mathsf{AccBind}')$  in  $I_1$  for Sch.
- (4) Let us consider any access in  $I_{\text{Accessed}}$  which is not an access in  $I_{\text{Accessed}}^{\dagger}$ . The binding for this access must include some element of Adom(W), so its matching tuples must be in W, which are all in  $I_{\text{Accessed}}$ . Hence, by construction any such accesses are valid for Sch.

This concludes the proof of Theorem 7.4 using Lemma 7.6, correcting each access according to the above process.  $\hfill \Box$ 

### 8. Decidability using Choice Simplification

In this section, we present the consequences of the choice simplifiability results of the previous section, in terms of decidability for expressive constraint languages.

**Decidable equality-free constraints.** Theorem 7.3 implies that monotone answerability is decidable for a wide variety of schemas. The approach applies to constraints that do not involve equality and have decidable query containment. We state here one complexity result for the class of *frontier-guarded TGDs* (FGTGDs): recall that these are TGDs whose body contains a single atom including all exported variables. The same approach applies to extensions of FGTGDs with disjunction and negation [BMMP16, BCS15].

**Theorem 8.1.** We can decide whether a CQ is monotonically answerable with respect to a schema with result bounds whose constraints are FGTGDs. The problem is 2EXPTIMEcomplete.

*Proof.* Hardness holds because of a reduction from query containment with FGTGDs (see, e.g., Prop. 3.16 in [BtCLT16]), already in the absence of result bounds, so we focus on  $2\mathsf{EXPTIME}$ -membership. By Theorem 7.3 we can assume that all result bounds are one, and by Proposition 4.8 we can replace the schema with the relaxed version that contains only result lower bounds. Now, a result lower bound of 1 can be expressed as an ID as was illustrated in Example 7.2. Thus, Proposition 4.9 allows us to reduce monotone answerability to a query containment problem with additional FGTGDs, and this is decidable in  $2\mathsf{EXPTIME}$  (see, e.g., [BGO10]).

**Complexity with UIDs and FDs.** We now turn to constraints that consist of UIDs and FDs, and use the choice simplifiability result of Theorem 7.4 to derive complexity results for monotone answerability with result-bounded access methods:

**Theorem 8.2.** We can decide monotone answerability with respect to a schema with result bounds whose constraints are UIDs and FDs. The problem is in 2EXPTIME.

Compared to Theorem 6.4, this result restricts to UIDs rather than IDs, and has a higher complexity, but it allows FD constraints. To the best of our knowledge, this result is new even in the setting without result bounds.

*Proof.* By choice simplifiability (Theorem 7.4) we can assume that all result bounds are one. By Proposition 4.9 we can reduce to a query containment problem  $Q \subseteq_{\Gamma} Q'$ . The constraints  $\Gamma$  include  $\Sigma$ , its copy  $\Sigma'$ , and accessibility axioms:

- $(\bigwedge_i \operatorname{accessible}(x_i)) \land R(\vec{x}, \vec{y}) \to R_{\operatorname{Accessed}}(\vec{x}, \vec{y})$  for each non-result-bounded method mt accessing relation R and having input positions  $\vec{x}$ ;
- $(\bigwedge_i \operatorname{accessible}(x_i)) \land \exists \vec{y} \ R(\vec{x}, \vec{y}) \to \exists \vec{z} \ R_{\operatorname{Accessed}}(\vec{x}, \vec{z})$  for each result-bounded method mt accessing relation R and having input positions  $\vec{x}$ ;
- $R_{\text{Accessed}}(\vec{w}) \to R(\vec{w}) \land R'(\vec{w}) \land \bigwedge_i \operatorname{accessible}(w_i)$  for each relation R.

Note that  $\Gamma$  includes FDs and non-unary IDs; containment for these in general is undecidable [Mit83]. To show decidability, we will explain how to rewrite these axioms in a way that makes  $\Gamma$  separable [CLR03]. That is, we will be able to drop the FDs of  $\Sigma$  and  $\Sigma'$ without impacting containment. First, by inlining  $R_{\text{Accessed}}$ , we can rewrite the above axioms as follows:

- for each non-result-bounded method mt accessing relation R with input positions  $\vec{x}$ , the axiom  $(\bigwedge_i \operatorname{accessible}(x_i)) \wedge R(\vec{x}, \vec{y}) \to R'(\vec{x}, \vec{y}) \wedge \bigwedge_i \operatorname{accessible}(y_i)$
- for each result-bounded method mt accessing relation R with input positions  $\vec{x}$ , the axiom  $(\bigwedge_i \operatorname{accessible}(x_i)) \wedge R(\vec{x}, \vec{y}) \to \exists \vec{z} \ [R(\vec{x}, \vec{z}) \wedge R'(\vec{x}, \vec{z}) \wedge \bigwedge_i \operatorname{accessible}(z_i)]$

We then modify the second type of axiom so that, in addition to the variables  $\vec{x}$  at input positions of mt in R, the axioms also export all variables at positions  $\mathsf{DetBy}(\mathsf{mt})$  of R that are determined by the input positions. In other words, the second bullet point becomes:

• for each result-bounded method **mt** accessing relation R with  $\vec{x}$  the variables at positions of  $\mathsf{DetBy}(\mathsf{mt}), (\bigwedge_i \mathsf{accessible}(x_i)) \land R(\vec{x}, \vec{y}) \to \exists \vec{z} [R(\vec{x}, \vec{z}) \land R'(\vec{x}, \vec{z}) \land \bigwedge_i \mathsf{accessible}(z_i)].$ 

This rewriting does not impact the soundness of the chase, as each chase step with a rewritten axiom can be mimicked by a step with an original axiom followed by FD applications.

Let us now argue that we can indeed drop the FDs of  $\Sigma$  and  $\Sigma'$ . That is, let us show that we never create a violation of an FD of  $\Sigma$  and  $\Sigma'$  in restricted chase proofs with the rewritten constraints. To argue this, it suffices to consider restricted chase proofs where we first fire the constraints in  $\Sigma$ , then the accessibility axioms as rewritten above, and last the constraints in  $\Sigma'$ . Indeed, at each of these three steps, we never create any new triggers for a preceding step. So let us show that these steps never introduce FD violations.

To show that the first steps do not introduce violations, remember that the restricted chase with UIDs can never introduce FD violations, because we only fire active triggers — this argument was spelled out at the end of the proof of Claim 7.7. The same reasoning shows that the third step cannot create FD violations either.

For the second step, assume by contradiction that firing the rewritten axioms creates an FD violation, and consider the first FD violation that is created. Either the violation is on a

primed relation, or it is on an unprimed relation. If it is on a primed relation, it consists of a first fact  $F'_1 = R'(\vec{c}, \vec{d})$ , and of a second fact  $F'_2 = R'(\vec{f}, \vec{g})$  which was just generated by firing an axiom on some fact  $F_2 = R(\vec{f}, \vec{h})$ . The accessibility axiom may be associated with an access method that is not result-bounded, in which case  $\vec{g}$  and  $\vec{h}$  are empty tuples; or it may relate to a result-bounded access method, in which case all values in  $\vec{g}$  are fresh. As we are only at the second step, we have not fired any dependencies from  $\Sigma'$  yet, so  $F'_1$  must also have been generated by firing an axiom on some fact  $F_1 = R(\vec{c}, \vec{e})$ , and again  $\vec{d}$  is either empty or only consists of fresh values. Now, we know that the determinant of the violated FD must be within the intersection of the positions of  $\vec{c}$  and of  $\vec{f}$ , because it cannot contain fresh values in any of the two facts  $F'_1$  and  $F'_2$ . Hence, by the modification that we did on the axioms, the determined position of the violated FD must also be within the intersection of the positions of  $\vec{c}$  and of  $\vec{f}$ . This means that  $F_1$  and  $F_2$  are already a violation of the FD, which means that  $F'_1, F'_2$  was not the first violation, a contradiction.

Now, if the violation is on an unprimed relation, it consists of a first fact  $F'_1 = R(\vec{c}, \vec{d})$ , and of a second fact  $F'_2 = R(\vec{f}, \vec{g})$  which was just generated by an axiom for a result-bounded access method. In this case, let  $F_2 = R(\vec{f}, \vec{h})$  be the fact on which the axiom was fired. Because the elements of  $\vec{g}$  are fresh, the determinant of the violated FD must be within positions of  $\vec{f}$ . Now, the positions of  $\vec{f}$  are exactly those positions determined by the input positions of the method, so the determined position of the violated FD must also be within positions of  $\vec{f}$ . This means that  $F'_1$  and  $F_2$  are already a violation of the FD, again contradicting that  $F_1$  and  $F_2$  were the first violation.

Thus, let  $\Gamma^{\mathsf{Sep}}$  denote the rewritten constraints without the FDs. We have shown that monotone answerability is equivalent to  $Q \subseteq_{\Gamma^{\mathsf{Sep}}} Q'$ . As  $\Gamma^{\mathsf{Sep}}$  contains only GTGDs, we can infer decidability in 2EXPTIME using [CGK08], which concludes the proof of Theorem 8.2.

#### 9. General First-Order Constraints

We have shown that, for many expressive constraint classes, the value of result bounds does not matter, and monotone answerability is decidable. A natural question is then to understand what happens with schema simplification and decidability for general FO constraints that may include the equality symbol. In this case, we find that choice simplifiability no longer holds:

**Example 9.1.** Consider a schema Sch with two relations P and U of arity 1. There is an input-free method  $\mathsf{mt}_P$  on P with result bound 5, and an input-free method  $\mathsf{mt}_U$  on Uwith no result bound. The first-order constraints  $\Sigma$  say that P has exactly 7 tuples, and if one of the tuples is in U, then 4 of these tuples must be in U. Consider the query  $Q: \exists x P(x) \land U(x)$ . The query is monotonically answerable on Sch: the plan simply accesses P with  $\mathsf{mt}_P$ , intersects the result with U using  $\mathsf{mt}_U$ , and projects to return true or false depending on whether the intersection is empty or not. Thanks to  $\Sigma$ , this will always return the correct result.

In the choice simplification  $\mathsf{Sch}^{\dagger}$  of  $\mathsf{Sch}$ , all we can do is access  $\mathsf{mt}_U$ , returning all of U, and access  $\mathsf{mt}_P$ , returning a single tuple. If this tuple is not in U, we have no information on whether or not Q holds. Hence, we can easily see that Q is not answerable on  $\mathsf{Sch}^{\dagger}$ .

The fact that simplification results fail does not immediately imply that monotone answerability problems are undecidable. However, we show that if we move to constraints where containment is undecidable, then the monotone answerability problem is also undecidable, even in cases such as equality-free FO which are choice simplifiable:

**Proposition 9.2.** It is undecidable to check if a conjunctive query Q is monotonically answerable with respect to equality-free FO constraints.

This result is true even without result bounds, and follows from results in [BtCLT16]: we give a self-contained argument here. Satisfiability for equality-free first-order constraints is undecidable [AHV95]. We will reduce from this to show undecidability of monotone answerability:

*Proof.* Assume that we are given an instance of a satisfiability problem consisting of equalityfree first-order constraints  $\Sigma$ . We produce from this an instance of the monotone answerability problem where the schema has no access methods and has constraints  $\Sigma$ , and we have a CQ *Q* consisting of a single 0-ary relation *A* not mentioned in  $\Sigma$ .

We claim that this gives a reduction from unsatisfiability to monotone answerability, and thus shows that the latter problem is undecidable for equality-free first-order constraints.

If  $\Sigma$  is unsatisfiable, then vacuously any plan answers Q: since answerability is a condition where we quantify over all instances satisfying the constraints, this is vacuously true when the constraints are unsatisfiable because we are quantifying over the empty set.

Conversely, if there is some instance I satisfying  $\Sigma$ , then we let  $I_1$  be formed from I by setting A to be true and  $I_2$  be formed by setting A to be false.  $I_1$  and  $I_2$  both satisfy  $\Sigma$  and have the same accessible part, so they form a counterexample to AMonDet. Thus, there cannot be any monotone plan for Q. This establishes the correctness of our reduction, and concludes the proof of Proposition 9.2.

The same undecidability result holds for other constraint languages where query containment is undecidable, such as general TGDs.

#### 10. Summary and Conclusion

We formalized the problem of answering queries in a complete way by accessing Web services that only return a bounded number of answers to each access, assuming integrity constraints on the data. We showed how to reduce this to a standard reasoning problem, query containment with constraints. We have further shown simplification results for many classes of constraints, limiting the ways in which a query can be answered using result-bounded plans, thus simplifying the corresponding query containment problem. By coupling these results with an analysis of query containment, we have derived complexity bounds for monotone answerability under several classes of constraints. Table 1 on p. 4 summarizes which simplifiability result holds for each constraint class, as well as the decidability and complexity results.

In our study of the answerability problem, we have have also introduced refinements of technical tools which we hope could be useful in a wider context. One example is the blowing-up method that we use in schema simplification results. Our results on bounded-width dependencies show that we can exploit the special form of query containments produced by answerability problems with access method – namely, they are guarded TGDs where the "side atoms" have a fixed signature. This leads us to a finer-grained analysis of the complexity of

guarded TGDs, tracking how a fixed side signature allows us to refine prior query answering techniques — like the linearization approach of [GMP14] and the tree-shrinking argument of [JK84]. The paper demonstrates how these model-theoretic and query-rewriting techniques can be applied to questions about answerability with access methods, a setting quite different from prior motivations. We believe the rewriting techniques in particular can be pushed to provide broader results on entailment with guarded TGDs, based on the distinction between the guard signature and the "side signature": for some attempts in this direction, see Appendix G of [AB18b].

We now discuss limitations and open questions.

**Complexity and expressiveness gaps.** Note that for the case of FDs and UIDs, the complexity bounds are not tight. The conference version sketches an approach to show that monotone answerability for this class is in EXPTIME, with details given in [AB18b]. We do not provide a full presentation of this in this work.

We leave open the complexity of monotone answerability with result bounds for some important cases: full TGDs, and more generally weakly-acyclic TGDs. Our choice approximation result applies here, but we do not know how to analyze the chase even for the simplified containment problem.

On the expressiveness side, we also leave open the question of whether choice simplifiability holds for general FDs and IDs; that is, not restricting to UIDs. We also leave open the question of whether UIDs and FDs, or even IDs and FDs, can be shown to be FD simplifiable

Note that all of our results forbid the use of constants in constraints. In particular, our definition of constraint classes like guarded TGDs forbids constants, differing in this respect from some prior presentations of these classes. We believe all of the results in the paper still hold in the presence of constants with roughly the same proofs, but we have not verified this.

Monotone vs general plans. We have restricted to *monotone* plans throughout the paper. As explained in Appendix D, the reduction to query containment still applies to plans that can use negation. Our schema simplification results also extend easily to answerability with such plans, but lead to a more involved query containment problem. Hence, we do not know how to show decidability of the answerability problem for UIDs and FDs with such plans.

In the case where constraints are dependencies, it is difficult to construct examples of CQs that require non-monotone plans. This suggests that the impact of considering richer plans is not large. But this is only anecdotal; and in addition, the situation is completely different with more general constraints — e.g., with disjunction and negation — where dealing with general plans is obviously critical.

Finite vs unrestricted equivalence. We have defined answerability by requiring that the query and the plan agree on all instances, finite and infinite. An alternative is to consider equivalence over finite instances only. We say that a plan PL finitely answers Q, if for any finite instance I satisfying the integrity constraints of PL, the only possible output of PLs is Q(I). Both finite and unrestricted answerability have been studied in past work on access methods in the absence of result bounds [BtCT16, BtCLT16], just as finite and unrestricted variants of other static analysis problems (e.g., query containment) have long been investigated in database theory (e.g., [JK84]). The unrestricted variants usually provide a cleaner theory and better algorithms, but the finite versions can be more precise.

In the presence of result bounds, we know nothing about the finite variants. Our analysis of the corresponding query containment problems can be extended to the finite variant of containment. But a major question is whether the reductions to query containment from Section 4 still hold in the finite case. The conference version of this paper [AB18a] claimed that these reductions could be extended, but the argument was found to be flawed in the review process for the present paper. Thus the issue is left as an open question for further work.

**Practical impact.** Our results provide a very comprehensive analysis of when there is an algorithm for answering queries in the presence of result bounds. But there is a question of how to interpret the "bottom line" of these results. For our expressiveness results, we feel it is reasonable to consider them as negative. Example 9.1 shows that in the presence of complex constraints, result-bounded methods can be useful for answering queries in extremely non-obvious ways. In contrast, our simplification results show that for many common constraint classes, result-bounded methods can be useful only in limited ways. In particular, we show that this limitation holds for many of the classes where we have decision procedures for the query answering problem. This limitation is related to the fact that our notion of answerability — the usual one considered for access methods and for views — is difficult to achieve for queries that intrinsically rely on result bounds. More relaxed notions have been explored in recent work [RPS20], but only in very restricted settings. In the setting of result bounds, weaker notions of answerability are an important topic for future investigation.

**Answering vs answerability.** In this paper we have focused only on the decision problem related to answerability — does there exists a plan that answers the query. But we did not deal with how to obtain the plans. Exactly the same complexity bounds apply to the plan-construction problem as to the decision problem in each case we consider. Indeed, in this work we have reduced the answerability question to a query containment question, and we then analyzed the complexity of determining whether there is a proof witnessing the containment resulting from the reduction. In the case where the constraints are dependencies, the corresponding proofs are just chase sequences. The temporary tables will store the state of the chase after each proof step. And there is a simple linear-time algorithm to extract a plan from a chase proof of the corresponding containment. In the case where there are no result bounds, the method is given in [BtCT16, BtCLT16]. In the plan we produce an access command for every firing of an accessibility axiom in the proof. When our existence-check or FD simplifiability results apply — for example the case of IDs given in Theorem 5.2 and FDs in Theorem 5.5 – we can eliminate result bounds completely, and then use these algorithms out of the box. But in the presence of results bounds, these algorithms generalize in the obvious way. When we fire an accessibility axiom that corresponds to a result-limited method, we generate an access command in the same way as in the absence of bounds. Note that for languages with disjunction, constructing a plan is more complex. Instead of a chase proof, one needs a tableau proof, and instead of the straightforward algorithm given in Chapter 4 of [BtCLT16], one uses interpolation. Still the algorithms are linear in the size of the proof, and extend to result-bounds. So again there is no distinction in the complexity between answerability and plan generation.

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# APPENDIX A. ALTERNATIVE SEMANTICS FOR PLANS

In the body of the paper we defined a semantics for plans using valid access selections, which assumed that multiple accesses with a result-bounded method always return the same output. We also claimed that all our results held without this assumption. We now formally define the alternative semantics where this assumption does not hold, and show that indeed the choice of semantics makes no difference. In this appendix, we will call *idempotent semantics* the one that we use in the main body of the paper, and *non-idempotent semantics* the one that we now define.

Intuitively, the idempotent semantics assumes that the access selection function is chosen for the entire plan, so that all calls with the same input to the same access method return the same output. The non-idempotent semantics makes no such assumption, and can choose a different valid access selection for each access. In both cases, the semantics is a function taking an instance I for the input schema and the input tables of the plan, and returning as output a set of *possible outputs* for each output table of the plan.

Formally, given a schema Sch and instance I, an access selection is a function mapping each access on I to an output of the access, as defined in the body of the paper, and it is valid if every output returned by the access selection is a valid output for the corresponding access. Given a plan, a multi-selection assignment associates a valid access selection to each access command in the plan. An idempotent multi-selection assignment is one that always assigns the same selection to a given method mt, even if it occurs in multiple commands. Given a multi-selection assignment F for plan PL, we can associate to each instance I an assignment mapping each variable in the plan to an instance of a relation, by induction on the number of commands. For an access command  $T \leftarrow_{\text{OutMap}} \text{mt} \leftarrow_{\text{InMap}} E$  the output is obtained by first evaluating E to get a collection of tuples. We then use the selection function that F associates with this command to get a set of results for each tuple, and put the union of the results into T. The semantics of middleware query commands is the usual semantics for relational algebra. The semantics of concatenation of commands is now defined via induction. The output of the plan under the function F is the value assigned to the output variable.

The difference between the output of a plan under the idempotent semantics and the output under the non-idempotent semantics relates to which assignments we consider. For the *idempotent semantics*, given I, the possible outputs are those that are returned by

any idempotent multi-selection assignment. For the *non-idempotent semantics* the possible outputs are those that are returned by any multi-selection assignment at all.

**Example A.1.** Consider a schema with a input-free access method mt with result bound 5 on relation R. Let PL be the plan that accesses mt twice and then determines whether the intersection of the results is non-empty:

 $T_1 \leftarrow \mathsf{mt} \leftarrow \emptyset;$   $T_2 \leftarrow \mathsf{mt} \leftarrow \emptyset;$   $T_0 \coloneqq \pi_{\emptyset}(T_1 \cap T_2);$  Return  $T_0$ .

As  $T_1$  and  $T_2$  are identical under the idempotent semantics, PL just tests if R is non-empty. Under the non-idempotent semantics, PL is non-deterministic, since it can return empty or non-empty when R contains at least 10 tuples.

Note that, in both semantics, when we use multiple access methods on the same relation, there is no requirement that an access selection be "consistent": if an instance I includes a fact R(a, b) and we have result-bounded access methods  $\mathsf{mt}_1$  on the first position of R and  $\mathsf{mt}_2$  on the second position of R, then an access to  $\mathsf{mt}_1$  on a might return (a, b) even if an access to  $\mathsf{mt}_2$  on b does not return (a, b). This captures the typical situation where distinct access methods use unrelated criteria to determine which tuples to return.

It is clear that if a query that has a plan that answers it under the non-idempotent semantics, then the same plan works under the idempotent semantics. Conversely, Example A.1 shows that that a given plan may answer a query under the idempotent semantics, while it does not answer any query under the non-idempotent semantics. However, if a query Q has some plan that answers it under the idempotent semantics, we can show that it also does under the non-idempotent semantics. We formally state this as follows, recalling that an RA plan is a plan using the full relational algebra (as introduced in the preliminaries):

**Proposition A.2.** For any CQQ over schema Sch, there is a monotone plan that answers Q under the idempotent semantics with respect to Sch iff there is a monotone plan that answers Q under the non-idempotent semantics. Likewise, there is an RA plan that answers Q under the idempotent semantics with respect to Sch iff there is an RA plan that answers Q under the non-idempotent semantics.

We first give the argument for RA plans (i.e., non-monotone plans, which allow arbitrary relational algebra expressions). If there is a plan PL that answers Q under the non-idempotent semantics, then clearly PL also answers Q under the idempotent semantics, because there are less possible outputs.

In the other direction, suppose PL answers Q under the idempotent semantics. Let cached(PL) be the function that executes PL, but whenever it encounters an access mt on a binding AccBind that has already been performed in a previous command, it uses the values output by the prior command rather than making a new access, i.e., it uses "cached values". Executing cached(PL) under the non-idempotent semantics gives exactly the same outputs as executing PL under the idempotent semantics, because cached(PL) never performs the same access twice. Further we can implement cached(PL) as an RA plan PL': for each access command  $T \Leftarrow mt \Leftarrow E$  in PL, we pre-process it in PL' by removing from the output of E any tuples previously accessed in mt, using a middleware query command with the relational difference operator. We then perform an access to mt with the remaining tuples, cache the output for further accesses, and post-process the output with a middleware query command to add back the output tuples cached from previous accesses. Thus PL' answers Q under the idempotent semantics as required.

Let us now give the argument for *monotone* plans (i.e., USPJ-plans), which are the plans used throughout the body of the paper. Of course the forward direction is proven in the same way, so we focus on the backward direction. Contrary to plans that can use negation, we can no longer avoid making accesses that were previously performed, because we can no longer remove input tuples that we do not wish to query. However, we can still cache the output of each access, and union it back when performing further accesses.

Let PL be a plan that answers Q under the idempotent semantics. We use Proposition 4.8 about the elimination of result upper bounds to assume without loss of generality that PL answers the query Q on the schema ElimUB(Sch), where all result bounds of Sch are replaced with result lower bounds only.

We define the plan  $\mathsf{PL}'$  from  $\mathsf{PL}$ , where access commands are modified in the following way: whenever we perform an access for a method **mt** in an access command *i*, we cache the input of access command *i* in a special intermediate table  $\mathrm{Inp}_{\mathsf{mt},i}$  and its output in another table  $\mathrm{Out}_{\mathsf{mt},i}$ , and then we add to the output of access command *i* the result of unioning, over all previously performed accesses with **mt** for j < i, the set of tuples in  $\mathrm{Out}_{\mathsf{mt},j}$  whose restriction to the input positions lie within  $\mathrm{Inp}_{\mathsf{mt},i} \cap \mathrm{Inp}_{\mathsf{mt},j}$ . This can be implemented using the relational join and project operators. Informally, whenever we perform an access with the same tuples on the same methods earlier in the plan. This can be implemented using USPJ operators. For each table defined on the left-hand side of an access or middleware command in  $\mathsf{PL}$ , we define its *corresponding table* as the table in  $\mathsf{PL}'$  where the same result is defined: for middleware commands, the correspondence is obvious because they are not changed from  $\mathsf{PL}$  to  $\mathsf{PL}'$ ; for access commands, the corresponding table is the one where we have performed the postprocessing to incorporate the previous tuple results.

We now make the following claim:

Claim A.3. Every possible output of PL' in the non-idempotent semantics is a subset of a possible output of PL in the idempotent semantics, and is a superset of a possible output of PL in the idempotent semantics.

This suffices to establish that  $\mathsf{PL}'$  answers the query Q in the non-idempotent semantics, because, as  $\mathsf{PL}$  answers Q in the idempotent semantics, its only possible output on an instance I in the idempotent semantics is Q(I), so Claim A.3 implies that the only possible output of  $\mathsf{PL}'$  on I is also Q(I), so  $\mathsf{PL}'$  answers Q under the non-idempotent semantics, concluding the proof. So it suffices to prove Claim A.3. We now do so:

*Proof.* Letting O be a result of  $\mathsf{PL}'$  under the non-idempotent semantics on an instance I, and letting  $\sigma_1 \ldots \sigma_n$  be the choice of valid access selections used for each access command of  $\mathsf{PL}'$  to obtain O, we first show that O is a superset of a possible output of  $\mathsf{PL}$  in the idempotent semantics, and then show that O is a subset of a possible output of  $\mathsf{PL}$  in the idempotent semantics.

To show the first inclusion, let us first consider the access selection  $\sigma^-$  on I defined in the following way: for each access binding AccBind on a method mt, letting  $\sigma_i$  be the access selection for the first access command of PL where the access on AccBind is performed on mt, we define  $\sigma^-(\text{mt}, \text{AccBind}) := \sigma_i(\text{mt}, \text{AccBind})$ ; if the access is never performed, define  $\sigma$ according to one of the  $\sigma_i$  (chosen arbitrarily). We see that  $\sigma^-$  is a valid access selection for I, because each  $\sigma_i$  is a valid access selection for i, and for each access  $\sigma^-$  returns the output of one of the  $\sigma_i$ , which is valid. Now, by induction on the length of the plan, it is clear that for every table in the execution of PL on I with  $\sigma^-$ , its contents are a *subset* of the contents of the corresponding table in the execution of  $\mathsf{PL}'$  on I with  $\sigma_1 \ldots \sigma_n$ . Indeed, the base case is trivial. The induction case for middleware commands follows from monotonicity of the USPJ operators. The induction case on access commands will follow because we perform an access with a subset of bindings. For each binding AccBind, if this is the first time we perform the access for this method on AccBind, we obtain the same output in PL as in PL'. And if this is not the first time, in PL we obtain the output as we did the first time, and in PL' we still obtain it because we retrieve it from the cached copy. The conclusion of the induction is that the output of PL on I under  $\sigma^-$  is a subset of the output O of PL' on I under  $\sigma_1 \ldots \sigma_n$ .

Let us now show the second inclusion by considering the access selection  $\sigma^+$  on I defined in the following way: for each access binding AccBind and method mt, we define  $\sigma^+(\mathsf{mt},\mathsf{AccBind}) := \bigcup_{1 \le i \le n} \sigma_i(\mathsf{mt},\mathsf{AccBind})$ . That is,  $\sigma^+$  returns all outputs that are returned in the execution of PL' on I in the non-idempotent semantics with  $\sigma_1 \ldots \sigma_n$ . This is a valid access selection, because for each access and binding it returns a superset of a valid output, so we are still obeying the result lower bounds, and there are no result upper bounds because we we are working with the schema ElimUB(Sch) where result upper bounds have been eliminated. Now, by induction on the length of the plan, analogously to the case above, we see that for every table in the execution of PL on I with  $\sigma^+$ , its contents are a *superset* of that of the corresponding table in the execution of PL' on I with  $\sigma_1 \ldots \sigma_n$ : the induction case is because each access on a binding in PL' cannot return more than the outputs of this access in all the  $\sigma_i$ , and this is the output obtained with  $\sigma^+$ . So we have shown that O is a subset of a possible output of PL, and that it is a superset of a possible output of PL, concluding the proof of the claim.

This concludes the proof of Proposition A.2.

# Appendix B. Proof of Theorem 6.13: COMPLETENESS OF THE DOWNWARD-FREE CHASE

Recall the statement:

For every tree-like chase sequence using single-headed GTGDs  $T_0 
dots T_n$ , there is a downward-free tree-like chase sequence  $T_0 = \overline{T_0}, \dots, \overline{T_m}$  such that there is a homomorphism h from the instance of  $T_n$  to the instance of  $\overline{T_m}$  with h(c) = c for any values c in the domain of the instance of  $T_0$ .

*Proof.* We prove the result by induction on n, calling  $h_n$  the homomorphism produced for n. We will ensure inductively that our homomorphism  $h_n$  preserves the tree structure of  $T_n$ . That is, there is additionally an injective homomorphism  $h_n^{\mathrm{T}}$  from the underlying tree of  $T_n$  to the underlying tree of  $\overline{T_m}$  such that for each node v of  $T_n$  and each fact  $G \in \mathsf{FactsOf}_n(v)$ , the node  $h_n^{\mathrm{T}}(v)$  contains the image fact of G obtained by mapping the elements of the fact following  $h_n$ .

For the base case n = 0, we simply set  $\overline{T_0} := T_0$ , take m = n = 0, and let both  $h_n$  and  $h_n^{\mathrm{T}}$  be the identity.

For the inductive case, there are two possibilities. The first possibility is that we performed a chase step when going from  $T_{n-1}$  to  $T_n$  to fire a trigger  $\rho$  at a node v to create a fact F, then we simply take the image  $h_{n-1}(\rho)$  of  $\rho$  by the homomorphism in the

node  $h_{n-1}^{\mathrm{T}}(v)$  and fire it there, creating the fact  $h_{n-1}(F)$  that we can use to extend the homomorphism.

The second possibility is the interesting one: we have performed a propagation step to go from  $T_{n-1}$  to  $T_n$ , and we must explain how to "mimic" it in  $\overline{T_m}$  while only performing upward propagation. To simplify the argument, letting F be the fact that was just created in  $T_{n-1}$  in a node v and is propagated in  $T_n$ , we assume that the propagation from  $T_{n-1}$  to  $T_n$ propagates F to all nodes that have a guard for its elements: this is the most challenging case.

We first perform the upward propagation in  $\overline{T_m}$ , that is, we consider the ancestors of v having a guard of the elements of F is propagated in  $T_n$ , take their image by  $h_{n-1}^{\mathrm{T}}$ , and propagate  $\overline{F} := h_{n-1}(F)$  to these ancestors. Let  $\overline{p}$  be the highest such ancestor in  $\overline{T_m}$ .

The key idea is now that we "mimic" downwards propagation by simply re-creating all the descendants of  $\overline{T_m}$ , which will "automatically" propagate the fact  $\overline{F}$  to them. More precisely, consider U the set of all domain elements that occur in strict descendants of  $\overline{p}$  but do not occur in  $\overline{p}$ , fix U' a disjoint set of fresh element names of the same cardinality, and fix a bijection h which maps U to U' and is the identity on the other elements of  $\overline{T_m}$ . Now, consider the sequence  $\overline{T_0}, \ldots, \overline{T_m}$  obtained thus far, which by induction does not contain any downwards propagation. Now, re-play that sequence but replacing the elements of U by U'. More formally, all triggers and all created facts are mapped through h. In particular, the non-full chase steps that created the children of  $\overline{p}$  will now create fresh child nodes, where the elements of U have been replaced by elements of U', further non-full chase steps on these children will continue creating a copy of their subtree, and full chase steps happening in their subtrees as well as upwards propagations are performed in the same way as in the original sequence. (Chase steps that create facts with no element of U are unchanged by the transformation, and doing them again recreates a fact that already exists, which has no effect.)

After this process, we have extended  $\overline{T_0}, \ldots, \overline{T_m}$  by a sequence  $\overline{T_{m+1}}, \ldots, \overline{T_{m'}}$ , and  $\overline{T_{m'}}$  is a superinstance of  $\overline{T_m}$  which differs in that every child of  $\overline{p}$  now exists in two copies, one featuring elements of U and the other one featuring the corresponding elements of U', these two copies being the roots of subtrees between which h is an isomorphism. Overall, the homomorphism h maps  $\overline{T_m}$  to  $\overline{T_{m'}}$  by mapping each original subtree to its copy. Let us call  $h^{\mathrm{T}}$  the corresponding injective homomorphism at the level of tree nodes. We can compose  $h_m$  and  $h_m^{\mathrm{T}}$  with h and  $h^{\mathrm{T}}$  respectively to obtain well-defined homomorphisms  $h_{m'}$  and  $h_{m'}^{\mathrm{T}}$ . Now, to show that they are suitable, the only point to verify is that we have correctly propagated the new fact, i.e., for all nodes v' of  $T_n$  where F is guarded, the node  $h_{m'}^{\mathrm{T}}$  indeed contains  $\overline{F}$ .

To understand why, notice that when we perform the sequence  $\overline{T_{m+1}}, \ldots, \overline{T_{m'}}$ , the node  $\overline{p}$  contains the new fact  $\overline{F}$  that we wished to downwards propagate. Hence, while we created the new subtrees,  $\overline{F}$  was added to every new child node whenever it was guarded by the elements of that node. Thus,  $\overline{F}$  now exists in each node of the new subtrees where it is guarded. This establishes that the chase sequence  $\overline{T_0}, \ldots, \overline{T_{m'}}$  and the homomorphisms  $h_{m'}$  and  $h_{m'}^{\mathrm{T}}$  satisfy the conditions. This shows the inductive case, and concludes the inductive proof, establishing the result.

APPENDIX C. PROOF OF THE SEMI-WIDTH RESULT (PROPOSITION 6.5)

In this appendix, we prove the NP bound on containment for bounded semi-width IDs, i.e., Proposition 6.5. Recall its statement:

For any fixed  $w \in \mathbb{N}$ , there is an NP algorithm for containment under IDs of semi-width at most w.

To prove the result, let  $\Sigma$  be the collection of IDs, and consider a chase sequence based on the canonical database  $I_0 := \mathsf{CanonDB}(Q)$  of the conjunctive query Q. Recall the notion of a *tree-like chase proof* from the body of the paper (after Proposition 6.14). This is a sequence of labelled trees — the *chase trees* of the proof — one for each instance in the chase sequence, where the tree associated with  $I_0$  consists of a single root node. In the case where the constraints are all IDs, we will modify the tree structure in this definition slightly, creating a new node even when firing full rules. We do not perform propagation of facts, which will never be needed for IDs. Thus the chase will have non-root nodes  $n_F$ in one-to-one correspondence with generated facts F. If performing a chase step on fact Fproduces fact F' in the sequence, then the node  $n_{F'}$  is a child of the node  $n_F$ .

Consider nodes n and n' in a chase tree within some tree-like chase proof, with n a strict ancestor of n'. We say n and n' are far apart if there are distinct generated facts  $F_1$  and  $F_2$  such that:

- the node  $n_1$  corresponding to  $F_1$  and the node  $n_2$  corresponding to  $F_2$  are both ancestors of n' and descendants of  $n_2$ ;
- $n_1$  is an ancestor of  $n_2$ ;
- $F_1$  and  $F_2$  were generated by the same rule of  $\Sigma$ ; and
- the equalities between values in positions within  $F_1$  are exactly the same as the equalities within  $F_2$ , and any values occurring in both  $F_1$  and  $F_2$  occur in the same positions within  $F_2$  as they do in  $F_1$ .

If such an n and n' are not far apart, we say that they are *near*.

A match of Q in the chase tree is a mapping from the variables of Q to the elements of the chase tree which is a homomorphism, i.e., it also maps every atom of Q to a fact in the chase tree. Given a match h of Q in the chase tree, its *augmented image* is the closure of its image under least common ancestors, including by convention the root node. If Q has size k then this has size  $\leq 2k + 1$ . For nodes n and n' in the augmented image, we call n the *image parent of* n' if n is the lowest ancestor of n' in the augmented image.

**Lemma C.1.** If Q has a match h in the final instance of a tree-like chase proof, where the final instance has chase tree T, then there is another tree-like chase proof with final tree T', and a match h' with the property that if n is the image parent of n' then n and n' are near.

*Proof.* We prove that given such an h and T, we can construct an h' and T' such that we decrease the sum of the depths of the violations.

If n is far apart from n', then there are witnesses  $F_1$  and  $F_2$  to this, corresponding to nodes  $n_1$  and  $n_2$  respectively. Informally, we will "pull up" the homomorphism by replacing witnesses below  $F_2$  with witnesses below  $F_1$ . Formally, we create T' by first removing each step of the chase proof that generates a node that is a descendent of  $n_1$ . Letting  $T_1$  be the nodes in T that do not lie below  $n_1$ , we will add nodes and the associated proof steps to T'. Let  $C_2$  be the chase steps in T that generate a node below  $n_2$ , ordered as in T, and let  $T_2$  be the nodes produced by these steps. We then add chase steps in T' for each chase step in  $C_2$ . More precisely, we expand T' by an induction on prefixes of  $C_2$ , building T' and a partial function m from the domains of facts in  $\{n_2\} \cup T_2$  into the domain of facts associated to  $n_1$ and its descendants in T'. The invariant is that m preserves each fact of T generated by the chase steps in  $C_2$  we have processed thus far in the induction, and that m is the identity on any values in  $F_1$ . We initialize the induction by mapping the elements associated to  $n_1$  to elements associated to  $n_2$ . Our assumptions on  $n_1$  and  $n_2$  suffice to guarantee that we can perform such a mapping satisfying the invariant. For the inductive case, suppose the next chase step s in  $C_2$  uses ID  $\delta$ , firing on the fact associated to  $v_i$  in T, producing node  $v_{i+1}$ . Then we perform a step s' using  $\delta$  and the fact associated to  $m(v_i)$  in T'. If  $\delta$  was a full ID we do not modify m, while if it is a non-full ID we extend m to map the generated elements of s to the corresponding elements of s'. We can thus form h' by revising h(x) when h(x)lies below  $n_1$ , setting h'(x) to m(h(x)). Note that there could not have been any elements in the augmented image of h in T that hang off the path between  $n_1$  and  $n_2$ , since n and n'were assumed to be adjacent in the augmented image.

In moving from T and h to T' and h' we reduce the sum of the depths of nodes in the image, while no new violations are created, since the image-parent relationships are preserved.

Call a match h of Q in the chase *tight* if it has the property given in the lemma above. The *depth* of the match is the depth of the lowest node in its image. The next observation, also due to Johnson and Klug, is that when the width is bounded, tight matches can not occur far down in the tree:

**Lemma C.2.** If  $\Sigma$  is a set of IDs of width w and the schema has arity bounded by m, then any tight match of size k has all of its nodes at depth at most  $k \cdot |\Sigma| \cdot m^{w+1} \cdot 2^w$ .

Proof. We claim that the length of the path between a match element h(x) and its image parent h(x') must be at most  $\Delta := |\Sigma| \cdot m^{w+1} \cdot 2^w$ . At most w values from h(x') are present in any fact on the path, and thus the number of configurations that can occur is at most  $m^{w+1}$ . Further, we multiply by a factor of  $|\Sigma|$  because we are accounting for the last rule used. We also multiply by a factor of  $2^w$  to account for the possible equality patterns among the values in the positions of the fact that do not contain a null. Thus after  $\Delta$  steps there will be two elements which repeat both the rule and the configuration of the values, which would contradict tightness. Since the augmented image contains the root, this implies the bound above.

Johnson and Klug's result follows from combining the previous two lemmas:

**Proposition C.3** [JK84]. For any fixed  $w \in \mathbb{N}$ , there is an NP algorithm for query containment under IDs of width at most w.

*Proof.* We know it suffices to determine whether there is a match in a chase proof, and the previous lemmas tell us that the portion of a chase proof required to find a match is not large. We thus guess a tree-like chase proof where the tree consists of k branches of depth at most  $k \cdot |\Sigma| \cdot m^{w+1} \cdot 2^w$ , along with a match in them, verifying the validity of the branches according to the rules of  $\Sigma$ .

We now give the extension of this argument for bounded semi-width. Recall from the body that a collection of IDs  $\Sigma$  has *semi-width* bounded by w if it can be decomposed as  $\Sigma = \Sigma_1 \cup \Sigma_2$  where  $\Sigma_1$  has width bounded by w and the basic position graph of  $\Sigma_2$  is acyclic. An easy modification of Proposition C.3 now completes the proof of our semi-width result (Proposition 6.5): *Proof.* We revisit the argument of Lemma C.2, claiming a bound with an extra factor of  $|\Sigma|$  in it. As in that argument, it suffices to show that, considering the extended image of a tight match of Q in a chase proof, then the distance between any node n' of the extended image and its closest ancestor n is bounded, i.e., it must be at most  $|\Sigma|^2 \cdot m^{w+1} \cdot 2^w$ . Indeed, as soon as we apply a rule of  $\Sigma_1$  along the path, at most w values are exported, and so the remaining path is bounded as before. Since  $\Sigma_2$  has an acyclic basic position graph, a value in n can propagate for at most  $|\Sigma_2|$  steps when using rules of  $\Sigma_2$  only. Thus after at most  $|\Sigma_2|$  edges in a path we will either have no values propagated (if we used only rules from  $\Sigma_2$ ) or at most w values (if we used a rule from  $\Sigma_1$ ). In particular, we cannot have a gap of more than  $|\Sigma_2| \cdot |\Sigma| \cdot m^{w+1} \cdot 2^w$  in a tight match.

#### APPENDIX D. GENERALIZATION OF RESULTS TO RA PLANS

In the body of the paper we dealt with monotone answerability. A relational algebra plan or just RA plan is defined as with a monotone plan, but in addition to the monotone relational algebra expressions we also allow as an operator a relational difference operator  $\setminus$ , which takes as input instances of two relations with the same arity. It is known that the queries defined by relational algebra are the same as those defined by first-order logic with the active-domain semantics [AHV95]. As we mentioned in the body of the paper, there are monotone queries that can be expressed using an RA plan, but not with a monotone plan. In the setting of views, this surprising fact, which contradicted prior claims in the literature (e.g., [SV05]), was uncovered in [NSV10]. These counterexamples notwithstanding, the bulk of the work in the literature on querying with access patterns has focused on monotone plans.

At the end of Section 3 and in Section 10, we claimed that many of the results in the paper, including the reduction to query containment and the schema simplification results, generalize in the "obvious way" to answerability where general relational algebra expressions are allowed. In addition, the results on complexity for monotone answerability that are shown in the body extend to answerability with RA plans, with one exception. The exception is that we do not have a decidability result for UIDs and FDs analogous to Theorem 8.2, because the containment problem is more complex.

We explain in the rest of the appendix how to adapt our results in the unrestricted setting from monotone answerability to RA answerability. In the specific case of IDs, we will show (Proposition D.8) that RA answerability and monotone answerability coincide. This generalizes a result known for views, and extends it to the setting with result bounds.

D.1. Variant of Reduction Results for RA Answerability. We first formally define the analog of AMonDet for the notion of RA answerability that we study in this appendix. In the absence of result bounds, this corresponds to the notion of *access-determinacy* [BtCLT16, BtCT16], which states that two instances with the same accessible part must agree on the query result. Here we generalize this to the setting with result bounds, where the accessible instance is not uniquely defined.

Given a schema Sch with constraints and methods which may have result lower bounds as well as result upper bounds, a query Q is said to be *access-determined* if for any two instances  $I_1$ ,  $I_2$  satisfying the constraints of Sch, if there is a valid access selection  $\sigma_1$  for  $I_1$  and a valid access selection  $\sigma_2$  for  $I_2$  such that  $AccPart(\sigma_1, I_1) = AccPart(\sigma_2, I_2)$ , then  $Q(I_1) = Q(I_2)$ .

We will now show that access-determinacy is equivalent to query containment, as with access monotonic determinacy. We will stick to the setting where Q is a CQ, for consistency with the body of the paper. This restriction will also be essential in the core results on expressiveness, decidability, and complexity to come. However, the results in this subsection, concerning reduction to query containment, hold also for a query Q in relational algebra.

As we did with AMonDet, it will be convenient to give an alternative definition of access-determinacy that talks only about a subinstance of a single instance.

For a schema Sch a common subinstance  $I_{\text{Accessed}}$  of  $I_1$  and  $I_2$  is *jointly access-valid* if, for any access performed with a method of Sch in  $I_{\text{Accessed}}$ , there is a set of matching tuples in  $I_{\text{Accessed}}$  which is a valid output to the access in  $I_1$  and in  $I_2$ . In other words, there is an access selection  $\sigma$  for  $I_{\text{Accessed}}$  whose outputs are valid in  $I_1$  and in  $I_2$ .

We now claim the analogue of Proposition 4.1, namely:

**Proposition D.1.** For any schema Sch with arbitrary constraints  $\Sigma$  and methods which may have result lower bounds and result upper bounds, a CQ Q is access-determined if and only if the following implication holds: for any two instances  $I_1, I_2$  satisfying  $\Sigma$ , if  $I_1$  and  $I_2$ have a common subinstance  $I_{\text{Accessed}}$  that is jointly access-valid, then  $Q(I_1) = Q(I_2)$ .

This result gives the alternative definition of access-determinacy that we will use in our proofs. Proposition D.1 follows immediately from the following proposition (the analogue of Proposition 4.2):

**Proposition D.2.** Again assume a schema with arbitrary constraints along with methods that may have result lower and upper bounds. The following are equivalent:

- (i)  $I_1$  and  $I_2$  have a common subinstance  $I_{\text{Accessed}}$  that is jointly access-valid.
- (ii) There is a common accessible part A of  $I_1$  and for  $I_2$ .

Proof. Suppose  $I_1$  and  $I_2$  have a common subinstance  $I_{\text{Accessed}}$  that is jointly access-valid. This means that we can define an access selection  $\sigma$  that takes any access performed with values of  $I_{\text{Accessed}}$  and a method of Sch, and maps it to a set of matching tuples in  $I_{\text{Accessed}}$ that is valid in  $I_1$  and in  $I_2$ . We can see that  $\sigma$  can be used as a valid access selection in  $I_1$ and  $I_2$  by extending it to return an arbitrary valid output to accesses in  $I_1$  that are not accesses in  $I_{\text{Accessed}}$ , and likewise to accesses in  $I_2$  that are not accesses in  $I_{\text{Accessed}}$ ; we then have  $\text{AccPart}(\sigma, I_1) = \text{AccPart}(\sigma, I_2)$  so we can define the accessible part A accordingly, noting that we have  $A \subseteq I_{\text{Accessed}}$ . Thus the first item implies the second.

Conversely, suppose that  $I_1$  and  $I_2$  have a common accessible part A, and let  $\sigma_1$  and  $\sigma_2$  be the witnessing valid access selections for  $I_1$  and  $I_2$ , i.e.,  $A = \mathsf{AccPart}(\sigma_1, I_1) = \mathsf{AccPart}(\sigma_2, I_2)$ . Let  $I_{\mathsf{Accessed}} := A$ , and let us show that  $I_{\mathsf{Accessed}}$  is a common subinstance of  $I_1$  and  $I_2$  that is jointly access-valid. By definition we have  $I_{\mathsf{Accessed}} \subseteq I_1$  and  $I_{\mathsf{Accessed}} \subseteq I_2$ . Now, to show that it is jointly access-valid in  $I_1$  and  $I_2$ , consider any access  $\mathsf{AccBind}$ , mt with values in  $I_{\mathsf{Accessed}}$ . We know that there is *i* such that  $\mathsf{AccBind}$  is in  $\mathsf{AccPart}_i(\sigma_1, I_1)$ , therefore by definition of the fixpoint process and of the access selection  $\sigma_1$  there is a valid output to the access in  $\mathsf{AccPart}_{i+1}(\sigma_1, I_1)$ , hence in  $I_{\mathsf{Accessed}}$ . Thus we can choose an output in  $I_{\mathsf{Accessed}}$  which is valid in  $I_1$ . But this output must also be in  $\mathsf{AccPart}(\sigma_2, I_2)$ , and thus it is valid in  $I_2$  as well. Thus,  $I_{\mathsf{Accessed}}$  is jointly access-valid. This shows the converse implication and concludes the proof. The following analogue of Proposition 4.4 motivates these two equivalent definitions of access-determinacy, showing that either one is equivalent to the existence of an RA-plan that answers Q:

**Proposition D.3.** Again assume a schema with arbitrary constraints, along with methods that may have result upper bounds and result lower bounds. If a CQ Q has an RA plan PL that answers it w.r.t. Sch, then Q is access-determined over Sch.

Proof. Assume that Q has an RA plan PL that answers it. Using Proposition D.1, consider two instances  $I_1$  and  $I_2$  satisfying the constraints of Sch, and having a common subinstance  $I_{\text{Accessed}}$  that is jointly access-valid. Let us show that  $Q(I_1) = Q(I_2)$ . Let  $\sigma$  be a valid access selection for  $I_{\text{Accessed}}$ , and extend it to a valid access selection  $\sigma_1$  for  $I_1$  and  $\sigma_2$  for  $I_2$ . Specifically, accesses with a binding in  $I_{\text{Accessed}}$  on  $\sigma_1$  and  $\sigma_2$  return the same result as  $\sigma$ , which by definition is valid in  $I_1$  and  $I_2$  in addition to being valid in  $I_{\text{Accessed}}$ . Further, accesses with a binding using values from  $\text{Adom}(I_1) \setminus \text{Adom}(I_{\text{Accessed}})$  for  $\sigma_1$  return some valid response for  $\sigma_1$ , and likewise for  $\sigma_2$ .

Now, a simple induction shows that the intermediate tables produced by a plan using  $\sigma_1$  on  $I_1$ , using  $\sigma_2$  on  $I_2$ , and using  $\sigma$  on  $I_{\text{Accessed}}$ , must be the same, and must all consist of values from  $\text{Adom}(I_{\text{Accessed}})$ .

Now, as PL answers Q, we know that the output of Q on  $I_1$  is equal to that of Q on  $I_2$ . This concludes the proof.

Analogously to Theorem 4.3, we can show that access-determinacy is equivalent to RA answerability. The proof starts the same way as that of Theorem 4.3, noting that in the absence of result bounds, this equivalence was shown in prior work:

**Theorem D.4** [BtCLT16, BtCT16]. For any  $CQ \ Q$  and schema Sch (with no result bounds) whose constraints  $\Sigma$  are expressible in active-domain first-order logic, the following are equivalent:

(1) Q has an RA plan that answers it over Sch.

(2) Q is access-determined over Sch.

The extension to result bounds is shown using the same reduction as for Theorem 4.3, by just "axiomatizing" the result bounds as additional constraints (by a direct analogue of Proposition 4.6). This gives the immediate generalization of Theorem D.4 to schemas that may include result bounds:

**Theorem D.5.** For any CQ Q and schema Sch whose constraints  $\Sigma$  are expressible in active-domain first-order logic, where methods may have result upper and result lower bounds, the following are equivalent:

- (1) Q has an RA plan that answers it over Sch.
- (2) Q is access-determined over Sch.

Hence, we have shown the analogue of Theorem 4.3 for the setting of RA answerability and RA plans studied in this appendix.

Elimination of result upper bounds for RA plans. As with monotone answerability, it suffices to consider only result lower bounds. Recall that ElimUB(Sch) is the schema obtained from Sch by removing result upper bounds and keeping only result lower bounds. We have:

**Proposition D.6.** Let Sch be a schema with arbitrary constraints and access methods which may have result lower bounds and result upper bounds. A query Q is RA answerable in Sch if and only if it is RA answerable in ElimUB(Sch).

*Proof.* The proof follows that of Proposition 4.8. We show the result for access-determinacy instead of RA answerability, thanks to Theorem D.5, and we use Proposition D.1. Consider arbitrary instances  $I_1$  and  $I_2$  that satisfy the constraints, and let us show that any common subinstance  $I_{\text{Accessed}}$  of  $I_1$  and  $I_2$  is jointly access-valid for Sch iff it is jointly access-valid for ElimUB(Sch): this implies the claimed result.

In the forward direction, if  $I_{\text{Accessed}}$  is jointly access-valid for Sch, then clearly it is jointly access-valid for ElimUB(Sch), as any output of an access on  $I_{\text{Accessed}}$  which is valid in  $I_1$  and in  $I_2$  for Sch is also valid for ElimUB(Sch).

In the backward direction, assume  $I_{\text{Accessed}}$  is jointly access-valid for ElimUB(Sch), and consider an access (mt, AccBind) with values from  $I_{\text{Accessed}}$ . If mt has no result lower bound, then there is only one possible output for the access, and it is valid also for Sch. Likewise, if mt has a result lower bound of k and there are  $\leq k$  matching tuples for the access in  $I_1$ or in  $I_2$ , then the definition of a result lower bound ensures that there is only one possible output which is valid for ElimUB(Sch) in  $I_1$  and  $I_2$ , and it is again valid for Sch. Finally, if there are > k matching tuples for the access, we let J be a set of tuples in  $I_{\text{Accessed}}$  which is is a valid output to the access in  $I_1$  and  $I_2$  for ElimUB(Sch), and take any subset J' of J with k tuples; it is clearly a valid output to the access for Sch in  $I_1$  and  $I_2$ . This establishes the backward direction, concluding the proof.

Based on this, from now on we will assume only result lower bounds in our schema.

**Reduction to query containment.** Since access-determinacy can be expresses as a query containment, in Theorem D.5 we already established an reduction of RA answerability to query containment. We will spell out what these axioms look like, focusing in the case where we have only result lower bounds. This is sufficient for our purposes by Proposition D.6. The constraints will be a more "more symmetrical" version of the axioms we saw in the case of access monotone determinacy.

Recall that accessible is a fresh unary relation, intuitively used to describe which elements are accessible. Given a schema Sch with constraints and access methods with result bounds, the *access-determinacy containment* for Q and Sch is the CQ containment  $Q \subseteq_{\Gamma} Q'$  where the constraints  $\Gamma$  are defined as follows: they include the original constraints  $\Sigma$ , the constraints  $\Sigma'$  on the relations R', and the following axioms (with implicit universal quantification):

• For each method **mt** that is not result-bounded, letting R be the relation accessed by **mt**:

$$\left(\bigwedge_{i} \operatorname{accessible}(x_{i})\right) \land R(\vec{x}, \vec{y}) \to R_{\operatorname{Accessed}}(\vec{x}, \vec{y})$$
$$\left(\bigwedge_{i} \operatorname{accessible}(x_{i})\right) \land R'(\vec{x}, \vec{y}) \to R_{\operatorname{Accessed}}(\vec{x}, \vec{y})$$

where  $\vec{x}$  denotes the input positions of mt in R and i ranges over these positions.

• For each method mt with a result lower bound of k, letting R be the relation accessed by mt, for all  $j \leq k$ :

$$\begin{split} & \left(\bigwedge_{i} \operatorname{accessible}(x_{i})\right) \wedge \exists^{\geq j} \vec{y} \ R(\vec{x}, \vec{y}) \to \exists^{\geq j} \vec{z} \ R_{\operatorname{Accessed}}(\vec{x}, \vec{z}) \\ & \left(\bigwedge_{i} \operatorname{accessible}(x_{i})\right) \wedge \exists^{\geq j} \vec{y} \ R'(\vec{x}, \vec{y}) \to \exists^{\geq j} \vec{z} \ R_{\operatorname{Accessed}}(\vec{x}, \vec{z}) \end{split}$$

where  $\vec{x}$  denotes the input positions of mt in R.

• For every relation R of the original signature:

$$R_{\text{Accessed}}(\vec{w}) \to R(\vec{w}) \land R'(\vec{w}) \land \bigwedge_{i} \operatorname{accessible}(w_{i}).$$

The intuition, like for AMonDet containment, is that the constraints  $\Gamma$  are axiomatizing the definition of access-determinacy, i.e., enforcing that  $I_{\text{Accessed}}$  is jointly access-valid. The only difference from the AMonDet containment is that the additional constraints are now symmetric in the two signatures, primed and unprimed. The analogue of Proposition 4.9 then follows immediately from Theorem D.5 and the definition of access-determinacy:

**Proposition D.7.** Let Q be a CQ, and let Sch be a schema with constraints expressible in active-domain first-order logic and with access methods that may have result upper and lower bounds. Then the following are equivalent:

- Q has an RA plan that answers it over Sch.
- Q is access-determined over Sch.
- The containment corresponding to access-determinacy holds.

Based on this reduction, all of our arguments about answerability with RA-plans can deal with the semantic notion of access-determinacy and the corresponding entailments, and we will always make use of this in what follows. Also following the convention in the body of the paper, in reasoning about access-determinacy and these entailments, we can restrict to the case of Boolean CQs, since non-Boolean CQs can be considered Boolean CQs with additional constants. We perform this restriction in proofs by default in the remainder of this section.

D.2. Full Answerability and Monotone Answerability. We show that there is no difference between full answerability and monotone answerability when constraints consist of IDs only. This is a generalization of an observation that is known for views (see, e.g., Proposition 2.15 in [BtCLT16]):

**Proposition D.8.** Let Sch be a schema with access methods and constraints  $\Sigma$  consisting of inclusion dependencies, and Q be a CQ that is access-determined. Then Q is AMonDet.

*Proof.* We know by Propositions 4.8 and D.6 that we can work with ElimUB(Sch) which has only result lower bounds, so we do so throughout this proof. Towards proving AMonDet, assume by way of contradiction that we have:

- instances  $I_1$  and  $I_2$  satisfying  $\Sigma$ ;
- an accessible part  $A_1$  of  $I_1$  with valid access selection  $\sigma_1$ , and an accessible part  $A_2$  of  $I_2$  with valid access selection  $\sigma_2$ ;

• 
$$A_1 \subseteq A_2;$$

• Q holding in  $I_1$  but not in  $I_2$ .

We first modify  $I_2$  and  $A_2$  to  $I_2^+$  and  $A_2^+$  by replacing each element that is in  $I_1$  but not in  $A_1$  by a copy that is not in  $I_1$ ; we modify the access selection from  $\sigma_2$  to  $\sigma_2^+$  accordingly. Since  $I_2^+$  is isomorphic to  $I_2$ , it is clearly true that the access selection  $\sigma_2^+$  is valid in  $I_2^+$ ,

that  $A_2^+$  is the accessible part of  $I_2^+$  corresponding to  $\sigma_2^+$ , that  $I_2^+$  satisfies  $\Sigma$  and that Q fails in  $I_2^+$ . Further we still have  $A_1 \subseteq A_2^+$  by construction. What we have ensured at this step is that values of  $I_2^+$  that are in  $I_1$  must be in  $A_1$ .

Consider now  $I_1^+ := I_1 \cup I_2^+$ . It is clear that Q holds in  $I_1^+$ , and  $I_1^+$  also satisfies  $\Sigma$  because IDs are preserved under taking unions. We will show that  $I_1^+$  and  $I_2^+$  have a common accessible part  $A_2^+$ , which will contradict the assumption that Q is access-determined.

Towards this goal, define an access selection  $\sigma_1^+$  on  $I_1^+$  as follows:

- For any access (mt, AccBind) made with a binding where all values are in  $A_1$ , we let  $\sigma_1^+(\mathsf{mt}, \mathsf{AccBind}) := \sigma_1(\mathsf{mt}, \mathsf{AccBind}) \cup \sigma_2^+(\mathsf{mt}, \mathsf{AccBind})$ : note that all returned tuples are in  $A_2^+$ , because the second member of the union is contained in  $A_2^+$ , while the first is contained in  $A_1$  which is a subset of  $A_2^+$ .
- For any access (mt, AccBind) made with a binding where all values are in  $A_2^+$  and some value is not in  $A_1$ , we let  $\sigma_1^+(\text{mt}, \text{AccBind}) := \sigma_2^+(\text{mt}, \text{AccBind})$ : again all tuples returned here are in  $A_2^+$ .
- For any access (mt, AccBind) made with a binding where some value is not in  $A_2^+$ , we choose an arbitrary set of tuples of  $I_1^+$  to form a valid output.

We claim that  $\sigma_1^+$  is a valid access selection and that performing the fixpoint process with this access selection yields  $A_2^+$  as an accessible part of  $I_1^+$ . To show this, first notice that performing the fixpoint process with  $\sigma_2^+$  indeed returns  $A_2^+$ : all facts of  $A_2^+$  are returned because this was already the case in  $I_2^+$ , and no other facts are returned because it is clear by induction that the fixpoint will only consider bindings in  $A_2^+$ , so that the choices made in the third point of the list above have no impact on the accessible part that we obtain.

So it suffices to show that  $\sigma_1^+$  is valid, i.e., that for any access (mt, AccBind) with a binding AccBind in  $A_2^+$ , the access selection  $\sigma_1^+$  returns a set of tuples which is a valid output to the access. For the first point in the list, we know that the selected tuples are the union of a valid result to the access in  $I_1$  and of a valid result to the access in  $I_2^+$ , so it is clear that it consists only of matching tuples in  $I_1^+$ . We then argue that it is valid by distinguishing two cases. If mt is not result-bounded, then the output is clearly valid, because it contains all matching tuples of  $I_1$  and all matching tuples of  $I_2^+$ , hence all matching tuples of  $I_1^+$ . Now suppose mt has a result lower bound of k. Suppose that for  $j \leq k$  there are  $\geq j$  matching tuples in  $I_1^+$ . We will show that the output of the access contains  $\geq j$  tuples. There are two sub-cases. The first sub-case is when there are  $\geq j$  matching tuples in  $I_1$ . In this sub-case we can conclude because  $\sigma_1(\mathsf{mt},\mathsf{AccBind})$  must return  $\geq j$  tuples. The second sub-case is when there are  $\langle j \rangle$  matching tuples in  $I_1$ . In this sub-case,  $\sigma_1(\mathsf{mt},\mathsf{AccBind})$  must return all of them, so these matching tuples are all in  $A_1$ . Hence they are all in  $A_2^+$  because  $A_1 \subseteq A_2^+$ . Thus the returned tuples are in  $I_2^+$ . Thus, in the second sub-case, all matching tuples in  $I_1^+$ for the access are actually in  $I_2^+$ , so we conclude because  $\sigma_2^+$  (mt, AccBind) must return  $\geq j$ tuples. This shows that the outputs of accesses defined in the first point are valid.

For accesses corresponding to the second point in the list, by the construction used to create  $I_2^+$  from  $I_2$ , we know that the value in AccBind which is not in  $A_1$  cannot be in  $I_1$  either. Thus all matching tuples of the access are in  $I_2^+$ . So we conclude because  $\sigma_2^+$  is a valid access selection of  $I_2^+$ . For accesses corresponding to the third point, the output is
always valid by definition. Hence, we have established that  $\sigma_1^+$  is valid, and that it yields  $A_2^+$  as an accessible part of  $I_1^+$ .

We have thus shown that  $I_1^+$  and  $I_2^+$  both have  $A_2^+$  as an accessible part. Since Q holds in  $I_1^+$ , by access-determinacy Q holds in  $I_2$ , and this contradicts our initial assumption, concluding the proof.

From Proposition D.8 we immediately see that in the case where the constraints consist of IDs only, all the results about monotone answerability with result bounds transfer to answerability. This includes simplification results and complexity bounds.

D.3. Blowup for RA Answerability. We now explain how the method of "blowing up counterexamples" introduced in the body extends to work with access-determinacy. We consider a counterexample to access-determinacy in the simplification (intuitively a pair of instances that satisfy the constraints and have a common subinstance that is jointly access-valid but one satisfy the query and one does not), and we show that we can blow it up to a counterexample to access-determinacy in the original schema. As we did in the body, we stick to Boolean CQs in all of our arguments — the results extend to the non-Boolean case by the usual method of changing free variables to constants. Formally, a *counterexample to access-determinacy* for a Boolean CQ Q and a schema Sch<sup>†</sup> is a pair of instances  $I_1^{\dagger}, I_2^{\dagger}$  both satisfying the schema constraints, such that  $I_1^{\dagger}$  satisfies Q while  $I_2^{\dagger}$  satisfies  $\neg Q$ , and  $I_1^{\dagger}$  and  $I_2^{\dagger}$  have a common subinstance  $I_{\text{Accessed}}^{\dagger}$  that is jointly access-valid.

It is clear that, whenever there is a counterexample to access-determinacy for schema Sch and query Q, then Q is *not* access-determined w.r.t. Sch. We now state the blowup lemma that we use. It is the direct analogue of Lemma 5.3, and the intuition is similar: we will obtain our counterexample for Sch by "blowing up" a counterexample to access-determinacy for Sch<sup>†</sup>. Here is the formal statement:

**Lemma D.9.** Let Sch and Sch<sup>†</sup> be schemas and Q a Boolean CQ on the common relations of Sch and Sch<sup>†</sup> such that Q is not access-determined in Sch<sup>†</sup>. Suppose that for some counterexample  $I_1^{\dagger}, I_2^{\dagger}$  to access-determinacy for Q in Sch<sup>†</sup> we can construct instances  $I_1$  and  $I_2$  that satisfy the constraints of Sch, that have a common subinstance  $I_{\text{Accessed}}^{\dagger}$  that is jointly access-valid for Sch, such that  $I_2$  has a homomorphism to  $I_2^{\dagger}$ , and the restriction of  $I_1^{\dagger}$  to the relations of Sch is a subinstance of  $I_1$ . Then Q is not access-determined in Sch.

*Proof.* We prove the contrapositive of the claim. Let Q be a query which is not accessdetermined in  $\mathsf{Sch}^{\dagger}$ , and let  $\{I_1^{\dagger}, I_2^{\dagger}\}$  be a counterexample. Using the hypothesis, we construct  $I_1$  and  $I_2$ . It suffices to observe that they are a counterexample to access-determinacy for Q and  $\mathsf{Sch}$ , which we show. First, they satisfy the constraints of  $\mathsf{Sch}$  and have a common subinstance which is jointly access-valid. Second, as  $I_1^{\dagger}$  satisfies Q, as all relations used in Q are on  $\mathsf{Sch}$ , and as the restriction of  $I_1^{\dagger}$  is a subset of  $I_1$ , we know that  $I_1$  satisfies Q. Finally, since  $I_2^{\dagger}$  does not satisfy Q and  $I_2$  has a homomorphism to  $I_2^{\dagger}$ , we know that  $I_2$  does not satisfy Q. Hence,  $I_1, I_2$  is a counterexample to access-determinacy of Q in  $\mathsf{Sch}$ , which concludes the proof. D.4. Choice Simplifiability for RA answerability. Recall that the choice simplification of a result-bounded schema is obtained by changing every result-bounded method to have bound 1. We say that a schema Sch is *choice simplifiable for RA plans* if any CQ that has an RA plan over Sch has one over its choice simplification. The following result is the counterpart to Theorem 7.3:

**Theorem D.10.** Let Sch be a schema with constraints in equality-free first-order logic (e.g., TGDs), and let Q be a CQ that is access-determined w.r.t. Sch. Then Q is also access-determined in the choice simplification Sch<sup>†</sup> of Sch.

The proof follows that of Theorem 7.3 with no surprises, using Lemma D.9.

Proof. We fix a counterexample  $I_1^{\dagger}, I_2^{\dagger}$  to access-determinacy in  $\mathsf{Sch}^{\dagger}$ : we know that  $I_1^{\dagger}$  satisfies the query,  $I_2^{\dagger}$  violates the query,  $I_1^{\dagger}$  and  $I_2^{\dagger}$  satisfy the equality-free first order constraints of  $\mathsf{Sch}$ , and  $I_1^{\dagger}$  and  $I_2^{\dagger}$  have a common subinstance  $I_{\mathsf{Accessed}}^{\dagger}$  which is jointly access-valid for  $\mathsf{Sch}^{\dagger}$ . We expand  $I_1^{\dagger}$  and  $I_2^{\dagger}$  to  $I_1$  and  $I_2$  that have a common subinstance that is jointly access-valid for  $\mathsf{Sch}^{\dagger}$ . We expand  $I_1^{\dagger}$  and  $I_2^{\dagger}$  to  $I_1$  and  $I_2$  that have a common subinstance that is jointly access-valid for  $\mathsf{Sch}$ , to conclude using Lemma D.9. Our construction is identical to the blow-up used in Theorem 7.3: for each element a in the domain of  $I_1^{\dagger}$ , introduce infinitely many fresh elements  $a^j$  for  $j \in \mathbb{N}_{>0}$ , and identify  $a^0 := a$ . Now, define  $I_1 := \mathsf{Blowup}(I_1^{\dagger})$ , where  $\mathsf{Blowup}(I_1^{\dagger})$  is the instance with facts  $\{R(a_1^{i_1} \dots a_n^{i_n}) \mid R(\vec{a}) \in I_1^{\dagger}, \vec{i} \in \mathbb{N}^n\}$ . Define  $I_2$  from  $I_2^{\dagger}$  in the same way.

The proof of Theorem 7.3 already showed that  $I_1^{\dagger}$  and  $I_1$  agree on all equality-free first-order constraints, that  $I_1^{\dagger}$  still satisfies the query, and  $I_2^{\dagger}$  still violates the query. All that remains is to construct a common subinstance that is jointly access-valid for Sch. We do this as in the proof of Theorem 7.3, setting  $I_{\text{Accessed}} := \text{Blowup}(I_{\text{Accessed}}^{\dagger})$ . To show that  $I_{\text{Accessed}}$ is jointly access-valid, consider any access (mt, AccBind) with values from  $I_{\text{Accessed}}$ . If there are no matching tuples in  $I_1^{\dagger}$  and in  $I_2^{\dagger}$ , then there are no matching tuples in  $I_1$  and  $I_2$  either. Otherwise, there must be some matching tuple in  $I_{\text{Accessed}}^{\dagger}$  because it is jointly access-valid in  $I_1^{\dagger}$  and  $I_2^{\dagger}$  for Sch<sup>†</sup>. Hence, sufficiently many copies exist in  $I_{\text{Accessed}}$  to satisfy the original result bounds, so we can find a valid response to the access in  $I_{\text{Accessed}}$ . Hence,  $I_{\text{Accessed}}$  is indeed jointly access-valid, which completes the proof.

As with choice simplification for AMonDet, this result can be applied immediately to TGDs. In particular, if we consider frontier-guarded TGDs, the above result says that we can assume any result bounds are 1, and thus the query containment problem produced by Proposition D.7 will involve only frontier-guarded TGDs. We thus get the following analog of Theorem 8.1:

**Theorem D.11.** We can decide whether a CQ is RA answerable with respect to a schema with result bounds whose constraints are frontier-guarded TGDs. The problem is 2EXPTIME-complete.

D.5. **FD** Simplifiability for **RA** plans. We now turn to FD simplification. Recall that the FD simplification of a result-bounded schema is intuitively defined by adding an auxiliary relation  $R_{\rm mt}$  for every result-bounded method **mt**, relating it with inclusion dependencies to the relation R accessed by **mt**, and replacing **mt** by a non-result-bounded method on  $R_{\rm mt}$ . The new method makes it possible to retrieve the values for the output positions that are

determined by the input positions of mt according to the FDs. The formal definition is given in Section 5. A schema is *FD simplifiable for RA plans* if every CQ having a plan over the schema has an RA plan in its FD simplification.

We now show that schemas whose constraints consist only of FDs are FD simplifiable, which is the analogue of Theorem 5.5:

**Theorem D.12.** Let Sch be a schema whose constraints are FDs, and let Q be a CQ that is RA answerable in Sch. Then Q is RA answerable in the FD simplification  $Sch^{\dagger}$  of Sch.

*Proof.* We use Lemma D.9 and assume that we have a counterexample  $I_1^{\dagger}$ ,  $I_2^{\dagger}$  to determinacy for Sch<sup>†</sup>, with Q holding in  $I_1^{\dagger}$ , with Q not holding in  $I_2^{\dagger}$ , and with  $I_1^{\dagger}$  and  $I_2^{\dagger}$  having a common subinstance  $I_{Accessed}^{\dagger}$  which is jointly access-valid in  $I_1^{\dagger}$  and  $I_2^{\dagger}$  for Sch<sup>†</sup>. We will upgrade these to  $I_1$ ,  $I_2$ ,  $I_{Accessed}$  having the same property for Sch, by blowing up accesses one after the other. We fix a valid access selection  $\sigma$  for  $I_{Accessed}^{\dagger}$  which returns outputs for accesses that are valid in  $I_1^{\dagger}$  and in  $I_2^{\dagger}$ .

We construct  $I_1$ ,  $I_2$  and  $I_{\text{Accessed}}$  exactly as in the proof of Theorem 5.5 with the access selection  $\sigma$ , performing the same blowing up process (recall that it distinguished between the "dangerous" and the "non-dangerous" methods). The only point to show is that  $I_{\text{Accessed}}$ is jointly access-valid in  $I_1$ . To do so, we distinguish several possibilities, again following the distinction in that proof. If AccBind contains values from Adom $(I_{\text{Accessed}}) \setminus \text{Adom}(I_{\text{Accessed}}^{\dagger})$ , then all matching tuples in either  $I_1$  or  $I_2$  are in  $I_{\text{Accessed}}$  and there is nothing to show. If the method used is not result-bounded, then the matching tuples in  $I_1$  and  $I_2$  are either tuples of  $I_1^{\dagger}$  and  $I_2^{\dagger}$  that were already in  $I_{\text{Accessed}}^{\dagger}$ , or tuples added to  $I_1$  and  $I_2$  that were added to  $I_{\text{Accessed}}$  as well. If the method is dangerous, then one possibility is that the corresponding access on  $I_{\text{Accessed}}^{\dagger}$  according to  $\sigma$  either returned no tuples, in which case there are no matching tuples in  $I_1$  and  $I_2$  and all potential matching tuples are in  $I_{\text{Accessed}} \setminus I_{\text{Accessed}}^{\dagger}$ . Or the access returned precisely one tuple, which was added to  $I_{\text{Accessed}}$ .

For the case of an access with a result-bounded and dangerous method, there are again two cases. If we did not blow up the access, then  $\sigma$  did not return a result, and there were no matching tuples in  $I_1^{\dagger}$  or  $I_2^{\dagger}$  for the access, so all potential matching tuples in  $I_1$  or  $I_2$  are in  $I_{\text{Accessed}}$ . If we did blow up the access, then we know by construction that  $I_{\text{Accessed}}$  contains infinitely many tuples, from which we can construct a response which is valid both in  $I_1$ and  $I_2$ . This concludes the proof using Lemma D.9.

D.6. Complexity of RA answerability for FDs. In Theorem 6.2 we showed that monotone answerability with FDs was decidable in the lowest possible complexity, i.e., NP.

The argument involved first showing FD simplifiability, which allowed us to eliminate result bounds at the cost of adding additional IDs. We then simplified the resulting rules to ensure that the chase would terminate. This relied on the fact that the axioms for AMonDet would include rules going from R to R', but not vice versa. Hence, the argument does not generalize for the rules that axiomatize RA plans.

However, we can repair the argument at the cost of adding an additional assumption. A schema Sch with access methods is *single method per relation*, abbreviated SMPR, if for every relation there is at most one access method. This assumption was made in many works on access methods [LC01a, Li03], although we do not make it by default elsewhere in this work. We can then show the following analogue of Theorem 6.2 with this additional assumption:

We will actually show something stronger: for SMPR schemas with constraints consisting of FDs only, there is no difference between full answerability and monotone answerability. Given Theorem 6.2, this immediately implies Theorem D.13.

**Proposition D.14.** Let Sch be a schema with access methods satisfying SMPR and constraints  $\Sigma$  consisting of functional dependencies, and Q be a CQ that is access-determined. Then Q is AMonDet.

*Proof.* We know from Theorem D.12 that the schema is FD simplifiable, so we can eliminate result bounds as follows. Recall that  $\mathsf{DetBy}(\mathsf{mt})$  denotes the positions of the relation of  $\mathsf{mt}$  that are determined by the input positions of  $\mathsf{mt}$  according to the FDs. Recall the form of the FD simplification:

- The signature of Sch<sup>†</sup> is that of Sch plus some new relations: for each result-bounded method mt, letting R be the relation accessed by mt, we add a relation  $R_{mt}$  whose arity is |DetBy(mt)|.
- The integrity constraints of Sch<sup>†</sup> are those of Sch plus, for each result-bounded method mt of Sch, two new ID constraints:

$$\begin{aligned} R(\vec{x}, \vec{y}, \vec{z}) &\to R_{\mathsf{mt}}(\vec{x}, \vec{y}) \\ R_{\mathsf{mt}}(\vec{x}, \vec{y}) &\to \exists \vec{z} \; R(\vec{x}, \vec{y}, \vec{z}) \end{aligned}$$

where  $\vec{x}$  denotes the input positions of mt and  $\vec{y}$  denotes the other positions of DetBy(mt).

• The methods of  $\mathsf{Sch}^{\dagger}$  are the methods of  $\mathsf{Sch}$  that have no result bounds, plus the following: for each result-bounded method  $\mathsf{mt}$  on relation R in  $\mathsf{Sch}$ , a method  $\mathsf{mt}^{\dagger}$  on  $R_{\mathsf{mt}}$  that has no result bounds and whose input positions are the positions of  $R_{\mathsf{mt}}$  corresponding to input positions of  $\mathsf{mt}$ .

By Proposition D.7 we know that Q is access-determined exactly when  $Q \subseteq_{\Gamma} Q'$ , where  $\Gamma$  contains two copies of the above schema and also axioms of the following form for each access method **mt**:

• (Forward):

$$\bigwedge_{i} \operatorname{accessible}(x_{i}) \land S(\vec{x}, \vec{y}) \to \left(\bigwedge_{i} \operatorname{accessible}(y_{i})\right) \land S'(\vec{x}, \vec{y}).$$

• (Backward):

$$\left(\bigwedge_{i} \operatorname{accessible}(x_{i})\right) \wedge S'(\vec{x}, \vec{y}) \rightarrow \left(\bigwedge_{i} \operatorname{accessible}(y_{i})\right) \wedge S(\vec{x}, \vec{y})$$

where  $\vec{x}$  denotes the input positions of mt. Note that S may be one of the original relations, or one of the relations  $R_{\rm mt}$  produced by the transformation above, depending on whether mt originally had result bounds or not.

We now show that chase proofs with  $\Gamma$  must in fact be very simple under the SMPR assumption:

Claim D.15. Assuming our schema is SMPR, consider any chase sequence for  $\Gamma$ . Then:

- Rules of the form  $R_{\mathsf{mt}}(\vec{x}, \vec{y}) \to \exists \vec{z} \ R(\vec{x}, \vec{y}, \vec{z})$  will never fire.
- Rules of the form  $R'(\vec{x}, \vec{y}, \vec{z}) \to R'_{\mathsf{mt}}(\vec{x}, \vec{y})$  will never fire.
- FDs will never fire (assuming they were satisfied on the initial instance).

## • (Backward) axioms will never fire.

Note that the last item suffices to conclude that Proposition D.14 holds, since a proof of access-determinacy in which (Backward) axioms never fire is a proof of AMonDet. So it suffices to prove the claim. We do so by induction on the length of a chase proof. We consider the first item. Consider a fact  $R_{mt}(\vec{c}, \vec{d})$ . Since the (Backward) axioms never fire (fourth point of the induction), the fact must have been produced from a fact  $R(\vec{c}, \vec{d}, \vec{e})$ . Hence the axiom can not fire on this fact, because we only fire active triggers.

We move to the second item, considering a fact  $R'(\vec{c}, \vec{d}, \vec{e})$ . By SMPR and the inductive assumption that FDs do not fire, this fact can only have been produced via applying a (Backward) axiom to a fact of the form  $R'_{mt}(\vec{c}, \vec{d})$ . Since inductively we know that such rules doe not fire, this completes the inductive step.

Turning to the third item, we first consider a potential violation of an FD  $D \rightarrow r$  on an unprimed relation R. This consists of facts  $R(\vec{c})$  and  $R(\vec{d})$  agreeing on positions in Dand disagreeing on position r. As the initial instance is always assumed to satisfy the FDs, these facts are not in the initial instance. But they could not have been otherwise produced, as we know by induction (first and fourth points) that none of the rules with an unprimed relation R in their head will fire. Now let us turn to facts that are potential violations of the primed copies of the FDs, for some relation R'. The existence of the violation implies that there is an access method on the corresponding relation R in the original schema, since otherwise there could be no relation  $R'_{mt}$ , and such a violation could not have occurred. By the SMPR assumption there is exactly one such method.

We first consider the case where this access method has result bounds. We know that the facts in the violation must have been produced by the rule going from  $R'_{mt}$  to R' (noting that in this case the Forward rule creates  $R'_{mt}$ -facts, not R'-facts). Let us write the facts of the violation as  $R'(\vec{c}_1, \vec{d}_1, \vec{e}_1)$  and  $R'(\vec{c}_2, \vec{d}_2, \vec{e}_2)$ . Assume that  $R'(\vec{c}_2, \vec{d}_2, \vec{e}_2)$  was the latter of the two facts to be created, then  $\vec{e}_2$  would have been chosen fresh. Hence the violation must occur within the positions corresponding to  $\vec{c}_1, \vec{d}_1$  and  $\vec{c}_2, \vec{d}_2$ . But by induction (third point), and by the SMPR assumption, these facts must have been created from facts  $R'_{mt}(\vec{c}_1, \vec{d}_1)$ and  $R'_{mt}(\vec{c}_2, \vec{d}_2)$  where mt is the only access method on R, and in turn these must have been created from facts  $R_{mt}(\vec{c}_1, \vec{d}_1)$  and  $R_{mt}(\vec{c}_2, \vec{d}_2)$ . These last must (again, by induction, using the third and fourth points) have been created from facts  $R(\vec{c}_1, \vec{d}_1, \vec{f}_1)$  and  $R(\vec{c}_1, \vec{d}_1, \vec{g}_1)$ . But then we have an earlier violation of the FDs on these two facts, which is a contradiction.

We now consider the second case, where the access method on R has no result bounds in the original schema. In this case there is no relation  $R'_{mt}$  and the facts of the violation must have been produced by applying the Forward rule, which can only apply to the relation R. But then the R-facts used to create them must themselves be an earlier violation of the corresponding FD on R, which is again a contradiction. Hence, we have shown the third item.

Turning to the last item, there are two kinds of Backward rules to consider. First, the ones involving a primed relation R' and the original relation R, where there is an access method without result bounds on R in the original schema. Secondly, the ones involving a primed relation  $R'_{mt}$  and the unprimed relation  $R_{mt}$  where there is an access method with result bounds on R in the original schema. For the first kind of axiom, any R'-fact can only have been created from an R-fact using the Forward axioms, and so the Backward axiom cannot fire. For the second kind of axiom, we show the claim by considering a fact  $R'_{mt}(\vec{c}, \vec{d})$ .

Using the second point of the induction, it can only have been generated by a fact  $R_{mt}(\vec{c}, d)$ , and thus (Backward) could not fire, which establishes the desired result.

Without SMPR, we can still argue that RA answerability is decidable, and show a singly exponential complexity upper bound:

## **Theorem D.16.** For general schemas with access methods and constraints $\Sigma$ consisting of FDs, RA answerability is decidable in EXPTIME.

*Proof.* We consider the query containment problem for RA answerability obtained after eliminating result bounds, and let  $\Gamma$  be the corresponding constraints as in Proposition D.14.

Instead of claiming that neither the FDs nor the backward axioms will fire, as in the case of SMPR, we argue only that the FDs will not fire. From this it follows that the constraints consist only of IDs and accessibility axioms, leading to an EXPTIME complexity upper bound: one can apply the EXPTIME complexity result without result bounds from [BBB13].

We consider a chase proof with  $\Gamma$ , and claim, for each relation R and each result-bounded method **mt** on R, the following invariant:

- Every  $R_{mt}$ -fact and every  $R'_{mt}$ -fact is a projection of some R-fact or some R'-fact.
- All the FDs are satisfied in the chase instance, and further for any relation R, the relation  $R \cup R'$  satisfies any FDs on relation R, That is: for any FD  $D \rightarrow r$  on relation R, we cannot have an R-fact and an R'-fact that agree on positions in D and disagree on some position in r.

The second item of the invariant implies that the FDs do not fire, which as we have argued is sufficient to conclude our complexity bound.

The invariant is initially true, by assumption that FDs are satisfied on the initial instance. When firing an R-to- $R_{mt}$  axiom or an R'-to- $R'_{mt}$  axiom, the first item is preserved by definition, and the second is trivially preserved since there are no FDs on  $R_{mt}$  or  $R'_{mt}$ .

When firing an accessibility axiom, either forward or backward, again the first and the second item are clearly preserved.

Now, consider the firing of an  $R_{mt}$ -to-R axiom. The first item is trivially preserved, so we must only show the second.

Consider the fact  $R_{\mathsf{mt}}(a_1 \ldots a_m)$  and the generated fact  $F = R(a_1 \ldots a_m, b_1 \ldots b_n)$ created by the rule firing. Assume that F is part of an FD violation with some other fact F' which is of the form  $R(a'_1 \ldots a'_m, b'_1 \ldots b'_m)$  or  $R'(a'_1 \ldots a'_m, b'_1 \ldots b'_m)$ .

We know that the left-hand-side of the FD cannot contain any of the positions of the  $b_i$ , because they are fresh nulls. Hence, the left-hand-side of the FD is included in the positions of  $a_1 \ldots a_m$ . But now, by definition of the FD simplification, the right-hand-side of the FD cannot correspond to one of the  $b_1 \ldots b_n$ , since otherwise that position would have been included in  $R_{\rm mt}$ . So the right-hand-side is also one of the positions of  $a_1 \ldots a_m$ , and in particular we must have  $a_i \neq a'_i$  for some  $1 \leq i \leq m$  in the right-hand-side of the FD.

Now we use the first item of the inductive invariant on the fact  $R_{mt}(a_1 \ldots a_m)$ : there was already a fact F'', either an R or R'-fact, with tuple of values  $(a_1 \ldots a_m, b''_1 \ldots b''_m)$ . As there is  $1 \le i \le m$  such that  $a'_i \ne a_i$ , the tuples of values of F' and F'' must be different. But now, as F and F' are an FD violation on the positions  $a_1 \ldots a_m$ , then F' and F'' are seen to also witness an FD violation in  $R \cup R'$  that existed before the firing. This contradicts the first point of the invariant, so we conclude that the second item is preserved when firing an  $R_{mt}$ -to-R axiom.

When firing  $R'_{mt}$ -to-R' rules, the symmetric argument applies.

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This completes the proof of the invariant, and concludes the proof of Theorem D.16.  $\Box$ 

D.7. Choice Simplifiability for RA plans with UIDs and FDs. We last turn to the adaptation of our choice simplifiability result for UIDs and FDs (Theorem 7.4). Here is the statement for the case of RA plans:

**Theorem D.17.** Let schema Sch have constraints given by UIDs and arbitrary FDs, and Q be a CQ that is access-determined w.r.t. Sch. Then Q is also access-determined in the choice simplification of Sch.

We will proceed in a similar fashion to Theorem 7.4, i.e., fixing one access at a time. Here is the analogue of the single-access blowup (Definition 7.5), where we simply replace the access-valid subinstance by a jointly access-valid subinstance:

**Definition D.18.** Let Sch be a schema and Sch<sup>†</sup> be its choice simplification, and let  $\Sigma$  be a set of constraints.

Consider two instances  $I_1^{\dagger}, I_2^{\dagger}$  that satisfy  $\Sigma$ , and a common subinstance  $I_{\text{Accessed}}^{\dagger}$  which is jointly access-valid in  $I_1^{\dagger}$  and  $I_2^{\dagger}$  for Sch<sup>†</sup>. Let (mt, AccBind) be an access in  $I_{\text{Accessed}}^{\dagger}$ 

A single-access RA blowup of  $I_1^{\dagger}$ ,  $I_2^{\dagger}$  and  $I_{\text{Accessed}}^{\dagger}$  for (mt, AccBind) is a pair of instances  $I_1, I_2$  that satisfy  $\Sigma$ , such that  $I_1$  is a superinstance of  $I_1^{\dagger}$ ,  $I_2$  has a homomorphism to  $I_2^{\dagger}$ ,  $I_1$  and  $I_2$  have a common subinstance  $I_{\text{Accessed}}$  which is jointly access-valid in  $I_1$  and  $I_2$  for Sch<sup>†</sup>, and the following hold:

- (1)  $I_{\text{Accessed}}$  is a superinstance of  $I_{\text{Accessed}}^{\dagger}$ ;
- (2) there is an output to the access mt, AccBind in  $I_{\text{Accessed}}$  which is valid in  $I_1$  for Sch;
- (3) for any access in  $I_{\text{Accessed}}^{\dagger}$  having an output in  $I_{\text{Accessed}}^{\dagger}$  which is valid for Sch in  $I_{1}^{\dagger}$ , there is an output to this access in  $I_{\text{Accessed}}$  which is valid for Sch in  $I_{1}$ ;
- (4) for any access in  $I_{\text{Accessed}}$  which is not an access in  $I_{\text{Accessed}}^{\dagger}$ , there is an output in  $I_{\text{Accessed}}$  which is valid for Sch in  $I_1$ ;

We use the following blowup lemma as an analogue of Lemma 7.6:

**Lemma D.19.** Let Sch be a schema and Sch<sup>†</sup> be its choice simplification, and let  $\Sigma$  be the set of constraints.

Assume that, for any CQ Q not access-determined in Sch<sup>†</sup>, for any counterexample  $I_1^{\dagger}, I_2^{\dagger}$ of access-determinacy for Q and Sch<sup>†</sup> with a common subinstance  $I_{Accessed}^{\dagger}$  jointly access-valid in  $I_1^{\dagger}$  and  $I_2^{\dagger}$  for Sch<sup>†</sup>, for any access mt, AccBind in  $I_{Accessed}^{\dagger}$ , we can construct a single-access RA blowup of  $I_1^{\dagger}, I_2^{\dagger}$  and  $I_{Accessed}^{\dagger}$  for (mt, AccBind).

Then any CQ which is access-determined in Sch is also access-determined in  $Sch^{\dagger}$ .

The proof of this lemma is exactly like that of Lemma 7.6.

We are now ready to prove Theorem D.17 using the process of Lemma D.19. We proceed similarly to the proof of Theorem 7.4.

*Proof.* Let Sch be the schema, let Sch<sup>†</sup> be its choice simplification, and let  $\Sigma$  be the set of constraints. Let Q be a CQ which is not access-determined in Sch<sup>†</sup>, let  $I_1^{\dagger}, I_2^{\dagger}$  be a counterexample to access-determinacy, and let  $I_{\text{Accessed}}^{\dagger}$  be a common subinstance of  $I_1^{\dagger}$  and  $I_2^{\dagger}$ for Sch<sup>†</sup> which is jointly access-valid in  $I_1^{\dagger}$  and  $I_2^{\dagger}$  for Sch<sup>†</sup>. Let (mt, AccBind) be an access on relation R in  $I_{\text{Accessed}}^{\dagger}$ : we know that this access has an output which is valid for Sch<sup>†</sup>, but it does not necessarily have one which is valid for Sch. Our proof is to follow the single-access RA blowup process and build superinstances  $I_1$ ,  $I_2$ , and  $I_{\text{Accessed}}$  of  $I_1^{\dagger}$ ,  $I_2^{\dagger}$ , and  $I_{\text{Accessed}}$  respectively, which satisfy the conditions.

As in the proof of Theorem D.17, if there are no matching tuples in  $I_1^{\dagger}$  for the access (mt, AccBind), then there are no matching tuples in  $I_{\text{Accessed}}^{\dagger}$  either, so the access (mt, AccBind) already has a valid output for Sch and there is nothing to do. The same holds if there are no matching tuples in  $I_2^{\dagger}$ . Now, if there is exactly one matching tuple in  $I_1^{\dagger}$  and exactly one matching tuple in  $I_2^{\dagger}$ , as  $I_{\text{Accessed}}^{\dagger}$  is jointly access-valid for Sch<sup>†</sup>, it necessarily contains these matching tuples, so that, as  $I_{\text{Accessed}}^{\dagger} \subseteq I_1^{\dagger}$  and  $I_{\text{Accessed}}^{\dagger} \subseteq I_2^{\dagger}$ , the matching tuple in  $I_1^{\dagger}$  and again there is nothing to do: the access (mt, AccBind) already has a valid output for Sch.

Hence, the only interesting case is when there is a matching tuple to the access in  $I_1^{\dagger}$ and in  $I_2^{\dagger}$ , and there is more than one matching tuple in one of the two. As  $I_1^{\dagger}$  and  $I_2^{\dagger}$  play a symmetric role in the hypotheses of Lemma D.19, we assume without loss of generality that it is  $I_1^{\dagger}$  which has multiple matching tuples for the access.

As  $I_{\text{Accessed}}^{\dagger}$  is access-valid in  $I_1^{\dagger}$  for  $\mathsf{Sch}^{\dagger}$ , we know that  $I_{\text{Accessed}}^{\dagger}$  contains at least one of these tuples, say  $\vec{t}_1$ . As  $I_{\text{Accessed}} \subseteq I_2^{\dagger}$ , then  $I_2^{\dagger}$  also contains  $\vec{t}_1$ . As in the proof of Theorem 7.4, we take  $\vec{t}_2$  a different matching tuple in  $I_1^{\dagger}$ , let C be the non-empty set of positions where  $\vec{t}_1$  and  $\vec{t}_2$  disagree, and observe that there is no FD implied from the complement of C to a position of C.

We define W as in the proof of Theorem 7.4, and construct  $I_1 := I_1^{\dagger} \cup W$  and  $I_2 := I_2^{\dagger} \cup W$ as in that proof. We show that  $(I_1, I_2)$  is a counterexample to determinacy for Q and Sch<sup>†</sup>:

- We know by Claim 7.7 that  $I_1$  and  $I_2$  satisfy the UIDs and the FDs of  $\Sigma$ .
- We clearly have  $I_1^{\dagger} \subseteq I_1$ .
- The homomorphism from  $I_2$  to  $I_2^{\dagger}$  is defined as in the proof of Theorem 7.4.
- We define  $I_{\text{Accessed}} := I_{\text{Accessed}}^{\dagger} \cup W$  a common subinstance of  $I_1$  and  $I_2$  and we must show that  $I_{\text{Accessed}}$  is jointly access-valid in  $I_1$  and  $I_2$  for  $\text{Sch}^{\dagger}$ . We do this as in the proof of Theorem 7.4. First, for accesses that include an element of  $\text{Adom}(I_{\text{Accessed}}) \setminus \text{Adom}(I_{\text{Accessed}}^{\dagger})$ , the matching tuples are all in W so they are in  $I_{\text{Accessed}}$ . Second, for accesses on  $\text{Adom}(I_{\text{Accessed}}^{\dagger})$ , the matching tuples include the result U of this access in  $I_{\text{Accessed}}^{\dagger}$ , which was valid in  $I_1^{\dagger}$  and  $I_2^{\dagger}$ , and possible additional matching tuples U' from W which are in  $I_{\text{Accessed}}$ , and these are the only possible matching tuples. Thus, we can construct a valid output to this access for  $\text{Sch}^{\dagger}$  from U and U'.

What remains to be able to use Lemma D.19 is to show the four additional conditions:

- (1) It is immediate that  $I_{\text{Accessed}} \supseteq I_{\text{Accessed}}^{\dagger}$ .
- (2) The access (mt, AccBind) has an output in  $I_{\text{Accessed}}$  which is valid for Sch in  $I_1$  and  $I_2$ . This is established as in the proof of Theorem 7.4: there are now infinitely many matching tuples for the access in  $I_1$  and  $I_2$ , so we can choose as many as we want in W to obtain an output in  $I_{\text{Accessed}}$  which is valid for Sch in  $I_1$  and  $I_2$ .
- (3) For every access of  $I_{\text{Accessed}}^{\dagger}$  that has an output which is valid for Sch in  $I_1^{\dagger}$  in  $I_2^{\dagger}$ , then we can construct such an output in  $I_{\text{Accessed}}$  which is valid for Sch in  $I_1$  and  $I_2$ . This is similar to the fourth bullet point above. From the output U to the access in  $I_{\text{Accessed}}^{\dagger}$  which is

Fragment	Simplification	Complexity
IDs	Existence-check (Thm 5.2, Prop. D.8)	EXPTIME-complete (Thm 6.3, Prop. D.8)
Bounded-width IDs	Existence-check (see above)	$NP ext{-complete}$ (Thm 6.4, Prop D.8)
FDs	FD (Thm D.12)	In EXPTIME (Thm D.16)
FDs under $SMPR$	FD (see above)	NP-complete (Thm D.13)
FDs and UIDs	Choice (Thm D.17)	Open
Equality-free FO	Choice (Thm D.10)	Undecidable (same proof as Prop 9.2)
Frontier-guarded TGDs	Choice (see above)	2EXPTIME-complete (Thm D.11)

Table 2: Summary of results on simplifiability and complexity of RA answerability

valid for  $I_1^{\dagger}$  and  $I_2^{\dagger}$ , we construct an output to the access in  $I_{\text{Accessed}}$  which is valid for  $I_1$  and  $I_2$ , using the tuples of U and the matching tuples in W.

(4) All accesses of  $I_{\text{Accessed}}$  which are not accesses of  $I_{\text{Accessed}}^{\dagger}$  have an output which is valid for Sch in  $I_1$  and  $I_2$ . As before, such accesses must include an element of W, so by the fourth bullet point all matching tuples are in W, so they are all in  $I_{\text{Accessed}}$ .

Hence, we have explained how to fix the access (mt, AccBind), so we can conclude using Lemma D.19 that we obtain a counterexample to access-determinacy of Q in Sch by fixing all accesses. This concludes the proof.

D.8. Summary of Extensions to Answerability with RA plans. Table 2 summarizes the expressiveness and complexity results for RA plans. There are two differences with the corresponding table for monotone answerability (Table 1 in the body):

- For RA plans, while we know that choice simplifiability holds with FDs and UIDs, we do not know whether answerability is decidable. Indeed, in the monotone case, when proving Theorem 8.2, we had used a separability argument to show that FDs could be ignored for FDs and UIDs (see the proof of Theorem 8.2 in Section 8). We do not have such an argument for answerability with RA plans.
- For RA plans, our tight complexity bound for answerability with FDs in isolation holds only under the SMPR assumption; see Appendix D.6 for details.