A Simple Algorithm for Consistent Query Answering Under Primary Keys

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Abstract

We consider the dichotomy conjecture for consistent query answering under primary key constraints. It states that, for every fixed Boolean conjunctive query q, testing whether q is certain (i.e. whether it evaluates to true over all repairs of a given inconsistent database) is either polynomial time or coNP-complete. This conjecture has been verified for self-join-free and path queries.

We propose a simple inflationary fixpoint algorithm for consistent query answering which, for a given database, naively computes a set Δ of subsets of database repairs with at most k facts, where k is the size of the query q. The algorithm runs in polynomial time and can be formally defined as:

1. Initialize Δ with all sets S of at most k facts such that $S \models q$.
2. Add any set S of at most k facts to Δ if there exists a block B (i.e., a maximal set of facts sharing the same key) such that for every fact $a \in B$ there is a set $S' \in \Delta$ contained in $S \cup \{a\}$.

The algorithm answers "q is certain" iff Δ eventually contains the empty set. The algorithm correctly computes certainty when the query q falls in the polynomial time cases of the known dichotomies for self-join-free queries and path queries. For arbitrary Boolean conjunctive queries, the algorithm is an under-approximation: the query is guaranteed to be certain if the algorithm claims so. However, there are polynomial time certain queries (with self-joins) which are not identified as such by the algorithm.

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1 Introduction

A database often comes with integrity constraints. The constraints are helpful in many ways, for instance in order to help optimizing query evaluation. When the database violates its integrity constraints we are faced with several possibilities. A first possibility is to clean the data until all integrity constraints are satisfied. This task is not easy as it is inherently non-deterministic: there could be many equally good ways to "repair" a database. A repair can be understood as a minimal way to change the database in order to satisfy the constraints.

Another possibility is to keep the database in its inconsistent state, postponing the problem until a query is asked to the database. In order to evaluate the query, the classical solution is to consider all possible repairs of the database and to output all the answers on the database D which are "certain", i.e., those answers that are in the output of the query when evaluated on *every* repair of D [2]. However, this method usually has an impact on the complexity of the query evaluation problem. The impact will of course depend on the type of integrity constraints and on the definition of a repair, but most often the worst case complexity increases by a factor at least exponential in the size of the database, as there could be exponentially many ways to repair a database.

Depending on the integrity constraints, what is a "good" notion of repair may be controversial. In this paper we consider primary key constraints, which are arguably the most common kind of integrity constraints in databases. For primary keys, there is a unanimously accepted notion of repair. Primary key constraints identify, for each relation, a set of attributes which are considered to be the relation *key*. An inconsistent database is therefore a database that has distinct tuples within a relation sharing the same key. For such constraints, the standard notion of a repair is any maximal subset of the database satisfying all the primary key constraints. This amounts to keeping exactly one among all tuples having the same key in each relation. A simple analysis shows that there can be exponentially many repairs for a given database, and therefore a naive evaluation algorithm would have to evaluate the query on each of these exponentially many repairs.

We consider Boolean conjunctive queries which can be evaluated efficiently over all databases, in polynomial time in data complexity. With the certain answer semantics described above, a query is certain on an inconsistent database if it is true on all its repairs. The data complexity of certain answers for conjunctive queries over inconsistent databases in the presence of primary key constraints is therefore in coNP since, in order to test whether the query is not certain, it is enough to guess a subset of the database which is a repair and which makes the query false. Further, it has been observed that for some conjunctive queries the certain answering problem is coNP-hard [4] while, for other queries, the certain answering problem can be solved in polynomial time. The main conjecture for inconsistent databases in the presence of primary keys is that there are no intermediate cases: for any conjunctive query, the certain answering problem is either solvable in polynomial time or is complete for coNP.

The conjecture has been proved for self-join-free Boolean conjunctive queries [8]. These are queries on which there are no two atoms using the same relation. It has been also proved for path queries [7]. However, the conjecture remains open for arbitrary conjunctive queries (with self-joins).

In this paper we revisit the two cases above where the conjecture is known to hold: self-join-free queries and path queries.

Contributions. Our main contribution is the design of a simple fixpoint algorithm for computing certain answers of queries over inconsistent databases in the presence of primary key constraints. For every $k \geq 1$, we describe a fixpoint algorithm parameterized by k. The algorithm is always an under-approximation of the certain answers: on Boolean queries, when it outputs "yes" then the query is certain, i.e., it is true on all repairs of the database. But there could false negatives: queries which are certain on which the algorithm outputs "no".

Our main result shows that for all self-join-free queries and path queries whose certain answering problem is computable in polynomial time there is a number k (namely, the number of atoms of the query) such that this simple algorithm correctly computes the certain answer. In other words, if for all k our algorithm gives a false negative answer for a self-join-free or path query it is because the query has a coNP-complete certain answering problem.

A natural question is then to wonder whether our algorithm always correctly computes the certain answering problem on all queries for which this problem is polynomial time computable. We answer negatively to this question, by exhibiting a conjunctive query (with self-joins) whose certain answers can be solved in polynomial time, but for all k the algorithm fails to give a correct answer.

Though our greedy fixpoint computation algorithm is simple, the proof of correctness is not. In the case of self-join-free queries, we provide a semantic condition and show that when the condition holds, the fixpoint gives always the correct answer, by setting the parameter k to be the number of atoms of the query. The proof is by contradiction: if the algorithm fails to give the correct answer, we use the fixpoint definition of the algorithm in order to produce (chase) an infinite sequence of distinct facts of the database, contradicting its finiteness. When the semantic condition does not hold, we show that it implies the condition of [8] characterizing those queries having a coNP-complete certain answers problem.

The situation is simpler for the case of path queries, as we show that for a suitable k (again the number of atoms of the query), our fixpoint algorithm can simulate the polynomial time algorithm of [7] for computing certain answers for q, assuming that certain answering for q is polynomial time solvable.

Related work. Our work is very much inspired by the results of Koutris and Wijsen [9, 8]. For self-join-free queries, the authors prove the polynomial-time case via a long sequence of reductions eventually producing a simple query whose certain answers can be solved efficiently. When unfolding the sequence of reductions this gives a complicated polynomial time algorithm with a complex proof of correctness. We have basically simplified the algorithm and pushed all the difficulty into the proof of correctness. Our algorithm is simple, but the proof of correctness is arguably as complex as theirs. Further, our algorithm does not give, a priori, the optimal LogSpace complexity result of [9] as we know that some of the path queries that can be solved with our algorithm are PTime complete [7]. The semantic condition that we provide for characterizing the polynomial case in the self-join-free case can be effectively tested, but not efficiently, unlike the simple syntactic characterization of [8] based on the so-called "attack graph" of the query.

In the case of path queries, [7] also provides a simple fixpoint algorithm for solving the polynomial cases. Though it seems that their algorithm is different in spirit from ours, the two algorithms have some similarities that we use in order to "simulate" their fixpoint computation using ours.

All missing details can be found in the appendix of the long version of this paper [3].

2 Preliminaries

A **database** is a finite relational structure. A **relational signature** is a finite set of relation symbols associated with an arity. A **finite relational structure** D over a relational signature σ is composed of: a finite set, the domain of D, and a function associating to each symbol R of σ a relation $R(D)$ of the appropriate arity over the domain of D.

An R**-fact** of a database D over a signature σ is a term of the form $R(\bar{a})$ where R is a symbol of σ and $\bar{a}$ a tuple in $R(D)$. A **fact** is an R-fact for some R, R is then the symbol associated to the fact and $\bar{a}$ the tuple associated to the fact. A database can then be viewed as a finite collection of facts. By the **size of a database** we mean the number of facts it contains. Assuming σ is fixed, which we will implicitly do in this paper, this is equivalent to the usual notion of size for a database, up to some polynomial function.

A **primary key constraint** over a signature σ is a special case of a functional dependency designating for a relation symbol R of σ a certain set of indices (columns) of R as a primary key. A database satisfies the primary key constraint if for every relation R over σ, whenever two R-facts agree on the key indices they must be equal. In a set of primary key constraints, each relation of σ has a unique primary key constraint. As all the sets of constraints we consider are primary key constraints we will henceforth omit the "primary" prefix. We use the letter Γ to denote the corresponding set of key constraints.

Given two facts u and v and a set Γ of key constraints, we say that u and v are Γ-equivalent, denoted by $u \sim_\Gamma v$, if u and v have the same associated symbol R and agree on the key of R as specified by Γ. Γ-equivalence is an equivalence relation and the equivalence classes are called **Γ-blocks**. We will omit Γ in our notations whenever it is clear from the context. A database is then a finite collection of blocks, each block being a finite collection of equivalent facts. When writing a query q we will always underline in an atom $R(\bar{x})$ the positions that are part of the key of R as specified by Γ. This will avoid describing explicitly Γ. For instance $R(\underline{x}\ y)$ says that the position of the variable x (i.e., the first position) is the key for the binary relational symbol R; and $R'(\underline{yz}\ x)$ says that the positions of the variables y and z form the key for the ternary relational symbol R'.

If a database D satisfies the key constraints Γ, denoted by $D \models \Gamma$, then each block of D has size one. If not, then a **repair** of D is a subset of the facts of D such that each block of D has exactly one representative in the repair. In particular a repair always satisfies the key constraints. Notice that there could be exponentially many repairs of a given database D.

In this paper a query is a Boolean conjunctive query. We view a query over a relational signature σ as a collection of atoms where an atom is a term $R(\bar{x})$ where R is a relation symbol and $\bar{x}$ is a tuple of variables of the appropriate arity. The query being Boolean, all variables are implicitly existentially quantified. We will consider atoms of a conjunctive query to be ordered in an arbitrary but fixed order. A database D satisfies a query q having atoms $A_1, \ldots, A_k$, denoted by $D \models q$, if there is a mapping μ from the variables of q to the elements of the domain of D such that the fact $\mu(A_i) \in D$ for all i. In this case the sequence $(\mu(A_1), \ldots, \mu(A_k))$ of (not necessarily distinct) facts of D is called a **solution** to q in D. Different mappings yield different solutions. The set of solutions to q in D is denoted by $q(D)$. We will also write $D \models q(\bar{u})$ to denote that the sequence of facts $\bar{u}$ is a solution to q in D. If $\bar{u} = (u_1, \ldots, u_k)$ is a solution to q we also say that u_i **matches** A_i in this solution, and that any subsequence $u_{i_1}, \ldots, u_{i_l}$ matches $A_{i_1}, \ldots, A_{i_l}$.

We say that a query q is **certain** for a database D if all repairs of D satisfy q. We study the complexity of determining whether a query is certain for a database D. We adopt the *data complexity* point of view. For each query q and set of key constraints Γ, we denote by $\mathbf{certain}_\Gamma(q)$ (or simply $\textsc{certain}(q)$ when Γ is understood from the context) the problem of determining, given a database D, whether q is certain for D. Clearly the problem is in coNP as one can guess a (polynomial sized) repair and test whether it does not satisfy q. It is known that for some queries q the problem $\textsc{certain}(q)$ is coNP-complete [4]. However, there are queries q for which $\textsc{certain}(q)$ is in PTime or even expressible in first-order logic (denoted by FO in the sequel) [6, 10].

The following dichotomy has been conjectured (cf [4, 1]):

▶ **Conjecture 1** (Dichotomy conjecture). *For each query q, the problem* $\textsc{certain}(q)$ *is either in* PTime *or* coNP*-complete.*

The conjecture has been proved in the case of self-join-free queries [8] and of path queries [7]; however, it remains open in the general case. A Boolean conjunctive query is **self-join-free** if all its atoms involve different relational symbols. A **path query** is a

Boolean conjunctive query with $n+1$ distinct variables $x_0, x_1, \cdots x_n$ and n atoms $A_1 \cdots A_n$ such that each $A_i = R_i(\underline{x_{i-1}}, x_i)$ for some symbol R_i of σ of arity two. The query may contain self-joins, i.e. $R_i = R_j$ for some $i \neq j$.

▶ **Example 2.** Consider the following example queries taken from [6, 7]. For the self-join-free query $q_1 : R_1(\underline{x}\ y) \wedge R_2(\underline{y}\ z)$ (recall that all variables are implicitly existentially quantified), it is easy to see that the problem CERTAIN(q_1) can be solved in polynomial time [6]. Actually, it can be expressed by the first-order formula $\exists xyz\ R_1(xy) \wedge R_2(yz) \wedge \forall y'(R_1(xy') \rightarrow \exists z' R_2(y'z'))$.

For the self-join-free query $q_2 : R_1(\underline{x}\ y) \wedge R_2(\underline{y}\ x)$ and the path query $q_2' : R(\underline{x_1}\ x_2) \wedge X(\underline{x_2}\ x_3) \wedge R(\underline{x_3}\ x_4) \wedge Y(\underline{x_4}\ x_5) \wedge R(\underline{x_5}\ x_6) \wedge Y(\underline{x_6}\ x_7)$, it has been shown, in [10] and [7] respectively, that CERTAIN(q_2) and CERTAIN(q_2') can be solved in polynomial time but cannot be expressed in first-order logic. Our algorithm works for q_1, q_2 and q_2'.

Finally, for the self-join-free query $q_3 : R_1(\underline{x}\ y) \wedge R_2(\underline{z}\ y)$ and the path query $q_3' : R(\underline{x_1}\ x_2) \wedge X(\underline{x_2}\ x_3) \wedge R(\underline{x_3}\ x_4) \wedge X(\underline{x_4}\ x_5) \wedge R(\underline{x_5}\ x_6) \wedge Y(\underline{x_6}\ x_7) \wedge R(\underline{x_7}\ x_8) \wedge Y(\underline{x_8}\ x_9)$, both CERTAIN($q_3$) and CERTAIN($q_3'$) are known to be coNP-complete [4, 7].

3 Polynomial-time algorithm

To solve CERTAIN(q), we describe a family of algorithms $\mathrm{Cert}_k(q)$, where $k \geq 1$ is a parameter. For a fixed k and query q, $\mathrm{Cert}_k(q)$ takes a database as input and runs in time polynomial in the size of the database, in such a way that $\mathrm{Cert}_k(q)$ is always an under-approximation of CERTAIN(q), i.e., whenever $\mathrm{Cert}_k(q)$ says "yes" then q is certain for the input database. However, $\mathrm{Cert}_k(q)$ could give false negative answers.

In Section 4 we will show that for self-join-free queries either $\mathrm{Cert}_k(q)$ computes CERTAIN(q) (where k is the number of atoms occurring in q) or CERTAIN(q) is complete for coNP. In Section 5 we show an analogous result for path queries.

The algorithm inductively computes sets of facts maintaining the invariant that every repair containing one of these sets makes the query true. The algorithm returns "yes" if the empty set is eventually derived (since all repairs contain the empty set).

We now describe the algorithm. Assume q, Γ and k are fixed. Let D be a database. A k-set over D is a set S of facts of D of size at most k such that no two elements of S are Γ-equivalent. In other words a k-set is a subset of a repair of D of size at most k. We denote by $\mathrm{Cert}_k(q)$ the following algorithm. On a database input D, the algorithm $\mathrm{Cert}_k(q)$ computes inductively a set $\Delta_k(q, D)$ of k-sets over D while maintaining the invariant:

If $S \in \Delta_k(q, D)$ and r is a repair of D containing S, then $r \models q$. (INV)

Initially $\Delta_k(q, D)$ contains all k-sets S such that $S \models q$. In other words, we start with all solutions to q in all repairs of D. Clearly, this satisfies the invariant (INV). Now we iteratively add a k-set S to $\Delta_k(q, D)$ if there exists a block B of D such that for every fact $u \in B$ there exists $S' \subseteq S \cup \{u\}$ such that $S' \in \Delta_k(q, D)$. Again, it is immediate to verify that the invariant (INV) is maintained.

This is an inflationary fixpoint algorithm and notice that the initial and inductive steps can be expressed in FO. If n is the number of facts of D, the fixpoint is reached in at most n^k steps. In the end, $\mathrm{Cert}_k(q)$ returns "yes" iff the empty set belongs to $\Delta_k(q, D)$. Equivalently, $\mathrm{Cert}_k(q)$ returns "yes" if there is a block B of D such that for all facts u of B the set $\{u\}$ belongs to $\Delta_k(q, D)$. We write $D \models \mathbf{Cert}_k(q)$ to denote the fact that $\mathrm{Cert}_k(q)$ returns "true" upon input D. Altogether we have shown:

▶ **Proposition 3.** *For all q, Γ, k, $\mathrm{Cert}_k(q)$ runs in time polynomial in the size of its input database D and, whenever $D \models \mathrm{Cert}_k(q)$ then q is certain for D.*

In order to simplify the notations, as we will mostly consider this case, we write $\Delta(q, D)$ and $\mathrm{Cert}(q)$ to denote $\Delta_k(q, D)$ and $\mathrm{Cert}_k(q)$ respectively, where k is the number of atoms of q. Also, for a fact u, we write $u \in \Delta_k(q, D)$ instead of $\{u\} \in \Delta_k(q, D)$.

▶ **Example 4.** Consider again the query $q_2 : R_1(\underline{x}\ y) \wedge R_2(\underline{y}\ x)$ from Example 2. Let $k = 2$ and consider the execution of $\mathrm{Cert}_2(q_2)$. Initially, $\Delta_2(q_2, D)$ contains all pairs of facts $\{R_1(ab), R_2(ba)\}$ such that both $R_1(ab)$ and $R_2(ba)$ are in D. The first iterative step adds to $\Delta_2(q_2, D)$ (i) all singletons $\{R_1(ab)\}$ such that $R_2(ba)$ is a fact of D whose block contains only $R_2(ba)$, and (ii) analogously all $\{R_2(ab)\}$ such that the block of $R_1(ba)$ is a singleton. And so it continues.

We show that $\mathrm{Cert}_2(q_2)$ computes $\textsc{certain}(q_2)$. In other words, for q_2, $\mathrm{Cert}_2(q_2)$ is not an *under* approximation but an *exact* computation of certainty.

Observe that, for every repair r and fact α therein, there is at most one other fact α' in r such that $\{\alpha, \alpha'\} \models q_2$. This is because in any repair the first atom of q_2 determines the second atom and vice-versa. This "mutual determinacy" is, in fact, what makes $\mathrm{Cert}_2(q_2)$ a complete procedure, as we shall see next.

In view of Proposition 3, it remains to show that if q_2 is certain for D then $\Delta_2(q_2, D)$ contains the empty set.

Let r be a repair of D. By $|q(r)|$ we denote the number of solutions to q in r, i.e., the cardinality of $q(r)$. We say that a repair r is **minimal** if there is no repair s such that $|q(s)| < |q(r)|$. We prove the following claim.

▷ Claim. If r is a minimal repair and $R_1(ab)$, $R_2(ba)$ are facts of r then $R_1(ab) \in \Delta_2(q_2, D)$.

Towards a contradiction, assume that $R_1(ab) \notin \Delta_2(q_2, D)$. We shall construct an infinite sequence $u_1, u_2, \ldots$ of distinct facts of D, contradicting the finiteness of D. We construct, at the same time, an infinite sequence $v_1, v_2, \ldots$ of facts of D and an infinite sequence of minimal repairs $r_1, r_2, \ldots$ maintaining the following invariant:

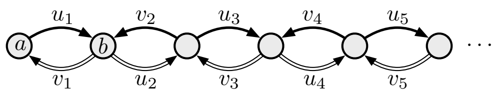
1. the u_i's are pairwise distinct;
2. $u_i \notin \Delta_2(q_2, D)$;
3. if $u_i = R_1(cd)$ then $v_i = R_2(dc)$ and if $u_i = R_2(cd)$ then $v_i = R_1(dc)$;
4. $u_{i+1} \sim v_i$ and $u_{i+1} \neq v_i$;
5. r_i is minimal and contain each u_j, $j \leq i$ together with v_i.

Initially $r_1 = r$, $u_1 = R_1(ab)$ and $v_1 = R_2(ba)$ and the invariant conditions are met, the second item being our initial hypothesis.

Consider step i. Consider the block B_i of v_i. As $u_i \notin \Delta_2(q_2, D)$ we know that B_i must contain an element u_{i+1} such that both $u_{i+1} \notin \Delta_2(q_2, D)$ and $\{u_i, u_{i+1}\} \notin \Delta_2(q_2, D)$. In particular $u_{i+1} \sim v_i$ but $u_{i+1} \neq v_i$ and items 2 and 4 of our inductive hypothesis are met. Towards the first item of our inductive hypothesis, if $u_{i+1} = u_j$ then by item 5 the repair r_i would contain two equivalent facts, v_i and $u_{i+1} = u_j$, which is not possible since we have already established that $u_{i+1} \neq v_i$.

Consider the repair r_{i+1} resulting from replacing v_i with u_{i+1}. Let v_{i+1} be the dual fact of u_{i+1} as required by the third item of the invariant. As $u_i v_i$ forms a solution to q in r_i and r_i is minimal, we must have $v_{i+1} \in r_{i+1}$. Finally notice that r_{i+1} is minimal as its solutions to q are exactly the same as for r_i except for $u_i v_i$ that has been removed and $u_{i+1} v_{i+1}$ that has been added (by the mutual determinacy of the atoms of q_2).

Here is a depiction of how the u_i's and v_i's are defined, where the full and hollow arrows correspond to R_1 and R_2 respectively.



This concludes the construction of the infinite sequence, showing that $R_1(ab) \in \Delta_2(q_2, D)$ for any minimal repair containing both $R_1(ab)$ and $R_2(ba)$.

To conclude that $\mathrm{Cert}_2(q_2)$ returns the correct answer, consider a minimal repair r of D. As q_2 is certain for D, we must have $r \models q$ and this is witnessed by two facts $R_1(ab)$ and $R_2(ba)$ of r. Let B be the block of $R_1(ab)$. Let us show that all facts of B are in $\Delta_2(q_2, D)$ and hence $\emptyset \in \Delta_2(q_2, D)$. Let $R_1(ab')$ be such a fact and consider the repair r' obtained by replacing $R_1(ab)$ with $R_1(ab')$. As r is minimal it follows immediately that r' is minimal and must contain $R_2(b'a)$ (again, this is ensured by the mutual determinacy of q_2). From the claim it follows that $R_1(ab') \in \Delta_2(q_2, D)$, as desired.

Observe that Cert_k does not always compute the certain answers. For instance, the query q_3 from Example 2 is so that $\textsc{certain}(q_3)$ is coNP-complete, and hence $\mathrm{Cert}_k(q_3)$ must have false negatives for all k, assuming coNP $\neq$ PTime (proving this without relying on complexity theoretic assumptions remains plausible, and would not impact our results).

4 Self-join-free queries

In this section we consider the case of self-join-free queries. We exhibit a condition named PCond (for Polynomial-time Condition) and show that any self-join-free query q satisfying PCond is such that $\mathrm{Cert}(q)$ computes $\textsc{certain}(q)$. When PCond fails, we show that $\textsc{certain}(q)$ is coNP-hard.

We start by defining PCond, which will require some extra definitions. Fix, for the rest of this section, a set Γ of primary key constraints. Let D be a database and r a repair of D. For a fact u of r, and for an equivalent fact $v \sim u$ from D, we denote by $r[u \to v]$ the repair obtained from r by replacing the fact u with v.

Consider a self-join-free query q with k atoms. Recall that we write $D \models q(\bar{u})$ when $\bar{u}$ is a solution to q in D. As q is self-join-free, for each fact a in a solution $\bar{u}$ there is a unique atom of q that a can match, namely the only fact of q having the same relation symbol as a. Hence, the order on $\bar{u}$ and on the atoms of q is not relevant. With some abuse of notation we will therefore often treat a solution $\bar{u}$, or the sequence of atoms of q, as a *set* rather than a *sequence*; we will often use different orders among the facts of a same solution, placing up front the most relevant facts. In particular we shall write, for a tuple $\bar{u}$ of facts, $\bar{u} \in \Delta(q, D)$ to denote that the k-set formed by the facts of $\bar{u}$ belongs to $\Delta(q, D)$.

Let A be an atom of q whose associated symbol is R. We denote by ***vars***(A) the set of variables of A and by ***key***(A) the set of variables of A occurring in a position belonging to the primary key of R. For instance $\mathit{key}(R(\underline{x}\, y))$ is $\{x\}$, $\mathit{key}(R'(\underline{yz}\, x))$ is $\{y, z\}$ and $\mathit{key}(R''(\underline{xzx}\, y))$ is $\{x, z\}$.

Given a set X of variables of q and a sequence $A_1 \dots A_n$ of atoms of q, we say that $X\ A_1 \dots A_n$ is a **Γ-derivation** from X to A_n in q if for each $1 \le i \le n$ we have that

$$\mathit{key}(A_i) \subseteq X \cup \bigcup_{1 \le j < i} \mathit{vars}(A_j).$$

If $X = \mathit{vars}(A_0)$, for some atom A_0 of q, we also say that the Γ-derivation is from A_0 to A_n, and we also write it as $A_0 A_1 \dots A_n$. We say that an atom A' is **Γ-determined** by the atom A if there exists a Γ-derivation from A to A'. Moreover, A and A' are **mutually Γ-determined** if A' is Γ-determined by A and A is Γ-determined by A'. This is an equivalence relation among atoms. A set S of atoms of q is said ***stable*** if each pair of facts of S are mutually Γ-determined. Note that a stable set is not necessarily an equivalence class of Γ-determinacy, it may also be a subset of it. As usual, we will omit Γ when it is clear from the context. The key property relating Γ-determinacy and query solutions is given by the lemma:

▶ **Lemma 5.** *Let q be a self-join-free query. Let D be a database instance and r, r' be two repairs of D. Let $A_1 \dots A_n$ be a Γ-derivation in q from atom A_1 to A_n. Let $r \models q(\bar{\alpha} a_1 \dots a_n \bar{\beta})$, and $r' \models q(\bar{\alpha}' a'_1 \dots a'_n \bar{\beta}')$ where for each i, a_i and a'_i match A_i and $\bar{\alpha}\bar{\beta}$ and $\bar{\alpha}'\bar{\beta}'$ match the rest of the atoms of q. If $a_1 = a'_1$ and $a_i \in r'$ for each $i < n$, then 1) $a_i = a'_i$ for each $i < n$ and 2) $a_n \sim a'_n$ (and therefore $a_n = a'_n$ if moreover $a_n \in r'$).*

We are now ready to define PCond. A **Γ-sequence** τ of q is a sequence $\tau = S_1 S_2 \cdots S_n$ where each S_i is a stable set of atoms of q, and the S_i's form a partition of q. In this context, we denote by $S_{\leq i}$ the set $\bigcup_{j \leq i} S_j$.

Let $\tau = S_1 S_2 \cdots S_n$ be a Γ-sequence of q. Let $1 \leq i < n$ and let A be an atom of S_{i+1}. We say that the query q satisfies $\mathbf{PCond}_\tau(A)$ and write $q \models \mathrm{PCond}_\tau(A)$ if the following is true for all databases D, all repairs r of D and all solutions $\bar{\alpha} u \bar{\beta}$ and $\bar{\alpha}' u' \bar{\beta}'$ to q in D such that $\bar{\alpha}$ and $\bar{\alpha}'$ match $S_{\leq i}$ and u and u' match A:

$$\text{If } \left\{ \begin{array}{l} r \models q(\bar{\alpha} u \bar{\beta}), \\ u \sim u', \text{ and} \\ r[u \to u'] \models q(\bar{\alpha}' u' \bar{\beta}') \end{array} \right\} \text{ then } \left\{ \begin{array}{l} r \models q(\bar{\alpha}' u \bar{\delta}) \text{ and} \\ r[u \to u'] \models q(\bar{\alpha} u' \bar{\delta}') \end{array} \right\} \text{ for some sequences } \bar{\delta} \text{ and } \bar{\delta}'.$$

We write $q \models \mathbf{PCond}_\tau(i)$ if q satisfies $\mathrm{PCond}_\tau(A)$ for all A of S_{i+1}, and we write $q \models \mathbf{PCond}_\tau$ if q satisfies $\mathrm{PCond}_\tau(i)$ for all $1 \leq i < n$. Since the condition is restricted to indices $i < n$, PCond_τ trivially holds for any τ having only one stable set. Finally, we write $q \models \mathbf{PCond}$ if there is a Γ-sequence τ of q such that $q \models \mathrm{PCond}_\tau$. Again, if q has only one Γ-determinacy class (for instance the query q_2 of Example 4) then $q \models \mathrm{PCond}$ in a trivial way.

Our goal is to show that $q \models \mathrm{PCond}$ implies that $\mathrm{Cert}(q)$ computes $\textsc{certain}(q)$. This is the main technical result of this section and is proved by Theorem 7. In Theorem 13 we will conclude the self-join-free case by showing that when PCond fails, then the certainty of the query is hard. Before we prove those results, some examples are in order.

▶ **Example 6.** We recall the three queries from Example 2. The query $q_2 = R_1(\underline{x}\ y) \wedge R_2(\underline{y}\ x)$ satisfies PCond since it has only one maximal stable set.

The query $q_1 = R_1(\underline{x}\ y) \wedge R_2(\underline{y}\ z)$ has two stable sets: $R_1(\underline{x}\ y)$ determines $R_2(\underline{y}\ z)$ but the converse is false. For $\tau = \{R_2(\underline{y}\ z)\}\{R_1(\underline{x}\ y)\}$ we have $q \not\models \mathrm{PCond}_\tau$ because we have $q_1(R_2(bc)R_1(ab))$ and $q_1(R_2(b'c)R_1(ab'))$ but not $q_1(R_2(bc)R_1(ab'))$. However for $\tau = \{R_1(\underline{x}\ y)\}\{R_2(\underline{y}\ z)\}$ it is easy to verify that $q_1 \models \mathrm{PCond}_\tau$. Hence, $q_1 \models \mathrm{PCond}$.

The query $q_3 = R_1(\underline{x}\ y) \wedge R_2(\underline{z}\ y)$ has also two stable sets, but no possible sequence τ makes PCond_τ true. This is because (i) $q_3(R_1(ab)\ R_2(cb))$ and $q_3(R_1(a'b')\ R_2(cb'))$ hold, but not $q_3(R_1(ab)\ R_2(cb'))$, and (ii) $q_3(R_2(ab)\ R_1(cb))$ and $q_3(R_2(a'b')\ R_1(cb'))$ hold, but not $q_3(R_2(ab)\ R_1(cb'))$. Therefore, $q_3 \not\models \mathrm{PCond}$.

▶ **Theorem 7.** *Let q be a self-join-free query. If $q \models \mathrm{PCond}$, then $\mathrm{Cert}(q)$ computes $\textsc{certain}(q)$.*

Suppose q has k atoms. Let $\tau = S_1 \cdots S_n$ be a Γ-sequence of q such that $q \models \mathrm{PCond}_\tau$. We need to show that $\mathrm{Cert}(q) = \mathrm{Cert}_k(q)$ computes precisely $\textsc{certain}(q)$.

We start with some extra notations. Recall that $q(r)$ denotes the set of solutions to q in a repair r; we additionally denote by $q_{\leq i}(r)$ the projection of $q(r)$ on the first i sets of τ. More precisely

$$q_{\leq i}(r) = \{\bar{v} \mid \exists \bar{u} \in q(r) \text{ s.t. } \bar{v} \text{ is the subset of } \bar{u} \text{ matching } S_{\leq i}\},$$

and if $\bar{v} \in q_{\leq i}(r)$ we write equivalently $r \models q_{\leq i}(\bar{v})$. Let D be a database and r a repair of D. We say that r is ***i*-minimal** if there is no repair r' such that $q_{\leq i}(r') \subsetneq q_{\leq i}(r)$. We say that a fact u of a database D is ***i*-compatible**, if it matches some atom of S_i. We will need the limit case when $i = 0$. In that case S_0 is the empty set, as well as $S_{\leq 0}$ (and hence $\mathrm{PCond}_\tau(0)$ is always true), $q_{\leq 0}(r)$ contains only the empty sequence ε for all r, and therefore all repairs are 0-minimal. The proof of the theorem will make use of an induction based on the following invariant property of the database, for each $0 \leq i \leq n$:

$$\mathrm{IND}_i = \text{For all } i\text{-minimal repair } s \text{ and facts } \bar{u} \text{ s.t. } s \models q_{\leq i}(\bar{u}), \text{ we have } \bar{u} \in \Delta(q, D).$$

▶ **Lemma 8.** *Given q, D and a Γ-sequence τ for q, for every $0 \leq i < n$, if IND_{i+1} and $\mathrm{PCond}_\tau(i)$, then IND_i.*

We first show how this statement already implies Theorem 7.

Proof of Theorem 7. From Proposition 3, we know that if D is a database such that $D \models \mathrm{Cert}(q)$ then all repairs of D satisfy q. It remains to show the converse.

Assume all repairs satisfy q and that $q \models \mathrm{PCond}_\tau$ for some sequence τ of length n, which means that $\mathrm{PCond}_\tau(i)$ holds for all i. Observe that IND_n holds true by the base case definition of $\Delta(q, D)$. Hence by n repeated applications of Lemma 8 we obtain that IND_0 holds true. Now take any repair r. By definition r is 0-minimal and by hypothesis it satisfies the query q. By IND_0 it follows that the empty set (denoted by the empty tuple) is in $\Delta(q, D)$, and hence $D \models \mathrm{Cert}(q)$. ◀

We are now left with the proof of Lemma 8, which is the main technical content of the section. Towards this, we define a stronger version of i-minimality. For $1 \leq i < n$, we say that an i-minimal repair s is **strong** if there exists no repair s' such that $q_{\leq i}(s') = q_{\leq i}(s)$ and $|q_{\leq i+1}(s')| < |q_{\leq i+1}(s)|$. Note that a strong i-minimal repair is in particular $(i+1)$-minimal.

▷ Claim 9. If there exists an i-minimal repair s such that $s \models q_{\leq i}(\bar{u})$, then there exists a strong i-minimal repair s' such that $s' \models q_{\leq i}(\bar{u})$.

For a given database D, for a repair r of D, we denote by $r_{|i+1}$ the set of facts of r which are not $(i+1)$-compatible. A sequence $\bar{p}$ of facts of the database is **connected** with respect to $D' \subseteq D$ if for every repair r containing $\bar{p}$ and D', and for every two consecutive facts $a\,b$ of $\bar{p}$, if $r \models q(\bar{\alpha}, a, \bar{\beta})$ for some $\bar{\alpha}, \bar{\beta}$, then $b \in \bar{\alpha}\bar{\beta}$. Note that if $\bar{p}$ is the empty tuple (or a tuple of size 1), then $\bar{p}$ is trivially connected with respect to every $D' \subseteq D$.

Proof of Lemma 8. By contradiction, suppose the statement of the lemma is false. Then, there is some i such that IND_{i+1} and $\mathrm{PCond}_\tau(i)$ holds, but for some i-minimal repair s and tuple $\bar{u}$ we have

$$s \models q_{\leq i}(\bar{u}) \text{ but } \bar{u} \notin \Delta(q, D). \tag{h1}$$

From Claim 9, we can assume that s is strong i-minimal. We will build an infinite sequence of pairwise distinct facts $p_1, p_2, \ldots$ from D, contradicting the finiteness of D. We also maintain another sequence of repairs $r_1, r_2, \ldots$. We set $r_0 = s$ and $\bar{p}_0$ to be the empty fact sequence. And for all $l > 0$, we define $\bar{p}_l = p_1, \ldots p_l$.

The sequence is constructed by induction with the following invariant for every $l \geq 0$, assuming $\bar{p} = \bar{p}_l$ and $r = r_l$:

(a) $\bar{p}$ contains only $(i+1)$-compatible facts of D;
(b) the elements of $\bar{p}$ are pairwise distinct;
(c) $\bar{p}$ is connected with respect to $r_{|i+1}$;
(d) r is strong i-minimal, $r \models q_{\leq i}(\bar{u})$ and, if $\bar{p}$ is not empty and v is the last fact of $\bar{p}$, then $r \models q(\bar{u}v\bar{\delta})$, for some $\bar{\delta}$;
(e) $\bar{u}\bar{c} \notin \Delta(q, D)$, where $\bar{c}$ is the maximal suffix of $\bar{p}$ satisfying $r' \models q(\bar{u}\bar{c}\bar{\beta})$ for some $\bar{\beta}$ and strong i-minimal repair r' containing $\bar{p}$ and $r_{|i+1}$.

Note that the invariant (b) leads to a contradiction when l is larger than the size of D.

Base case. When $l = 0$, we have $r_0 = s$ and $\bar{p}$ is the empty sequence. Hence (a), (b) and (c) are trivially true by emptiness of $\bar{p}$; (d) holds since $s \models q_{\leq i}(\bar{u})$ (note that we have assumed s to be strong i-minimal); finally (e) holds with empty $\bar{c}$ since $\bar{u} \notin \Delta(q, D)$ by (h1).

Inductive step. Assume we have $r = r_{l-1}$ and $\bar{p} = p_1, \ldots p_{l-1}$ (possibly empty) satisfying the five properties above. Consider the maximal suffix $\bar{c}$ concerned by property (e). That is, for some $\bar{\beta}$ and strong i-minimal repair r' containing $\bar{p}$ and $r_{|i+1}$ we have:

$$\bar{u}\bar{c} \notin \Delta(q, D) \text{ and } r' \models q(\bar{u}\bar{c}\bar{\beta}) \tag{h2}$$

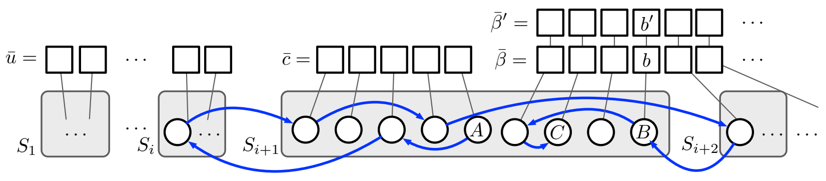
First let $\bar{\beta} = d_1 d_2, \ldots d_t$. Since $\bar{u}\bar{c} \notin \Delta(q, D)$, by definition of $\Delta(q, D)$ there exists some $d'_1 \sim d_1$ such that $\bar{u}\bar{c}d'_1 \notin \Delta(q, D)$. This again implies that there exists some $d'_2 \sim d_2$ such that $\bar{u}\bar{c}d'_1 d'_2 \notin \Delta(q, D)$. Since k is the number of atoms in q, we can continue this to obtain $\bar{\beta}' = d'_1 d'_2, \ldots d'_t$ where $d'_i \sim d_i$ but $\bar{u}\bar{c}\beta'$ contains no k-set in $\Delta(q, D)$. Also note that $\bar{\beta}'$ matches all atoms of q not already matched by $\bar{u}\bar{c}$.

Further, we show that $\bar{c}$ cannot match the entire set S_{i+1}. Suppose, by means of contradiction, that $r' \models q_{\leq i+1}(\bar{u}\bar{c})$. As r' is strong i-minimal, it is $(i+1)$-minimal. Hence, since $\textsc{Ind}_{i+1}$ holds by hypothesis, $\bar{u}\bar{c} \in \Delta(q, D)$, which is in contradiction with (h2). Then,

$$r' \not\models q_{\leq i+1}(\bar{u}\bar{c}). \tag{h3}$$

This means that, since $r' \models q(\bar{u}\bar{c}\bar{\beta})$ by (h2), and $\bar{c}$ matches a subset of S_{i+1}, there must be an atom C of S_{i+1} that is not matched by any fact of $\bar{c}$. Consider the atom A of S_{i+1} matching the last element of $\bar{c}$. If instead $\bar{c}$ is empty, choose A as an arbitrary atom of S_{i+1}.

Since A and C are both in S_{i+1}, which is stable, there exists a Γ-derivation σ from A to C. (Notice that σ may contain atoms outside S_{i+1}.) Consider the first atom B of σ which is in S_{i+1} and which is not matched by any fact of $\bar{c}$. The following depiction may help to see the situation:



In the picture directed edges connecting atoms of the query represent the successor relation in the Γ-derivation from A to C.

Let b be the fact of $\bar{\beta}$ matching B and $b' \sim b$ be the fact matching B in $\bar{\beta}'$. We show that

$$b \notin \bar{p}. \tag{h4}$$

Suppose b is in $\bar{p}$, by connectedness of $\bar{p}$ with respect to $r_{|i+1}$, this implies that the suffix $\bar{b}$ of $\bar{p}$ starting with b is part of the solution $\bar{u}\bar{c}\bar{\beta}$, that is, $r' \models q(\bar{u}\bar{b}\bar{\gamma})$ for some $\bar{\gamma}$. By construction, b is not in $\bar{c}$, thus it must occur before $\bar{c}$ in $\bar{p}$ and hence $\bar{b}$ strictly contains $\bar{c}$. This contradicts the maximality of $\bar{c}$ imposed by (e), thus proving that (h4) holds. Note that this also implies $b' \notin \bar{p}$, otherwise if $b' \in \bar{p}$, we have that $b' \sim b$ are both in r', thus $b = b' \in \bar{p}$, contradicting (h4).

Assign $p_l = b'$, so we have $\bar{p}' = \bar{p} \cdot p_l$ and let $r_l = r'[b \to b']$. (To avoid many subscripts, let $r_l = s'$). Observe that

$$s' \text{ contains } \bar{p}' \text{ and } r_{|i+1}. \tag{h5}$$

In fact s' contains $\bar{p}$, as observed earlier, and s' contains b' by construction; moreover s' contains $r'_{|i+1}$ which contains $r_{|i+1}$ by (e). We now show that $\bar{p}'$ and s' have all the desired properties.

(a) By construction b' is $(i+1)$-compatible.

(b) The elements of $\bar{p}'$ are pairwise distinct, as $b' \notin \bar{p}$.

(c) By our choice of b we show that $\bar{p}'$ is connected with respect to $s'_{|i+1}$. Without loss of generality assume that $\bar{p}'$ has at least size 2 (otherwise it is trivially connected). Therefore, $\bar{p}$ is not empty. Since $s'_{|i+1}$ contains $r_{|i+1}$ by (h5), the connectedness property of $\bar{p}$ with respect to $r_{|i+1}$ implies that for every repair containing $\bar{p}'$ and $s'_{|i+1}$ and for every pair of consecutive facts $a\,b$ in $\bar{p}$, every solution in s' containing a also contains b.

It remains to show the same property for the last fact a of $\bar{p}$. Consider a repair t containing $\bar{p}'$ and $s'_{|i+1}$ and suppose $t \models q(\bar{\gamma}a\bar{\delta})$ for some $\bar{\gamma}$ and $\bar{\delta}$. We have to show $b' \in \bar{\gamma}\bar{\delta}$. Let σ_{AB} be the prefix of the Γ-derivation σ going from A to B. (Notice that, since p is not empty $A \neq B$.) By property (d) of $\bar{p}$, since $\bar{p}$ is not empty, a is the last fact in $\bar{c}$. Recall that by (h2) $r' \models q(\bar{u}\bar{c}\bar{\beta})$; thus in this solution the atom A is matched by a. So we can apply Lemma 5 to r' and t with solutions $(\bar{u}\bar{c}\bar{\beta})$ and $(\bar{\gamma}a\bar{\delta})$ respectively, and Γ-derivation σ_{AB}. The hypotheses of Lemma 5 are satisfied since:

- in both solutions A is matched by a;
- by construction of B, for each atom D strictly preceding B in σ_{AB}, the fact matching D in $(\bar{u}\bar{c}\bar{\beta})$ is either in $\bar{c}$ or in $r'_{|i+1}$, both contained in t (in fact $t \supseteq \bar{p}' \supseteq \bar{p} \supseteq \bar{c}$ and $t \supseteq s'_{|i+1} \supseteq r'_{|i+1}$).

We conclude, by Lemma 5, that the facts matching B in the two solutions are equivalent, i.e., the fact matching B in $(\bar{\gamma}a\bar{\delta})$ is equivalent to b (which is the fact matching B in $\bar{u}\bar{c}\bar{\beta}$).

In t the unique fact equivalent to b is b' (since $b' \in \bar{p}' \subseteq t$), thus the fact matching B in $(\bar{\gamma}a\bar{\delta})$ is b'. We have thus proved that any solution in t containing the last fact a of p also contains b'.

(d) The following claim together with strong i-minimality of r' and $r' \models q(\bar{u}b\bar{\gamma})$ for some $\bar{\gamma}$, shows that

(I) s' is also strong i-minimal,
(II) $s' \models q_{\leq i}(\bar{u})$, and
(III) $s' \models q(\bar{u}b'\bar{\delta})$ for some $\bar{\delta}$.

▷ Claim 10. Assume $\text{PCond}_\tau(i)$. Let s be a strong i-minimal repair such that $s \models q(\bar{\alpha}a\bar{\beta})$ where $\bar{\alpha}$ matches $S_{\leq i}$ and a is $(i+1)$-compatible. Then for any $a' \sim a$ we have that $s' = s[a \mapsto a']$ is strong i-minimal and $s' \models q(\bar{\alpha}a'\bar{\delta})$ for some $\bar{\delta}$.

(e) Let $\bar{e}$ be the maximal suffix of $\bar{p}'$ such that, for a strong i-minimal repair t containing $\bar{p}'$ and $s'_{|i+1}$ we have $t \models q(\bar{u}\bar{e}\bar{\delta})$ for some $\bar{\delta}$. Since $s' \models q(\bar{u}\bar{b}'\bar{\delta}')$ for some $\bar{\delta}'$ by item (III) above, $\bar{e}$ cannot be empty. Then let $\bar{e} = \bar{d}\bar{b}'$, where $\bar{d}$ is a suffix of $\bar{p}$.

Since $s'_{|i+1}$ contains $r_{|i+1}$ by (h5), in particular t is a strong i-minimal repair containing $\bar{p}$ and $r_{|i+1}$. Then, by maximality of $\bar{c}$, $\bar{d}$ must be a suffix of $\bar{c}$, implying that $\bar{u}\bar{d}\bar{b}'$ is a subset of $\bar{u}\bar{c}\bar{\beta}'$. Since by definition $\bar{u}\bar{c}\bar{\beta}'$ does not contain any k-set in $\Delta(q, D)$, we have $\bar{u}\bar{d}\bar{b}' \notin \Delta(q, D)$ as needed.

This completes the proof of Lemma 8. ◀

▶ Remark 11. One can verify from the proof that if $q \models \text{PCond}_\tau$ where in the sequence τ each set S_i contains exactly one atom of q, then the fixpoint computing $\text{Cert}(q)$ is bounded, i.e., $\text{Cert}(q)$ can be expressed in FO.

It remains to show that when a self-join-free query q does not satisfy PCond, computing $\textsc{certain}(q)$ is coNP-hard. Towards this, we build on the dichotomy result of [8] based on the notion of attack graph. First we recall this notion using our notation.

Let q be a query, let Γ be a set of primary key constraints. Given an atom A of q let

$$\begin{aligned} A^+ = \{B \text{ atom of } q \mid & \text{ there exist a } \Gamma\text{-derivation } X\ B_1 \dots B_n \\ & \text{where } X = \mathit{key}(A),\ B_n = B, \text{ and for all } i,\ B_i \neq A\} \end{aligned}$$

Let $\mathit{vars}(A^+) = \bigcup_{B \in A^+} \mathit{vars}(B)$. Given two atoms A and B of q we say that A *attacks* B if there exists a sequence $F_0, F_1, \dots, F_n$ of atoms of q and $x_1, x_2, \dots, x_n$ of variables not in $\mathit{vars}(A^+)$ such that $A = F_0, B = F_n$ and for all $i > 0$, x_i is a variable occurring both in F_{i-1} and F_i. The attack from A to B is said to be *weak* if B is Γ-determined by A. The *attack graph* of q and Γ is the graph whose vertices are the atoms of q and whose edges are the attacks. A cycle in this graph is weak if all the attacks involved are weak.

The dichotomy result of [8] can be stated as:

▶ **Theorem 12** ([8], Theorem 3.2). *Let q be a self-join-free query and Γ a set of primary key constraints. If every cycle in the attack graph of q and Γ is weak, then* $\textsc{certain}(q)$ *can be computed in polynomial time; otherwise* $\textsc{certain}(q)$ *is* coNP*-complete.*

To show that our polynomial time algorithm covers all polynomial-time cases, we prove that if the attack graph of q and Γ contains only weak cycles, then PCond holds.

▶ **Theorem 13.** *Assume q is a self-join-free query and Γ a set of primary key constraints. If the attack graph of q and Γ contains only weak cycles then $q \models$* PCond.

5 Path queries

The dichotomy conjecture has also been shown to hold for *path queries* [7]. Recall that a path query of length n is a Boolean conjunctive query with $n+1$ distinct variables $x_0, x_1, \cdots, x_n$ and n atoms $A_1, \cdots, A_n$ such that $A_i = R_i(\underline{x_{i-1}}\ x_i)$ for some symbol R_i of σ. The query may contain self-joins, i.e., there could be $R_i = R_j$ for $i \neq j$.

For this section, assume that the relational signature σ contains only symbols of arity two and that the set Γ of constraints assigns to each symbol R of σ its first component as a primary key. Note that a path query can be described by a word over σ (e.g., the word describing q is $R_1 \cdots R_n \in \sigma^*$). For simplicity, we will henceforth blur the distinction between path queries and words over σ.

Following [7] we define the language $\mathcal{L}^{\looparrowright}(q)$ as the regular language defined by the following finite state automaton $\mathcal{A}^q$ with epsilon-transitions (we use $s, t, \dots$ to denote words over σ). The set of states of $\mathcal{A}^q$ is the set of all prefixes of q, including the empty prefix ε, which is the initial state. There is only one accepting state, which is q. There is a transition reading R from state s to the state sR. Moreover, there is an ε-transition in $\mathcal{A}^q$ from any state sR to any state tR such that tR is a prefix of s.

The dichotomy result of [7] can be formulated as follows[1]:

▶ **Theorem 14** ([7], Theorem 3.2)**.** *Let q be a path query. If q is a factor of all the words in the language $\mathcal{L}^{\looparrowright}(q)$, then* CERTAIN$(q)$ *can be evaluated in* PTIME*; otherwise,* CERTAIN(q) *is* coNP*-complete.*

We will show that, also in this case, $\text{Cert}(q)$ captures CERTAIN(q) for all polynomial-time path queries q (recall that $\text{Cert}(q)$ denotes $\text{Cert}_k(q)$ with $k = |q|$).

▶ **Theorem 15.** *Let q be a path query of length n. If q is a factor of all the words in the language $\mathcal{L}^{\looparrowright}(q)$, then* CERTAIN$(q) = \text{Cert}(q)$.

The rest of this section is devoted to the proof of Theorem 15. We will make use of the following fixpoint computation introduced by [7, Fig. 5]. For a fixed path query q and database instance D, let $N(q, D)$ be the set of pairs $\langle c, s\rangle$, where $c \in adom(D)$ and s is a prefix of q, computed via the following fixpoint algorithm.

Initialization Step: $N(q, D) \leftarrow \{\langle c, q\rangle \mid c \in adom(D)\}$
Iterative Step: If s is a prefix of q, add $\langle c, s\rangle$ to $N(q, D)$ if one of the following holds:

1. sR is a prefix of q and there is a fact $R(\underline{c}\ a)$ of D such that for every fact $R(\underline{c}\ b)$ of D we have $\langle b, sR\rangle \in N(q, D)$;
2. There is an ε transition from s to t in $\mathcal{A}^q$ and there is a fact $R(\underline{c}\ a)$ of D such that for every fact $R(\underline{c}\ b)$ of D we have $\langle b, tR\rangle \in N(q, D)$.

Let $N(q)$ be the set of all databases D such that there exists $c \in adom(D)$ with $\langle c, \varepsilon\rangle \in N(q, D)$.

▶ **Lemma 16** ([7], (proof of) Lemma 6.4)**.** *For every path query q, if q is a factor of every word in the language $\mathcal{L}^{\looparrowright}(q)$, then* CERTAIN$(q) = N(q)$.

In view of Lemma 16, Theorem 15 is now a direct consequence of the following proposition.

▶ **Proposition 17.** *For every path query q of length n, and assuming every word of $\mathcal{L}^{\looparrowright}(q)$ contains q as factor, we have $N(q) = \text{Cert}(q)$.*

Note that $\text{Cert}(q) \subseteq N(q)$ follows from $\text{Cert}(q) \subseteq$ CERTAIN(q) (Proposition 3) combined with CERTAIN$(q) = N(q)$ (Lemma 16). So we are left with proving $N(q) \subseteq \text{Cert}(q)$. Let $D \in N(q)$. We will prove that $D \in \text{Cert}(q)$.

For all $l \geq 0$ let s_l be the prefix of q of length l (i.e., $s_0 = \varepsilon$ and $s_n = q$). For every database D and fact $u = R(\underline{a}\ b)$ in D, let us define $trace(u) = R$, $key(u) = a$, and $last(u) = b$. For a sequence of (possibly repeating) facts $\Pi = u_1, \dots, u_k$ of a database D, we define $last(\Pi) = last(u_k)$ and $trace(\Pi) = trace(u_1) \cdots trace(u_k) \in \Sigma_q^*$. Also, let $S_\Pi = \{u_1, \dots, u_k\}$ be the *set* of facts in the sequence. Further, Π is called a **valid path** if (i) S_Π is a partial

[1] Actually, [7] provides a much finer tetrachotomy between FO, NL-complete, PTIME-complete and coNP-complete. Here we restrict our attention to the dichotomy between PTIME and coNP-complete.

repair of D, (ii) for all $i < k$ we have $\mathit{last}(u_i) = \mathit{key}(u_{i+1})$, and (iii) $\mathit{trace}(\Pi)$ is a prefix of q. In particular, for any valid path Π of length k, we have $\mathit{trace}(\Pi) = s_k$. Further, for any prefix s_l of q we write $\boldsymbol{\mathit{trace}}(\Pi) \sim s_l$ if there exists a run of the automaton $\mathcal{A}^q$ on $\mathit{trace}(\Pi)$ ending in state s_l.

Let $D \in N(q)$. Let $N^i(q,D)$ and $\Delta^i(q,D)$ be the fix-point computations of $N(q,D)$ and $\Delta(q,D)$ at their i^{th} steps, respectively. To prove that $D \in \mathrm{Cert}(q)$, we will use the following claim:

▷ Claim 18. For all $i \geq 0$, For $c \in \mathit{adom}(D)$ and for all prefix s_l of q if $\langle c, s_l \rangle \in N^i(q,D)$ then for all valid path Π where $\mathit{last}(\Pi) = c$ and $\mathit{trace}(\Pi) \sim s_l$ we have $S_\Pi \in \Delta^i(q,D)$.

Let us show that the claim implies $D \in \mathrm{Cert}(q)$. As $D \in N(q)$, there exists $c \in \mathit{adom}(D)$ such that $\langle c, \varepsilon \rangle \in N^m(q,D)$ for some step m. But note that $\langle c, \varepsilon \rangle \in N^m(q,D)$ can only be produced by application of Rule 1 in the *Iteration step* (Rule 2 is not possible since ε transitions do not start at the state ε). This implies that if R is the first relation occurring in q then there exists a fact of the form $R(\underline{c}\ a)$ and for all facts of the form $R(\underline{c}\ b)$ in D we have $\langle b, R \rangle \in N^{m-1}(q,D)$. For each such b we can apply the claim with the valid path $\Pi = R(\underline{c}\ b)$, obtaining $\{R(\underline{c}\ b)\} \in \Delta^{m-1}(q,D)$ for every $R(\underline{c}\ b)$. Hence, $\emptyset \in \Delta^m(q,D)$ which implies $D \in \mathrm{Cert}(q)$.

6 Cert$_k$ does not capture all polynomial-time queries

We have shown that for all self-join free and path queries whose certainty is solvable in polynomial time, the algorithm Cert_k computes CERTAIN(q) with $k = |q|$. A natural question is whether this extends to all queries for which certainty is solvable in polynomial time. In this section, we show that this is not the case. There exists query q whose certain answers can be computed in polynomial time but the algorithm $\mathrm{Cert}_k(q)$ will always have a false negative for any choice of k.

▶ **Theorem 19.** *Let q_4 be the query $q_4 = R(\underline{x}\,yz) \wedge R(\underline{z}\,xy)$. Then* CERTAIN($q_4$) *is in polynomial time but cannot be computed by $\mathrm{Cert}_k(q_4)$, for any choice of k.*

Before proving the theorem we discuss some special properties of the query q_4. Note that q_4 contains only two atoms but has self join. For any database D and facts $a, b, c \in D$, we have that if $D \models q_4(ab) \wedge q_4(ac)$ then $b = c$, and if $D \models q_4(ba) \wedge q_4(ca)$ then $b = c$. Also, if $D \models q_4(ab) \wedge q_4(bc)$ then $D \models q_4(ca)$.

Since q_4 contains only two atoms, for a database D, it is convenient to describe the set of solutions to q_4 as a graph. More precisely we say that the facts $a, b \in D$ are *q_4-related* if $D \models q_4(ab)$ or $D \models q_4(ba)$. We define the solution graph of D, denoted by G_D to be an undirected graph whose vertices are the facts of D and pairs of q_4-related facts form the edges. From the properties of q_4 it follows that every connected component in G_D is always a clique of size less than or equal to 3. If a clique has exactly three vertices we call it a *triangle*.

First we show that CERTAIN(q_4) is in polynomial time by reducing it to bipartite matching.

▶ **Lemma 20.** CERTAIN(q_4) *is in* PTIME.

Proof. Fix an input database D. Without loss of generality, assume that there are no facts $a \in D$ such that $D \models q_4(aa)$[2]. We reduce $\textsc{certain}(q_4, D)$ to a bipartite graph matching problem. Consider the bipartite graph $G = (V_1 \cup V_2, E)$ where V_1 is the set of all blocks and V_2 is the set of maximal cliques in G_D. Let $(v_1, v_2) \in E$ if the block v_1 contains a fact which is in the clique v_2.

Suppose that there is a V_1-saturating matching, that is, an injective function $f : V_1 \to V_2$ such that $(v_1, f(v_1)) \in E$ for every $v_1 \in V_1$. We construct a repair r where for every block B of D, we pick the fact (or one of the facts, if there are more than one) which is in $f(B)$. In this way, no two chosen facts will be in the same clique, and also since there is no solution of the form $q_4(aa)$ in D, no two chosen facts will form a solution to q_4. Thus, $r \not\models q_4$.

Conversely, if q_4 is not certain in D, let r be a repair such that $r \not\models q_4$. For each block B of D let $r(B)$ be the fact of B belonging to r. Note that, since V_2 is a partition of D, each $r(B)$ belongs to a unique clique in V_2. Define $f : V_1 \to V_2$ such that each block $B \in V_1$ is mapped to the clique in V_2 where $r(B)$ lies. To verify that f is a witness function of a V_1-saturating matching for G, note that for every $B \in V_1$ we have $(B, f(B)) \in E$, as B and $f(B)$ both contain $r(B)$. Moreover f is injective, otherwise if f maps two distinct blocks to the same clique, this clique contains at least two elements of r; these two elements are therefore q_4-related, and thus $r \models q_4$.

Thus, to check if $D \in \textsc{certain}(q_4)$, it is sufficient to check if there is a bipartite matching of G that saturates V_1. This is known to be in PTime [5]. ◀

We now prove that for all k, $\mathrm{Cert}_k(q_4)$ does not compute $\textsc{certain}(q_4)$. To this end, for every $n \geq 4$ we exhibit a database D_n such that

- $D_n \models \textsc{certain}(q_4)$ (Proposition 21);
- $D_n \not\models \mathrm{Cert}_{n-2}(q_4)$ (Proposition 22).

Fix some $n \geq 4$. The database D_n has n blocks of the form $B_1, \cdots, B_n$ where each B_i consists of $n-1$ facts denoted $b_i^1, \cdots, b_i^{n-1}$. Further, D_n also has $(n-1)(n-3)$ blocks of the form E_l^j for every $1 \leq j \leq n-1$ and $1 \leq l \leq n-3$, where each E_l^j has two facts denoted by u_l^j and v_l^j. The solution graph of D_n is depicted in Figure 1.

D_n is defined in such a way that every fact of D_n is part of a "triangle". More precisely, we have the following triangles in the solution graph of D_n: For every $1 \leq j \leq n-1$, the triples $\{b_1^j, b_2^j, u_1^j\}$ and $\{b_{n-1}^j, b_n^j, v_{n-3}^j\}$ form triangles and for every $1 \leq l < n-3$ we have a triangle $\{v_l^j, u_{l+1}^j, b_{l+2}^j\}$.

▶ **Proposition 21.** *For every $n \geq 2$, $D_n \models \textsc{certain}(q_4)$.*

To see this, note that there are $n + (n-1)(n-3)$ blocks in D_n and there are $(n-1)(n-2)$ cliques (all triangles) in the solution graph of D_n. Thus, in the corresponding bipartite graph (cf. Lemma 20) size of V_1 is strictly smaller than the size of V_2. Hence, there cannot be a V_1-saturating matching which implies $D_n \models \textsc{certain}(q_4)$.

▶ **Proposition 22.** *Let $k \geq 2$. $D_{k+2} \not\models \mathrm{Cert}_k(q_4)$.*

Proof sketch. To prove the proposition, for a set of blocks $\mathbb{X} = \{X_1, \ldots X_k\}$ of D_{k+2}, if $W = \{a_1, \ldots a_k\}$ is a set of facts where each $a_i \in X_i$, then we call W a partial repair of $\mathbb{X}$. Further, W is called an **obstruction set** of $\mathbb{X}$ if W satisfies some "desired properties". In

[2] If there is a fact $a \in D$ such that $D \models q(aa)$ then suppose the block containing a is a singleton set then clearly $D \models \textsc{certain}(q_4)$. Otherwise, $D \models \textsc{certain}(q_4)$ iff $D \setminus \{a\} \models \textsc{certain}(q_4)$, so we can consider the smaller database instance.

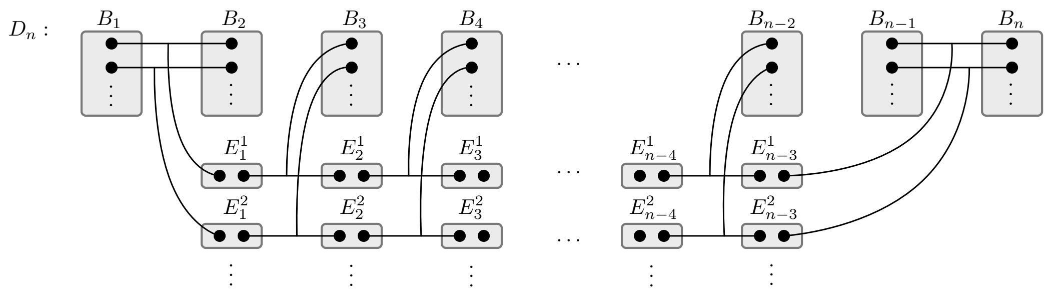


Figure 1 Solution graph for database D_n. Black dots denote facts, rectangles denote blocs, and three-pointed edges denote "triangles" in the solution graph of D_n. There are $n-1$ facts in each B_i and two facts in every E_k^j.

particular we will show that if W is an obstruction set then $W \not\models q_4$. Next we will prove that for any set of blocks $\mathbb{X} = \{X_1, \ldots X_k\}$ of D_{k+2}, we can always pick a partial repair W of $\mathbb{X}$ such that W is an obstruction set.

Now suppose $D_{k+2} \in \text{Cert}_k(q_4)$ then it follows that there has to exist at least one obstruction set $W \in \Delta_k(q_4, D_{k+2})$. We pick the minimum i such that there is some obstruction set in i^{th} step of $\Delta_k(q_4, D_{k+2})$ computation. Note that $i = 0$ is not possible since obstruction sets do not contain a solution to q_4. Thus, to obtain a contradiction, we will show that if there is an obstruction set in $\Delta_k(q_4, D_{k+2})$ at i^{th} step, then there has to exist an obstruction set in $\Delta_k(q_4, D_{k+2})$ in $(i-1)^{th}$ step. ◀

▶ **Theorem 23.** *Let $q_4 = R(\underline{x}\ yz) \wedge R(\underline{z}\ xy)$. Then $\neg$CERTAIN(q_4) is complete for bipartite matching under* LogSpace*-reductions.*

Proof. From the proof of Lemma 20 it follows that we can reduce $\neg$CERTAIN(q_4) to bipartite matching. The reader can verify that the reduction is in LogSpace. We now prove the other direction.

Given a bipartite graph $G = (V_1 \cup V_2, E)$, let $V_1 = \{s_1, \ldots s_n\}$ and $V_2 = \{t_1, \ldots t_m\}$. Consider the problem of determining whether there exists a matching that saturates V_1. We will reduce this problem to $\neg$CERTAIN(q_4).

For all $s_j \in V_1$ let $N(s_j) \subseteq V_2$ denote the neighbours of s_j and similarly for all $t_i \in V_2$ let $N(t_i) \subseteq V_1$ denote the neighbours of t_j.

First note that if there is some $s_j \in V_1$ such that $N(s_j) = \emptyset$, then clearly there cannot be a matching that saturates V_1. So assume that for every $s_j \in V_1$, $N(s_j) \neq \emptyset$. Similarly, if there is some $t_i \in V_2$ such that $N(t_i) = \emptyset$, then t_i does not contribute to any matching and hence can be removed from the input. So we can also assume that for every $t_i \in V_2$, $N(t_i) \neq \emptyset$. Further, suppose there is some t_i such that $|N(t_i)| = 1$, let s_j be the single neighbour of t_i. In this case, if there exists a matching that saturates V_1 then there is a matching that saturates V_1 where s_j is matched with t_i. So we can remove the pair (s_j, t_i) from the input. This means that we can assume that for every $t_i \in V_2$, $|N(t_i)| \geq 2$.

Altogether, we have $|N(s_j)| \geq 1$ for all $s_j \in V_1$ and $|N(t_i)| \geq 2$ for all $t_i \in V_2$. Note that these properties can be checked in LogSpace.

Now we define the database D_G. Note that this construction is very similar to the construction of D_n that we used to prove Theorem 19.

- For every vertex in $s_j \in V_1$ create a block B_j in D_G.
- For every $s_j \in V_1$ and $t_i \in V_2$, if $t_i \in N(s_j)$ then there is a fact denoted by b_j^i in the block B_j. By assumption $N(s_j) \geq 1$ and hence every block B_j is non-empty.

- For every $t_i \in V_2$ if $|N(t_i)| = l$ then let $s_{i_1}, \dots s_{i_l} \in V_1$ be the neighbours of t. By the above construction, for every $j \leq l$, there is a fact of the form $b^i_{i_j}$ in B_{i_j} that corresponds to the vertex t_i.

  Now if $l = 2$ then define $b^i_{i_1}$ and $b^i_{i_2}$ such that they form a solution to q_4. Otherwise, if $l = 3$ then define $b^i_{i_1}, b^i_{i_2}$ and $b^i_{i_3}$ such that they pair-wise form a solution to q_4 (the three facts form a triangle).

  If $l \geq 4$ then create $l - 3$ new blocks denoted by $E^i_1, \dots E^i_{l-3}$ where each E^i_j contains exactly two facts u^i_j and v^i_j. Moreover, in the same way as described in the definition of D_n earlier, define the facts appropriately such that $\{b^i_{i_1}, b^i_{i_2}, u^i_1\}$ and $\{b^i_{i_{l-1}}, b^i_{i_l}, v^i_{l-3}\}$ form triangles and for every $1 \leq j < l - 3$ we have a triangle $\{v^i_j, u^i_{j+1}, b^i_{j+2}\}$.

The reader can verify that this is exactly the construction used to define D_n. Again, this construction is in LogSpace. For each such j and l define $U(i, l) = \{u^i_k \mid 1 \leq k \leq l - 2\}$ and $V(i, l) = \{v^i_k \mid l - 1 \leq k \leq l - 3\}$.

Now suppose there is a matching that saturates V_1 and let us show that the query is not certain. Consider the repair r where for each block B_j we pick b^i_j if s_j is matched with t_i. Further, pick $U(i, l) \cup V(i, l)$ which gives a partial repair over $E^i_1 \dots E^i_l$.

If some $t_i \in V_2$ is not matched with any vertex in V_1 then pick $U(i, 1) \cup V(i, 1)$ which gives a partial repair over $E^i_1 \dots E^i_l$. It can be verified that the obtained repair does not contain any solution.

Finally, suppose there is a repair over D_G that falsifies the query then note that if b^i_j is picked in block B_j then for all other blocks $B_{j'}$, the fact $b^i_{j'}$ cannot be in the repair since that will make the query true. Also $b^i_j \in B_j$ only if there is an edge between s_j and t_i. Hence we can define the matching that maps every $s_j \in V_i$ to $t_i \in V_2$ where b^i_j is the fact in the falsifying repair from the block B_j. ◀

7 Conclusion

We have presented a simple polynomial time algorithm for certain query answering over inconsistent databases under primary key constraints. The query is always certain when the algorithm outputs "yes", but it may produce false negative answers. We showed that for any self-join-free or path query which is not coNP-hard, the algorithm correctly computes all certain answers. A similar fixpoint algorithm can be obtained for other kinds of constraints. It needs a few hypothesis such that being able to check in PTime whether a set of facts belongs to a repair. However, the analysis of this algorithm under other kinds of constraints is yet to be studied.

It is clear that when the fixpoint of the algorithm is bounded (i.e., it converges after a number of steps which is independent of the input database) the certainty of the query can be expressed in first-order logic, see Remark 11. It turns out that the converse is also true. Using the characterizations of [8] for self-join-free queries and of [7] for path queries, we can show that when the certainty can be expressed in first-order logic, then our algorithm is bounded. This will appear in the journal version of this paper.

As we have shown, our algorithm does not solve all the known cases where certainty can be solved in polynomial time. Hence, it would be interesting to have a (decidable) characterization of the queries whose certainty can be solved using our algorithm; we leave this for future work.

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