Finite Open-World Query Answering with Number Restrictions

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Abstract—Open-world query answering is the problem of deciding, given a set of facts, conjunction of constraints, and query, whether the facts and constraints imply the query. This amounts to reasoning over all instances that include the facts and satisfy the constraints. We study finite open-world query answering (FQA), which assumes that the underlying world is finite and thus only considers the finite completions of the instance. The major known decidable cases of FQA derive from the following: the guarded fragment of first-order logic, which can express referential constraints (data in one place points to data in another) but cannot express number restrictions such as functional dependencies; and the guarded fragment with number restrictions but on a signature of arity only two. In this paper, we give the first decidability results for FQA that combine both referential constraints and number restrictions for arbitrary signatures: we show that, for unary inclusion dependencies and functional dependencies, the finiteness assumption of FQA can be lifted up to taking the finite implication closure of the dependencies [5]. Our result relies on new techniques to construct finite universal models of such constraints, for any bound on the maximal query size.

I. INTRODUCTION

A longstanding goal in computational logic is to design logical languages that are both decidable and expressive. One approach is to distinguish integrity constraints and queries, and have separate languages for them. We would then seek decidability of the query answering with constraints problem: given a query $q$, a conjunction of constraints $\Sigma$, and a finite instance $I$, determine which answers to $q$ are certain to hold over any instance $I'$ that extends $I$ and satisfies $\Sigma$. This problem is often called open-world query answering. It is fundamental for deciding query containment under constraints, querying in the presence of ontologies, or reformulating queries with constraints. Thus it has been the subject of intense study within several communities for decades (e.g. [8], [3], [2], [12], [7]).

In many cases (e.g., in databases) the instances $I'$ of interest are the finite ones, and hence we can define finite open-world query answering (denoted here as FQA), which restricts the quantification to finite extensions $I'$ of $I$. In contrast, by unrestricted open-world query answering (UQA) we refer to the problem where $I'$ can be either finite or infinite. Generally the class of queries is taken to be the conjunctive queries (CQs) — queries built up from relational atoms via existential quantification and conjunction. We will restrict to CQs here, and thus omit explicit mention of the query language, focusing on the constraint language.

A first constraint class known to have tractable open-world query answering problems are inclusion dependencies (IDs) — constraints of the form, e.g., $\forall xyz R(x,y,z) \rightarrow \exists vw S(z,v,w,y)$. The fundamental results of Johnson and Klug [8] and Rosati [15] show that both FQA and UQA are decidable for ID and that, in fact, they coincide. When this happens, the constraints are said to be finitely controllable. These results have been generalized by Bárány et al. [2] to a much richer class of constraints, the guarded fragment of first-order logic.

However, those results do not cover a second important kind of constraints, namely number restrictions, which express, e.g., uniqueness. We represent them by the class of functional dependencies (FDs) — of the form $\forall xy (R(x_1, \ldots, x_n) \land \neg \bigwedge_{i \in \mathbb{N}} x_i = y_i) \rightarrow x_r = y_r$. The implication problem (does one FD follow from a set of others) is decidable for FDs, and coincides with implication restricted to finite instances [1]. Trivially, the FQA and UQA problems are also decidable for FDs alone, and coincide.

Trying to combine IDs and FDs makes both UQA and FQA undecidable in general [3]. However, UQA is known to be decidable when the FDs and the IDs are non-conflicting [8], [3]. Intuitively, this condition guarantees that the FDs can be ignored, as long as they hold on the initial instance $I$, and one can then solve the query answering problem by considering the IDs alone. But the non-conflicting condition only applies to UQA and not to FQA. In fact it is known that even for very simple classes of IDs and FDs, including non-conflicting classes, FQA and UQA do not coincide. Rosati [15] showed that FQA is undecidable for non-conflicting IDs and FDs (indeed, for IDs and keys, which are less rich than FDs).

Thus a general question is to what extent these classes, FDs and IDs, can be combined while retaining decidable FQA. The only decidable cases impose very severe requirements. For example, the constraint class of “single KDs and FKs” introduced in [15] has decidable FQA, but such constraints cannot model, e.g., FDs which are not keys. Further, in contrast with the general case of FDs and IDs, single KDs and FKs are always finitely controllable, which limits their expressiveness. Indeed, we know of no tools to deal with FQA for non-finitely-controllable constraints on relations of arbitrary arity.

A second decidable case is where all relation symbols and
all subformulas of the constraints have arity at most two. In this context, results of Pratt-Hartmann [12] imply the decidability of both FQA and UQA for a very rich non-finitely-controllable sublogic of first-order logic. For some fragments of this arity-two logic, the complexity of FQA has recently been isolated by Ibáñez-García et al. [7]. Yet these results do not apply to arbitrary arity signatures.

The contribution of this paper is to provide the first result about finite query answering for non-finitely-controllable IDs and FDs over relations of arbitrary arity. As the problem is undecidable in general, we must naturally make some restriction. Our choice is to limit to Unary IDs (UIDs), which export only one variable: for example, $\forall x \exists y \exists z \ldots R(x,y,z)$ $\rightarrow \exists w \forall s(w,x)$. UIDs and FDs are an interesting class to study because they are not finitely controllable, and allow the modeling, e.g., of single-attribute foreign keys, a common use case in database systems. The decidability of UQA for UIDs and FDs is known because they are always non-conflicting. In this paper, we show that finite query answering is decidable for UIDs and FDs, and obtain tight bounds on its complexity.

The idea is to reduce the finite case to the unrestricted case, but in a more complex way than by finite controllability. We make use of a technique originating in Cosmadakis et al. [5] to study finite implication on UIDs and FDs: the finite closure operation which takes a conjunction of UIDs and FDs and determines exactly which additional UIDs and FDs are implied over finite instances. Rosati [14] and Ibáñez-García [7] make use of the closure operation in their study of constraint classes over schemas of arity two. They show that finite query answering for a query $q$, instance $I$, and constraints $\Sigma$ reduces to unrestricted query answering for $I$, $q$, and the finite closure $\Sigma'$ of $\Sigma$. In other words, the closure construction which is sound for implication is also sound for query answering.

We show that the same general approach applies to arbitrary arity signatures, with constraints being UIDs and FDs. Our main result thus reduces finite query answering to unrestricted query answering, for UIDs and FDs in arbitrary arity:

**Theorem I.1.** For any finite instance $I$, conjunctive query $q$, and constraints $\Sigma$ consisting of UIDs and FDs, the finite open-world query answering problem for $I,q$ under $\Sigma$ has the same answer as the unrestricted open-world query answering problem for $I,q$ under the finite closure of $\Sigma$.

Using the known results about the complexity of UQA for UIDs, we isolate the precise complexity of finite query answering with respect to UIDs and FDs, showing that it matches that of UQA:

**Corollary I.2.** The combined complexity of the finite open-world query answering problem for UIDs and FDs is NP-complete, and it is PTIME in data complexity (that is, when the constraints and query are fixed).

Our proof of Theorem I.1 is quite involved, since dealing with arbitrary arity models introduces many new difficulties that do not arise in the arity-two case or in the case of IDs in isolation. We borrow and adapt a variety of techniques from prior work: using $k$-bounded simulations to preserve small acyclic CQs [7], dealing with UIDs following a topological sort [5], [7], performing a chase that reuses sufficiently similar elements [15], and taking the product with groups of large girth to blow up cycles [11]. However, we must also develop some new infrastructure to deal with number restrictions in an arbitrary arity setting: distinguishing between so-called dangerous and non-dangerous positions when chasing, constructing realizations for relations in a piecewise manner following the FDs, reusing elements in a combinatorial way that shuffles them to avoid violating the higher-arity FDs, and a new notion of mixed product to blow cycles up while preserving fact overlaps to avoid violating the higher-arity FDs.

**Paper structure.** The general scheme, presented in Section III, is to construct models of UIDs and FDs that are universal up to a certain query size $k$, which we call $k$-universal models. We start with only unary FDs (UFDs) and acyclic CQs (ACQs), and by assuming that the UIDs and UFDs are reversible, a condition inspired by the finite closure construction.

As a warm-up, Section IV proves the weakened result for a much weaker notion than $k$-universality, starting with binary signatures and generalizing to arbitrary arity. We extend the result to $k$-universality in Section V, maintaining a $k$-bounded simulation to the chase, and performing thrifty chase steps that reuse sufficiently similar elements without violating UFDs. We also rely on a structural observation about the chase under UIDs (Theorem V.11). Section VI eliminates the assumption that dependencies are reversible, by partitioning the UIDs into classes that are either reversible or trivial, and satisfying successively each class following a certain ordering.

We then generalize our result to higher-arity (non-unary) FDs in Section VII. This requires us to define a new notion of thrifty chase steps that apply to instances with many ways to reuse elements; the existence of these instances relies on a combinatorial construction of models of FDs with a high number of facts but a small domain (Theorem VII.7). Last, in Section VIII, we apply a cycle blowup process to the result of the previous constructions, to go from acyclic to arbitrary CQs through a product with acyclic groups. The technique is inspired by Otto [11] but must be adapted to respect FDs. We conclude in Section IX.
the projection $\pi_R(I)$ of $I$ to $R'$ as the set of the elements of $\text{dom}(I)$ that occur at position $R'$ in $I$. For $L \subseteq \text{Pos}(R)$, the projection $\pi_R(I)$ is a set of $|L|$-tuples defined analogously; for convenience, departing from the unnamed perspective, we index those tuples by the positions of $L$. A superinstance of $I$ is a (not necessarily finite) instance $I'$ such that $I \subseteq I'$. A homomorphism from an instance $I$ to an instance $F$ is a mapping $h : \text{dom}(I) \rightarrow \text{dom}(F)$ such that, for every fact $F = R(a)$ of $I$, the fact $h(F) := R(h(a_1), \ldots, h(a_{|R|}))$ is in $I'$.

Constraints. We consider integrity constraints (or dependencies) which are special sentences of first-order logic. As usual in the relational setting, we do not allow function symbols. The definition of an instance $I$ satisfying a constraint $\Sigma$, written $I \models \Sigma$, is standard.

An inclusion dependency ID is a sentence of the form $\tau : \forall x R(x_1, \ldots, x_n) \rightarrow \exists y S(z_1, \ldots, z_m)$, where $\tau \subseteq x \cup y$ and no variable occurs twice in $\tau$. The exported variables are the variables of $x$ that occur in $\tau$, and the arity of the dependency is the number of such variables. This work only studies unary inclusion dependencies (UIDs) which are the IDs with arity $1$. If $\tau$ is a UID, we write $\tau$ as $R' \subseteq S'$, where $R'$ and $S'$ are the positions of $R(x)$ and $S(z)$ where the exported variable occurs. For instance, the UID $\forall x y R(x, y) \rightarrow \exists z S(x, y, z)$ is written $R' \subseteq S'$. We assume without loss of generality that there are no trivial UIDs of the form $R' \subseteq R'$.

We say that a conjunction $\Sigma_{UID}$ of UIDs is transitively closed if it is closed under the transitivity rule: if $R' \subseteq S'$ and $S' \subseteq T'$ are in $\Sigma_{UID}$, then so is $R' \subseteq T'$ unless it is trivial. The transitive closure of $\Sigma_{UID}$ can clearly be computed in PTIME in $\Sigma_{UID}$, and it contains all non-trivial UIDs implied by $\Sigma_{UID}$ over finite or unrestricted instances [4]. We say a UID $\tau : R' \subseteq S'$ is reversible relative to $\Sigma_{UID}$ if both $\tau$ and its reverse $\tau^{-1} := S' \subseteq R'$ are in $\Sigma_{UID}$.

A functional dependency FD is a sentence of the form $\phi : \forall x y (R(x_1, \ldots, x_n) \wedge \forall R'(x, y) = y) \rightarrow x = y$, where $L \subseteq \text{Pos}(R)$ and $R' \subseteq \text{Pos}(R)$. For brevity, we write $\phi$ as $R^L \rightarrow R'$. We call $\phi$ a functionally dependent UFD if $|L| = 1$; otherwise it is higher-arity. For instance, $\forall x' \forall y' R(x', x') \wedge R(y, y') \wedge x' = y' \rightarrow x = y$ is a UFD, and we write it $R'^2 \rightarrow R^1$. We assume that $|L| > 0$, i.e., we do not allow nonstandard or degenerate FIDs. We call $\phi$ trivial if $R' \subseteq R^2$, in which case $\phi$ always holds. Two facts $R(a)$ and $R(b)$ violate a non-trivial FD $\phi$ if $\pi_L(a) = \pi_L(b)$ but $a \neq b$.

The key dependency $K : R^L \rightarrow R$, for $L \subseteq \text{Pos}(R)$, is the conjunction of FIDs $R_i \rightarrow R$ for all $R' \subseteq \text{Pos}(R)$; it is unary if $|L| = 1$. If $K$ holds, we call $L$ a (key) or unary key of $R$.

Queries. An atom $A = R(t)$ consists of a relation name $R$ and a $|R|$-tuple $t$ of variables or constants. A conjunctive query CQ is an existentially quantified conjunction of atoms. In this paper we focus for simplicity on Boolean queries (queries without free variables), but all our results hold for non-Boolean queries as well, by the standard method of enumerating the assignments. The size $|\phi|$ of a CQ $\phi$ is its number of atoms.

A Berge cycle in a Boolean CQ $\phi$ is a sequence $A_1, x_1, A_2, x_2, \ldots, A_n, x_n$ with $n \geq 2$, where the $A_i$ are pairwise distinct atoms of $\phi$, the $x_i$ are pairwise distinct variables of $\phi$, and $x_i$ occurs in $A_i$ and $A_{i+1}$ for $1 \leq i \leq n$ (with addition modulo $n$, so $x_n$ occurs in $A_1$). We call $\phi$ acyclic if $\phi$ has no Berge cycle and if no variable of $\phi$ occurs more than once in the same atom. We write $\text{ACQ}$ for the class of acyclic CQs.

A Boolean CQ $\phi$ holds in an instance $I$ exactly when there is a homomorphism $h$ from the atoms of $\phi$ to $I$ such that $h$ is the identity on the constants of $\phi$ (we call this a homomorphism from $\phi$ to $I$). The image of $h$ is called a match of $\phi$ in $I$.

QA problems. We define the unrestricted open-world query answering problem (UQA) as follows: given a finite instance $I$, a conjunction of constraints $\Sigma$, and a Boolean CQ $\phi$, decide whether there is a superinstance of $I$ that satisfies $\Sigma$ and violates $\phi$. If there is none, we say that $I$ and $\Sigma$ entail $\phi$ and write $(I, \Sigma) \models_{\text{ent}} \phi$.

This work focuses on the finite query answering problem (FQA), which is the variant of open-world query answering where we require the counterexample superinstance to be finite; if none exists, we write $(I, \Sigma) \models_{\text{fqa}} \phi$. Of course $(I, \Sigma) \models_{\text{fqa}} \phi$ implies $(I, \Sigma) \models_{\text{ent}} \phi$. We say a conjunction of constraints $\Sigma$ is finitely controllable if FQA and UQA coincide: for every finite instance $I$ and every Boolean CQ $\phi$, $(I, \Sigma) \models_{\text{ent}} \phi$ if $(I, \Sigma) \models_{\text{fqa}} \phi$.

The combined complexity of the UQA and FQA problems, for a fixed class of constraints, is the complexity of deciding it when all of $I$, $\Sigma$ (in the constraint class) and $\phi$ are given as input. The data complexity is defined by assuming that $\Sigma$ and $\phi$ are fixed, and only $I$ is given as input.

Chase. We say that a superinstance $I'$ of an instance $I$ is universal for constraints $\Sigma$ if $I' \models \Sigma$ and if for any Boolean CQ $\phi$, $I' \models \phi$ iff $(I, \Sigma) \models_{\text{ent}} \phi$. We now recall the definition of the chase [1], [10], a standard construction of (generally infinite) universal superinstances. We assume that we have fixed an infinite set $\mathbb{N}$ of non-nulls which is disjoint from $\text{dom}(I)$. We only define the chase for transitively closed UIDs, which we call the UID chase.

We say that a fact $F_0 = R(a)$ of an instance $I$ is an active fact for a UID $\tau : R' \subseteq S'$ if, writing $\tau : \forall x R(x) \rightarrow \exists y S(x, \exists)$, there is a homomorphism from $R(x)$ to $F_0$ but no such homomorphism can be extended to a homomorphism from $\{R(x), S(x, \exists)\}$ to $I$. In this case we say that $a$ wants to occur at position $S'$ in $I$, written $a \in \text{Wants}(I, S')$, and that we want to apply the UID $\tau$ to $a$, written $a \in \text{Wants}(I, \tau)$. Note that $\text{Wants}(I, \tau) = \pi_{R_0}(I) \setminus \pi_{S'}(I)$.

The result of a chase step on the active fact $F_0$ for $\tau$ in $I$ (we call this applying $\tau$ to $F_0$) is the superinstance $I'$ of $I$ obtained by adding a new fact $F_0 = S(b)$ defined as follows: we set $b := a$, which we call the exported element (and $S'$ the exported position of $F_0$), and use fresh nulls from $\mathbb{N}$ to instantiate the existentially quantified variables of $\tau$ and complete $F_0$; we say the corresponding elements are introduced at $F_0$. This ensures that $F_0$ is no longer an active fact in $I'$ for $\tau$.

A chase round of a conjunction $\Sigma_{UID}$ of UIDs on $I$ is the result of applying simultaneous chase steps on all active facts...
for all UIDs of $\Sigma_{UID}$, using distinct fresh elements. The UID chase $\text{Chase}(I, \Sigma_{UID})$ of $I$ by $\Sigma_{UID}$ is the (generally infinite) fixpoint of applying chase rounds. It is a universal superinstance for $\Sigma_{UID}$ [6].

As we are chasing by transitively closed UIDs, if we perform the core chase [10] rather than the UID chase defined above, we can ensure the following Unique Witness Property: for any element $a \in \text{dom}(\text{Chase}(I, \Sigma_{UID}))$ and position $R^0$ of $\sigma$, if two different facts of $\text{Chase}(I, \Sigma_{UID})$ contain $a$ at position $R^0$, then they are both facts of $I$. In our context, however, the core chase matches the UID chase defined above, except at the first round. Thus, modulo the first round, by $\text{Chase}(I, \Sigma_{UID})$ we refer to the UID chase, which has the Unique Witness Property.

Finite closure. Rosati [13], [15] showed that, while conjunctions of IDs are finitely controllable, even conjunctions of UIDs and FDs may not be. However, Cosmadakis et al. [5] showed how to decide in PTIME the finite implication problem for UIDs and FDs: given a conjunction $\Sigma$ of such dependencies, decide whether a UID or FD is implied by $\Sigma$ over finite instances. The finite closure of $\Sigma$ is the set of the UIDs and FDs thus implied by $\Sigma$ in the finite.

Rosati [14] later showed that the finite closure could be used to reduce UQA to FQA for some constraints on relations of arity at most two. Following the same idea, we say that a conjunction of constraints $\Sigma$ is finitely controllable up to finite closure if for every finite instance $I$, and Boolean CQ $q$, $(I, \Sigma) \models \text{fin q}$ iff $(I, \Sigma') \models \text{fin q}$, where $\Sigma'$ is the finite closure of $\Sigma$. This implies that we can reduce FQA to UQA, even if finite controllability does not hold.

III. MAIN RESULT AND OVERALL APPROACH

We study open-world query answering for FDs and UIDs. For unrestricted query answering (UQA), the following is already known, from bounds on UQA for UIDs:

Proposition III.1. UQA for FDs and UIDs has PTIME data complexity and NP-complete combined complexity.

However, for the finite case, even the decidability of FQA for FDs and UIDs is not known. Here is our main result, which is proved in the rest of this paper:

Theorem III.2 (Main theorem). Conjunctions of FDs and UIDs are finitely controllable up to finite closure.

From these two results, and an efficient computation of the closure, we deduce that the complexity of FQA matches that of UQA:

Corollary III.3. FQA for FDs and UIDs has PTIME data complexity and NP-complete combined complexity.

A. Rephrasing with universal models

We prove the main theorem via the notions of $k$-sound and $k$-universal instances.

Definition III.4. For $k \in \mathbb{N}$, we say that a superinstance $I$ of an instance $I_0$ is $k$-sound for constraints $\Sigma$ (and for $I_0$) if for every constant-free CQ $q$ of size $\leq k$ such that $I \models q$, we have $(I_0, \Sigma) \models_{\text{unr}} q$. We say it is $k$-universal if the converse also holds: $I \models q$ whenever $(I_0, \Sigma) \models_{\text{unr}} q$.

The assumption that $q$ is constant-free is without loss of generality: we can always assume that, for each constant $c \in \text{dom}(I_0)$, a fact $P(c)$ has been added to $I_0$ for a fresh unary relation $P_1$, and $c$ was replaced in $q$ by a existentially quantified variable $x$, with the atom $P_1(x)$ added to $q$. Hence, for simplicity, we assume from now on that queries are constant-free.

Theorem III.2 is implied by the following:

Theorem III.5 (Universal models). For every conjunction $\Sigma$ of FDs $\Sigma_{FD}$ and UIDs $\Sigma_{UID}$ closed under finite implication, for every finite instance $I_0$ that satisfies $\Sigma_{FD}$, for any $k \in \mathbb{N}$, there exists a finite superinstance $I$ of $I_0$ that is $k$-sound for $\Sigma$ and satisfies $\Sigma$ (and hence is $k$-universal).

The fact that such an $I$ is $k$-universal is because any superinstance of $I_0$ that satisfies $\Sigma$ must satisfy all CQs $q$ such that $(I_0, \Sigma) \models_{\text{unr}} q$, by definition of $\models_{\text{unr}}$.

We now fix the conjunction $\Sigma$ of FDs $\Sigma_{FD}$ and UIDs $\Sigma_{UID}$. We assume that $\Sigma$ is closed under finite implication; in particular, $\Sigma_{FD}$ and $\Sigma_{UID}$ in isolation are closed under implication, which implies that $\Sigma_{UID}$ is transitively closed. We also fix the instance $I_0$ such that $I_0 \models \Sigma_{FD}$, and the maximal query size $k \in \mathbb{N}$.

Our goal in the rest of this paper is to construct the finite $k$-sound superinstance of $I_0$ that satisfies the constraints $\Sigma$, thus proving the Universal Models Theorem and hence the Main Theorem.

B. Restricting to ACQs, UFDS, and reversible constraints

We first prove the Universal Models Theorem for a restricted class of queries and dependencies, which we now define. We will lift these restrictions later.

First, we define $\Sigma_{UFD}$ to be the unary FDs of $\Sigma_{FD}$, and write $\Sigma_U := \Sigma_{UFD} \wedge \Sigma_{UID}$. Note that, as we assumed that $\Sigma$ is closed under finite implication for UFDS and UIDs, the characterization of [5] implies that $\Sigma_U$ also is. We will first construct a $k$-sound superinstance that only satisfies $\Sigma_U$; in Section VII we will show how to adapt the process to also satisfy $\Sigma$.

Second, we will first construct a superinstance that is $k$-sound only for acyclic Boolean queries; in Section VIII we will show how to make the resulting superinstance sufficiently acyclic to be sound for cyclic queries as well.

Hence, in Sections IV, V and VI, we prove the following weakening of the Universal Models Theorem. The restrictions will be lifted in Sections VII and VIII.

Theorem III.6 (Acyclic unary universal models). There exists a finite superinstance of $I_0$ that satisfies $\Sigma_U$ and is $k$-sound for $\Sigma_U$ and ACQ (and hence $k$-universal for $\Sigma_U$ and ACQ).

To prove the Acyclic Unary Universal Models Theorem, in Sections IV and V, we will assume the following condition on the structure of the dependencies:
The following holds about \( \Sigma_U \):
- all \( \text{UIDs} \) in \( \Sigma_{\text{UID}} \) are reversible (remember this means that the reverse \( \tau^{-1} \) of any \( \tau \in \Sigma_{\text{UID}} \) is also in \( \Sigma_{\text{UID}} \));
- for any positions \( R^0 \) and \( R^0 \) occurring in \( \text{UIDs} \) of \( \Sigma_{\text{UID}} \), if \( R^0 \rightarrow R^0 \) is in \( \Sigma_{\text{UFD}} \) then so is \( R^0 \rightarrow R^0 \).

Intuitively, assumption reversible is connected to the finite close characterization of \([5]\), which adds to \( \Sigma_U \) the reverses of any \( \text{UIDs} \) and \( \text{UFDs} \) that form a certain cyclic pattern.

Working under assumption reversible, Section IV proves an even weaker version of the Acyclic Unary Universal Models Theorem, which replaces \( k \)-soundness by weak-soundness; Section V proves the actual theorem. Assumption reversible is lifted in Section VI to conclude the proof.

IV. Weak-Soundness and Reversible \( \text{UIDs} \)

The goal of this section is to prove the Acyclic Unary Universal Models Theorem (Theorem III.6) under assumption reversible, replacing \( k \)-soundness by weak-soundness.

Definition IV.1. A superinstance \( I' \) of an instance \( I \) is weakly-sound if the following holds:
- for any \( a \in \text{dom}(I) \) and \( R^p \in \text{Pos}(\sigma) \), if \( a \in \pi_{R^p}(I') \), then either \( a \in \pi_{R^p}(I) \) or \( a \in \text{Wants}(I, R^p) \);
- for any \( a \in \text{dom}(I') \) and \( R^p \) and \( R^q \in \text{Pos}(\sigma) \), if \( a \in \pi_{R^q}(I') \) and \( a \in \pi_{R^p}(I') \) then \( R^p = S^q \) or \( R^p \subseteq S^q \) is in \( \Sigma_{\text{UID}} \).

Intuitively, a superinstance is weakly-sound if existing elements were only added to positions where they wanted to appear, and new elements only occur at positions which are connected in \( \Sigma_{\text{UID}} \). This section shows the following:

**Proposition IV.2** (Acyclic unary weak-sound models). Under assumption reversible, there exists a finite superinstance of \( I \) that satisfies \( \Sigma_U \) and is weakly-sound.

The proposition itself will not be reused in the sequel, but the proof introduces some useful concepts to prove the actual Acyclic Unary Universal Models Theorem in Section V.

A. Binary signatures and balanced instances

For simplicity, we first focus on a simplified case with a binary signature, making the following assumption that will be lifted later in this section:

**binary:** all relations have arity 2 and \( \Sigma_{\text{UFD}} \) contains the \( \text{UFDs} \)

\[
R^1 \rightarrow R^2 \text{ and } R^2 \rightarrow R^1 \text{ for any relation } R.
\]

Our approach to construct a weakly-sound superinstance \( I' \) of \( I \) that satisfies \( \Sigma_U \) is then to perform a completion process that adds new (binary) facts to connect together elements. As all possible \( \text{UFDs} \) hold, \( I' \) can only contain a new fact \( R(a_1, b_2) \) if, for \( i \in \{1, 2\} \), \( a_2 \notin \pi_{R^i}(I) \), so that if \( a_i \in \text{dom}(I) \) then \( a_i \in \text{Wants}(I, R^i) \) by weak soundness.

One easy situation is when \( I_0 \) is balanced: for every relation \( R \), we can construct a bijection between the elements that want to be in \( R^1 \) and those that want to be in \( R^2 \):

**Definition IV.3.** An instance \( I \) is balanced if, for every two positions \( R^0 \) and \( R^0 \) such that \( R^0 \rightarrow R^0 \) and \( R^0 \rightarrow R^0 \) are in \( \Sigma_{\text{UFD}} \), we have \( |\text{Wants}(I, R^0)| = |\text{Wants}(I, R^0)| \).

If \( I_0 \) is balanced, we can show the Acyclic Unary Weakly-Sound Models Proposition under assumption binary, simply by pairing together elements, without adding any new ones:

**Proposition IV.4.** Assuming binary and reversible, any balanced finite instance \( I \) satisfying \( \Sigma_{\text{UFD}} \) has a finite weakly-sound superinstance \( I' \) that satisfies \( \Sigma_U \), with \( \text{dom}(I') = \text{dom}(I) \).

However, our instance \( I_0 \) may not be balanced. The idea is then to balance it by adding “helper” elements and assigning them to positions, as the following example shows:

**Example IV.5.** Consider three binary relations \( R, S, T \), with the \( \text{UIDs} \)

\[
R^2 \subseteq S^1, S^2 \subseteq T^1, T^2 \subseteq R^1
\]

and their reverses, and the \( \text{FDs} \) prescribed by assumption binary. Consider \( I_0 := \{ (a, b) \} \). We have \( a \in \text{Wants}(I_0, T^2) \) and \( b \in \text{Wants}(I_0, S^1) \); however \( \text{Wants}(I_0, S^2) = \text{Wants}(I_0, T^1) = \emptyset \), so \( I_0 \) is not balanced.

Still, we can construct the weak-sound superinstance \( I := \{ R(a, b), S(b, c), T(c, a) \} \) that satisfies the constraints.

Intuitively, we have added a “helper” element \( c \) and “assigned” it to the positions \( S^1 \) and \( T^2 \), which are connected by the \( \text{UIDs} \).

We now formalize this idea of constructing weakly-sound superinstances where the domain is augmented with helper elements. We first need to understand at which positions the helpers can appear to avoid violating weak-soundness.

**Definition IV.6.** For any two positions \( R^0 \) and \( S^1 \), we write \( R^0 \sim_{\text{ID}} S^1 \) when \( R^0 = S^1 \) or \( R^0 \subseteq S^1 \), and hence \( S^1 \subseteq R^0 \) by assumption reversible, are in \( \Sigma_{\text{UID}} \).

As \( \Sigma_{\text{UID}} \) is transitively closed, \( \sim_{\text{ID}} \) is an equivalence relation. Our idea to construct weakly-sound superinstances is thus to first decide on the helpers that we want to add, and the \( \sim_{\text{ID}} \)-class to which we want to assign them, following the definition of weak-soundness. We represent this choice as a partially-specified superinstance, or pssinstance:

**Definition IV.7.** A pssinstance of an instance \( I \) is a triple \( P = (I, H, \lambda) \) where \( H \) is a finite set of helpers and \( \lambda \) maps each \( h \in H \) to an \( \sim_{\text{ID}} \)-class \( \lambda(h) \).

We define \( \text{Wants}(P, R^0) := \text{Wants}(I, R^0) \cup \{ h \in H | R^0 \in \lambda(h) \} \). This allows us to talk of \( P \) being balanced following Definition IV.3.

A superinstance \( I' \) of \( I \) is a realization of \( P \) if \( \text{dom}(I') = \text{dom}(I) \cup H \), and, for any fact \( R(a) \) of \( I' \) and \( R^0 \in \text{Pos}(R) \), we have \( a_p \in \text{Wants}(P, R^0) \).

**Example IV.8.** In Example IV.5, a pssinstance of \( I_0 \) is \( P := (I_0, \{c\}, \lambda) \) where \( \lambda(c) := \{S^1, T^2\} \), and \( I \) is a realization of \( P \).

It is always possible to balance an instance by adding helpers:

**Lemma IV.9** (Balancing). For any finite instance \( I \), if \( I \) satisfies \( \Sigma_{\text{UFD}} \) then it has a balanced pssinstance.

From there, we can construct realizations like we constructed superinstances in Lemma IV.4.

**Lemma IV.10** (Binary realizations). For any balanced pssinstance \( P \) of an instance \( I \) that satisfies \( \Sigma_{\text{UFD}} \), we can construct a realization of \( P \) that satisfies \( \Sigma_U \).  

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We then observe that realizations are weakly-sound superinstances of $I_0$.

Lemma IV.11 (Binary realizations are completions). If $I$ is a realization of a pssinstance of $I$ then it is a weakly-sound superinstance of $I$.

We have thus proved the Acyclic Unary Weakly-Sound Models Proposition under assumptions binary and reversible, using the completion process formed by combining the three above lemmas.

B. Arbitrary arity and piecewise realizations

We now lift assumption binary (but retain assumption reversible). We show how to generalize the previous constructions to the arbitrary arity case. Contrary to the binary situation, we will see later that the resulting completion process needs to assume that a certain saturation process has been applied to $I_0$ beforehand.

The definition of balanced instances (Definition IV.3) generalizes to arbitrary arity, and we can show that the Balancing Lemma (Lemma IV.9) still holds. We keep the definition of pssinstance (Definition IV.7) but need to change the notion of realization. We replace it by piecewise realizations, which are defined on subsets of positions that are connected in $\Sigma_{UFD}$.

Definition IV.12. For any two positions $R^0$ and $R^n$, we write $R^0 \leftrightarrow_{\text{FUN}} R^n$ whenever $R^0 \rightarrow R^n$ and $R^n \rightarrow R^0$ are in $\Sigma_{UFD}$.

By transitivity of $\Sigma_{UFD}$, $\leftrightarrow_{\text{FUN}}$ is clearly an equivalence relation. We number the $\leftrightarrow_{\text{FUN}}$-classes of $\text{Pos}(\sigma)$ as $\Pi_1, \ldots, \Pi_n$ and define piecewise instances by their projections to the $\Pi_i$.

Definition IV.13. A piecewise instance is an $n$-tuple $PI = (K_1, \ldots, K_n)$, where each $K_i$ is a set of $[|\Pi_i|]$-tuples, indexed by $\Pi_i$ for convenience. The domain of $PI$ is $\text{dom}(PI) := \bigcup_i \text{dom}(K_i)$. For $1 \leq i \leq n$ and $R^0 \in \Pi_i$, we write $\pi_{R^0}(PI) := \pi_{R^0}(K_i)$.

We use this to define piecewise realizations of pssinstances:

Definition IV.14. A piecewise instance $PI = (K_1, \ldots, K_n)$ is a piecewise realization of the pssinstance $P = (I, \mathcal{H}, \lambda)$ if:

- $\pi_{K_i}(I) \subseteq K_i$ for all $1 \leq i \leq n$,
- $\text{dom}(PI) = \text{dom}(I) \cup \mathcal{H}$,
- for all $1 \leq i \leq n$, for all $R^p \in \Pi_i$, for every tuple $a \in K_i \setminus \pi_{K_i}(I)$, we have $a_{R^p} \in \text{Wants}(P, R^p)$.

In order to generalize the Binary Realizations Lemma (Lemma IV.10), we need to talk of a piecewise instance $PI$ “satisfying” $\Sigma_U$. For $\Sigma_{UFD}$, we require that $PI$ respects the UFDs within each $\leftrightarrow_{\text{FUN}}$-class. For $\Sigma_{UID}$, we define it directly from the projections of $PI$.

Definition IV.15. A piecewise instance $PI$ is $\Sigma_{UFD}$-compliant if, for all $1 \leq i \leq n$, there are no two tuples $a \neq b$ in $K_i$ such that $a_{R^p} = b_{R^p}$ for some $R^p \in \Pi_i$. $PI$ is $\Sigma_{UFD}$-compliant if $\text{Wants}(PI, \tau) := \pi_{R^0}(PI) \setminus \pi_{S^0}(PI)$ is empty for all $\tau \in \Sigma_{UFD}$.

$PI$ is $\Sigma_U$-compliant if $\text{Wants}(PI, \tau) := \pi_{R^0}(PI) \setminus \pi_{S^0}(PI)$ is empty for all $\tau \in \Sigma_{UID}$.

We can then generalize the Binary Realizations Lemma:

Lemma IV.16 (Realizations). For any balanced pssinstance $P$ of an instance $I$ that satisfies $\Sigma_{UID}$, we can construct a $\Sigma_U$-compliant piecewise realization of $P$.

Example IV.17. Consider a 4-ary relation $R$ and the UID $\tau : R_1 \subseteq R_2$, $\tau' : R_3 \subseteq R_4$ and their reverses, and the UFDs $\phi : R_1 \rightarrow R_2$, $\phi' : R_3 \rightarrow R_4$ and their reverses. We have $\Pi_1 = \{R_1, R_2\}$ and $\Pi_2 = \{R_3, R_4\}$. Consider $I_0 := \{R(a, b, c, d)\}$, which is balanced, and the balanced pssinstance $P := \{(a, b, c, d)\}$.

We now transform the $\Sigma_U$-compliant piecewise realization $PI$ into a weakly-sound superinstance, generalizing the “Binary Realizations Are Completions” Lemma (Lemma IV.11), and completing the description of our completion process. The idea is to expand each tuple of each $K_i$ to an entire fact $F_i$ of the corresponding relation.

However, to fill the other positions of $F_i$, we will need to reuse existing elements of $I_0$. For this, we want $I_0$ to contain some $R$-fact for every relation $R$ that occurs in $\text{Chase}(I_0, \Sigma_{UID})$.

Definition IV.18. A relation $R$ is achieved (by $I$ and $\Sigma_{UID}$) if there is some $R$-fact in $\text{Chase}(I, \Sigma_{UID})$.

A superinstance $I'$ of an instance $I$ is relation-saturated (for $\Sigma_{UID}$) if every achieved relation (by $I$ and $\Sigma_{UID}$) occurs in $I'$.

Example IV.19. Consider two binary relations $R(T)$ and $T$ and a unary relation $S$, the UID $\tau : S \subseteq R_1$, $\tau' : R_3 \subseteq T^4$ and their reverses, no UFDs, and the non-relation-saturated instance $I_0 := \{S(a)\}$ which is trivially balanced.

$P := \{(a, b, \lambda), (a, c, \lambda), (a, d, \lambda), (a, e, \lambda), (a, f, \lambda), (a, g, \lambda), (a, h, \lambda), (a, i, \lambda)\}$, and $\Sigma_{UID}$ is a $\Sigma_U$-compliant piecewise realization of $P$. However, we cannot easily complete $PI$ to a superinstance of $I_0$ satisfying $\tau$ and $\tau'$, because to create the fact $R(a, \bullet)$, we need to create an element to fill position $R^2$, and this would introduce a violation of $\tau'$. Intuitively, this is because $I_0$ is not relation-saturated.

Consider instead the instance $I_1 := I_0 \cup \{S(c), R(c, d), T(d)\}$. We can complete $I_1$ to satisfy $\tau$ and $\tau'$ by adding the fact $R(a, d)$, reusing the element $d$ to fill position $R^2$.

Clearly, initial chasing on $I_0$ ensures relation-saturation:

Lemma IV.20 (Relation-saturated solutions). The result of performing sufficiently many chase rounds on any instance $I$ is relation-saturated.

Relation-saturation ensures that we can reuse existing elements when completing $PI$. This allows us to perform the last step of the completion process:

Lemma IV.21 (Using realizations to get completions). For any finite relation-saturated instance $I$ that satisfies $\Sigma_{UID}$, from a $\Sigma_U$-compliant piecewise realization $PI$ of a pssinstance of $I$, we can construct a finite weakly-sound superinstance of $I$ that satisfies $\Sigma_U$. 

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We can now prove the Acyclic Unary Weakly-Sound Models Proposition. Consider our initial finite instance $I_0$, that satisfies $\Sigma_{URD}$, and chase it to a finite relation-saturated superinstance $I'_0$ using the Relation-Saturated Solutions Lemma. By the Unique Witness Property, $I'_0$ still satisfies $\Sigma_{URD}$, and it is clearly a weakly-sound superinstance of $I_0$.

Now, perform the completion process: construct a balanced simulation $P$ of $I'_0$ using the Balancing Lemma (Lemma IV.9), and a finite $\Sigma_w$-compliant piecewise realization $PI$ of $P$ by the Realizations Lemma (Lemma IV.16). Then, use the realization $PI$ with Lemma IV.21 to construct the finite weakly-sound superinstance $I$ of $I'_0$ that satisfies $\Sigma_w$. $I$ is clearly also a weakly-sound superinstance of $I_0$, so the result is proven.

V. k-Soundness and Reversible UIDs

We now move from weak-soundness to $k$-soundness, to prove the Acyclic Unary Universal Models Theorem (Theorem III.6), still making assumption reversible.

We first introduce the notion of aligned superinstances that we use to maintain $k$-soundness, and give the saturation process that generalizes relation-saturation. We then define a notion of thrifty chase steps, and a completion process that uses these chase steps to repair UID violations in the instance.

A. Aligned superinstances and fact-saturation

We ensure $k$-soundness by maintaining a $k$-bounded simulation from our superinstance of $I_0$ to Chase$(I_0, \Sigma_{URD})$. Indeed, Chase$(I_0, \Sigma_{URD})$ is a universal model for $\Sigma_{URD}$, and it satisfies $\Sigma_{FD}$ (by the Unique Witness Property, and because $I_0$ does). Hence, it is in particular $k$-sound for $\Sigma$. Now, as acyclic queries of size $\leq k$ are preserved through $k$-bounded simulations, superinstances of $I_0$ with a $k$-bounded simulation to Chase$(I_0, \Sigma_{URD})$ are indeed $k$-sound for ACQ.

**Definition V.1.** For $I, I'$ two instances, $a \in \text{dom}(I), b \in \text{dom}(I')$, and $n \in \mathbb{N}$, we write $(I,a) \leq_n (I',b)$ if, for any fact $R(a)$ of $I$ with $a_p = a$ for some $R' \in \text{Pos}(R)$, there exists a fact $R(b)$ of $I'$ such that $b_p = b$, and $(I,a) \leq_{n-1} (I',b)$ for all $R' \in \text{Pos}(R)$. The base case $(I,a) \leq_0 (I',b)$ always holds.

An $n$-bounded simulation from $I$ to $I'$ is a mapping sim such that for all $a \in \text{dom}(I)$, $(I,a) \leq_n (I',\text{sim}(a))$.

We write $a \equiv_n b$ for $a, b \in \text{dom}(I)$ if both $(I,a) \leq_n (I,b)$ and $(I,b) \leq_n (I,a)$; this is an equivalence relation on dom$(I)$.

**Lemma V.2.** For any instance $I$ and ACQ $q$ of size $\leq n$ such that $I \models q$, if there is an $n$-bounded simulation from $I$ to $I'$, then $I' \models q$.

We accordingly give a name to superinstances of $I_0$ that have a $k$-bounded simulation to the chase. For convenience, we also require them to be finite and satisfy $\Sigma_{URD}$. For technical reasons we require that the simulation is the identity on $I_0$, that it does not map other elements to $I_0$, and that elements occur in the superinstance at least at the position where their sim-image was introduced in the chase:

**Definition V.3.** An aligned superinstance $J = (I, \text{sim})$ of $I_0$ is a finite superinstance of $I_0$ that satisfies $\Sigma_{URD}$, and a $k$-bounded simulation sim from $I$ to Chase$(I_0, \Sigma_{URD})$ such that sim$_b$ is the identity and sim$_{(I,a)}$ maps to Chase$(I_0, \Sigma_{URD}) \setminus I_0$.

Further, for any $a \in \text{dom}(I) \setminus \text{dom}(I_0)$, letting $R^a$ be the position where sim$_a$ was introduced in Chase$(I_0, \Sigma_{URD})$, we require that $a \in \Pi^R(I)$.

Before we perform the completion process that allows us to satisfy $\Sigma_{URD}$, we need to perform a saturation process, like relation-saturation in the previous section. Instead of achieving all relations, we want the aligned superinstance to achieve all fact classes:

**Definition V.4.** A fact class is a pair $(R^a, C)$ of a position $R^a \in \text{Pos}(\sigma)$ and a $\Sigma$-tuple of $\Sigma_k$-classes of elements of Chase$(I_0, \Sigma_{URD})$. The dependency on $k$ is omitted for brevity.

The fact class of a fact $F = R(a)$ of Chase$(I_0, \Sigma_{URD}) \setminus I_0$ is $(R^a, C)$, where $a_p$ is the exported element of $F$ and $C_i$ is the $\Sigma_k$-class of $a_i$ in Chase$(I_0, \Sigma_{URD})$ for all $R^i \in \text{Pos}(R)$.

A fact class $(R^a, C)$ is achieved if it is the fact class of some fact of Chase$(I_0, \Sigma_{URD}) \setminus I_0$. We write $\text{AFactCl}$ for the set of all achieved fact classes (for brevity, the dependence on $I_0, \Sigma_{URD}$, and $k$ is omitted from notation).

An aligned superinstance $J = (I, \text{sim})$ is fact-saturated if, for any achieved fact class $D = (R^a, C)$ in $\text{AFactCl}$, there is a fact $I_D = R(a)$ of $I \setminus I_0$ such that sim$_{(I,a)} \in C_i$ for all $R^i \in \text{Pos}(R)$. We say $I_D$ achieves $D$ in $J$.

**Lemma V.5.** For any initial instance $I_0$, set $\Sigma_{URD}$ of UIDs, and $k \in \mathbb{N}$, $\text{AFactCl}$ is finite.

We now define our saturation process: chase $I_0$ until all fact classes are achieved, which is possible in finitely many rounds thanks to the above lemma. The result is easily seen to be a fact-saturated aligned superinstance:

**Lemma V.6** (Fact-saturated solutions). The result $I$ of performing sufficiently many chase rounds on $I_0$ is such that $I_0 = (I, \text{id})$ is a fact-saturated aligned superinstance of $I_0$.

We thus obtain a fact-saturated aligned superinstance $J_0$ of $I_0$, which we now want to complete to one that satisfies $\Sigma_{URD}$.

B. Fact-thrifty completion

Our general method to repair UID violations in $J_0$ is to apply a form of chase step on aligned superinstances, which may reuse elements: thrifty chase steps. To define them, we first distinguish dangerous and non-dangerous positions, which determine how we may reuse elements when chasing.

**Definition V.7.** We say a position $S' \in \text{Pos}(\sigma)$ is dangerous for a position $S' \neq S'$ if $S' \rightarrow S'$ is in $\Sigma_{URD}$, and write $S' \in \text{Dng}(S')$. Otherwise, $S'$ is non-dangerous, written $S' \in \text{Ndg}(S')$. Note that $\{S'\} \cup \text{Dng}(S') \cup \text{Ndg}(S') = \text{Pos}(S)$.

**Definition V.8 (Thrifty chase steps).** Let $J = (I, \text{sim})$ be an aligned superinstance of $I_0$, let $\tau: R^a \subseteq S'$ be a UID of $\Sigma_{URD}$, and let $F_a = R(a)$ be an active fact for $\tau$ in $I$. 

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Because sim is a 1-bounded simulation, sim(a_p) \in \pi_\text{r}\text{p}(\text{Chase}(I_0, \Sigma_{\text{UID}})), so, because the chase satisfies \tau, there is a fact \(F_0 = S(b'_0)\) in Chase\((I_0, \Sigma_{\text{UID}})\) with \(b'_0 = \text{sim}(a_p)\); we call \(F_0\) the chase witness.

Applying a thrifty chase step on \(F_0\) for \(\tau\) yields an aligned superinstance \(J' = (I', \text{sim})\). We define \(I'\) as \(I\) plus a new fact \(F_0 = S(b'_0)\), where \(b_0 = a_p\), and the \(b_i\) for \(S' \neq S\) may be elements of dom(\(I\)) or fresh elements. We require that:

1. for \(S' \in \text{NDng}(S')\), \(b_i \in \pi_\text{r}\text{p}(J)\) (so they are not fresh)
2. for \(S' \in \text{Dng}(S')\), \(b_i \notin \pi_\text{r}\text{p}(J)\) (so they may be fresh)
3. for \(S' \neq S\), if \(b_i\) is not fresh then \(\text{sim}(b_i) \simeq_k b'_i\).

We define \(\text{sim}'\) by extending sim to dom(\(J'\)) : we set \(\text{sim}'(b_i) := b'_i\) whenever \(b_i\) is fresh.

A fact-thrifty chase step is a thrifty chase step where we choose one fact \(F_i = S(c_i)\) of \(J \setminus I_0\) that achieves the fact class of \(F_0\) (that is, \(\text{sim}(c_i) \simeq_k b'_i\) for all \(i\)), and use \(F_i\) to define \(b_i := c_i\), for all \(S' \in \text{NDng}(S')\).

The chase step is fresh if \(b_i\) is fresh for all \(S' \in \text{Dng}(S')\).

Thrifty chase steps may in general violate \(\Sigma_{\text{UID}}\), but fact-thrifty chase steps never do. For this reason, we will only use fact-thrifty chase steps in this section. The point of working with fact-saturated aligned superinstances is that we can ensure that a suitable \(F_0\) always exists. We thus claim:

**Lemma V.9 (Fact-thrifty chase steps).** For any fact-saturated aligned superinstance \(J\), the result \(J'\) of a fact-thrifty chase step on \(J\) is indeed a well-defined aligned superinstance where the former active fact \(F_0\) is no longer active.

We now claim that we can expand fact-saturated superinstances to satisfy \(\Sigma_{\text{UID}}\), using fact-thrifty chase steps:

**Proposition V.10 (Fact-thrifty completion).** Under assumption reversible, for any fact-saturated aligned superinstance \(J\) of \(I_0\), we can expand \(J\) by fact-thrifty chase steps to a fact-saturated aligned superinstance \(J'\) of \(I_0\) that satisfies \(\Sigma_{\text{UID}}\).

This proposition allows us to prove the Acyclic Unary Universal Models Theorem (Theorem III.6) under assumption reversible. Indeed, consider the fact-saturated aligned superinstance \(J_0\) produced by the Fact-Saturated Solutions Lemma (Lemma V.6). Applying the Fact-Thrifty Completion Proposition to \(J_0\) yields a fact-saturated aligned superinstance \(J^*\), which is a finite \(k\)-sound superinstance of \(I_0\) that satisfies \(\Sigma_{\text{UID}}\) and satisfies \(\Sigma_{\text{UID}}\).

The rest of this section sketches the proof of the Proposition. The idea is to construct, as in Section IV, a balanced pssinstance \(P\) of the input aligned superinstance \(J\), and a \(\Sigma_{\text{r}}\)-compliant piecewise realization \(PI\) of \(P\). Now, instead of completing the facts of \(PI\) to add them directly to \(J\), we add them one by one, using fact-thrifty chase steps, to ensure that alignedness is preserved.

The only problematic point is that \(PI\) could connect together elements that have dissimilar sim-images, violating alignedness. However, we show that, up to chasing for \(k + 1\) rounds on the initial \(J\) with fresh fact-thrifty chase steps before constructing \(P\), we can ensure what we call \(k\)-reversibility: all elements that want to be at some position \(R^p\) in \(J\) have a sim-image whose \(\simeq_k\)-class only depends on \(R^p\). Once we have ensured this, we can essentially stop worrying about sim-images, because respecting weak-soundness, as \(PI\) does, is sufficient.

The reason why \(k + 1\) chasing rounds suffice to ensure this is by a general structural observation on the UID chase: when the last \(k\) UIDs applied to an element \(a\) of Chase\((I_0, \Sigma_{\text{UID}})\) are reversible (as is the case here, by assumption reversible), the \(\simeq_k\)-class of \(a\) only depends on the \(\simeq_{\text{UID}}\)-class of the position where it was introduced, and not on its exact history. Formally:

**Theorem V.11** (Chase locality theorem). For any instance \(I_0\), transitively closed set of UIDs \(\Sigma_{\text{UID}}\), and \(n \in \mathbb{N}\), for any two elements \(a\) and \(b\) respectively introduced at positions \(R^p\) and \(S^i\) in Chase\((I_0, \Sigma_{\text{UID}})\) such that \(R^p \simeq_{\text{UID}} S^i\), if the last \(n\) UIDs applied to create \(a\) and \(b\) are reversible, then \(a \simeq_{\text{n}} b\).

VI. ARBITRARY UIDS: LIFTING ASSUMPTION REVERSIBLE

This section concludes the proof of the Acyclic Unary Universal Models Theorem (Theorem III.6) by removing assumption reversibility. We do so by splitting \(\Sigma_{\text{UID}}\) in subsets that can be satisfied sequentially:

**Definition VI.1.** For any \(\tau, \tau' \in \Sigma_{\text{UID}}\), we write \(\tau \rightarrow \tau'\) when we can write \(\tau = R^p \subseteq S^i\) and \(\tau' = S^i \subseteq T^j\) with \(S^i \neq T^j\), and the UFD \(S^i \rightarrow S_j\) is in \(\Sigma_{\text{UID}}\). An ordered partition \((P_1, \ldots, P_n)\) of \(\Sigma_{\text{UID}}\) is a partition of \(\Sigma_{\text{UID}}\) (i.e., \(\Sigma_{\text{UID}} = \bigsqcup \Pi_{i} P_i\)) such that for any \(\tau \in P_i\), \(\tau' \in P_j\), if \(\tau \rightarrow \tau'\) then \(i \leq j\).

The notion of ordered partition is useful because thrifty chase steps can only cause new UID violations at the dangerous positions of the new fact. This implies the following:

**Lemma VI.2.** Let \(I\) be an aligned superinstance of \(I_0\) and \(J\) be the result of applying a thrifty chase step on \(I\) for a UID \(\tau\) of \(\Sigma_{\text{UID}}\). Assume that a UID \(\tau'\) of \(\Sigma_{\text{UID}}\) was satisfied by \(J\) but is not satisfied by \(J'\). Then \(\tau \rightarrow \tau'\).

Hence, given an ordered partition of \(\Sigma_{\text{UID}}\), once we have satisfied the UIDs of the first \(i\) classes \(P_1, \ldots, P_i\), then this property is preserved while we do thrifty chasing with \(P_j\), \(j > i\). So if we can satisfy each \(P_i\) individually with thrifty chase steps, then we can satisfy \(\Sigma_{\text{UID}}\) by satisfying \(P_1, \ldots, P_n\).

Of course, the point of partitioning \(\Sigma_{\text{UID}}\) is to be able to control the structure of the UIDs in each class:

**Definition VI.3.** We call \(P \subseteq \Sigma_{\text{UID}}\) reversible if it is transitively closed (as \(\Sigma_{\text{UID}}\) is) and satisfies assumption reversible.

We say \(P \subseteq \Sigma_{\text{UID}}\) is trivial if we have \(P = \{\tau\}\) for some \(\tau \in \Sigma_{\text{UID}}\) such that \(\tau \not\rightarrow \tau\). An ordered partition is manageable if all of its classes are either reversible or trivial.

If \(P \subseteq \Sigma_{\text{UID}}\) is reversible, then the previous section describes how to complete with thrifty chase steps any fact-saturated aligned superinstance of \(I_0\) to one that satisfies \(P\). If \(P\) is trivial, it follows directly from Lemma VI.2 that we can satisfy it.

**Corollary VI.4.** For any trivial class \(\{\tau\}\), performing one chase round on an aligned fact-saturated superinstance \(J\)
of \( I_0 \) by fresh fact-thrifty chase steps for \( \tau \) yields an aligned superinstance \( J' \) of \( I_0 \) that satisfies \( \tau \).

We now claim that we can construct a manageable partition of \( \Sigma_{UID} \). We build it as a topological sort of the strongly connected components (SCCs) of the directed graph on \( \Sigma_{UID} \) defined by \( \rightarrow \), with the technical complication that SCCs must be closed under UID reversal. The construction relies on the fact that \( \Sigma_{UID} \) is closed under finite implication, as characterized by Cosmadakis et al. [5].

**Lemma VI.5.** Any conjunction \( \Sigma_{UID} \) of UIDs closed under finite implication has a manageable partition.

**Example VI.6.** Consider the UIDs \( \tau_R : R^1 \subseteq R^2 \), \( \tau_S : S^1 \subseteq S^2 \), \( \tau : R^2 \subseteq S^3 \), and the UFDs \( \phi_R : R^1 \rightarrow R^2 \), \( \phi_S : S^1 \rightarrow S^2 \), \( \phi_0 : R^1 \rightarrow R^3 \), and \( \phi_1 : S^1 \rightarrow S^3 \). The UIDs \( \tau_R^{-1} \) and \( \tau_S^{-1} \), and UFDs \( \phi_R^{-1} \), \( \phi_S^{-1} \), and \( R^2 \rightarrow R^3 \), \( S^2 \rightarrow S^3 \), are finitely implied. A manageable partition is \( \{ \{ \tau_R, \tau_R^{-1} \}, \{ \tau_S, \tau_S^{-1} \} \} \), where the first and third classes are reversible and the second is trivial.

We can now conclude the proof of the Acyclic Unary Universal Models Theorem (Theorem III.6). We first note that the Fact-Saturated Solutions Lemma (Lemma VI.6) does not use assumption reversible, so we apply it (with \( \Sigma_{UID} \)) to obtain from \( I_0 \) an aligned fact-saturated superinstance \( J_1 \) of \( I_0 \). This is the saturation process.

We now satisfy \( \Sigma_{UID} \) by a completion process. Build a manageable partition \( (P_1, \ldots, P_n) \) of \( \Sigma_{UID} \), by Lemma VI.5. Now, for \( 1 \leq i \leq n \), use fact-thrifty chase steps by UIDs of \( P_i \) to extend the fact-saturated aligned superinstance \( J_i \) to a larger one \( J_{i+1} \) that satisfies \( P_i \). If \( P_i \) is trivial, use Corollary VI.4. If \( P_i \) is reversible, apply the Fact-Thrifty Completion Proposition (Proposition VI.10), taking \( \Sigma_{UID} \) to be \( P_i \). By Lemma VI.2, the result \( J_{i+1} \) satisfies \( \bigcup_{1 \leq i \leq n} P_i \).

Hence the result \( J_{n+1} \) of the completion process is an aligned superinstance of \( I_0 \) that satisfies \( \Sigma_{UID} \); as an aligned superinstance, it is also finite, satisfies \( \Sigma_{UFD} \), and is \( k \)-sound for \( ACQ \); so it is \( k \)-universal for \( \Sigma_{UFD} \) and \( ACQ \). This concludes the proof of the Acyclic Unary Universal Models Theorem.

**VII. Higher-Arity FDs**

We now bootstrap the Acyclic Unary Universal Models Theorem (Theorem III.6) to the Universal Models Theorem (Theorem III.5). The first step is to change our construction to avoid violating higher-arity FDs, namely, show the following, which applies to \( \Sigma = \Sigma_{UID} \land \Sigma_{FD} \) rather than \( \Sigma = \Sigma_{UID} \land \Sigma_{UFD} \):

**Theorem VII.1** (Acyclic universal models). There is a finite superinstance of \( I_0 \) that is \( k \)-universal for \( \Sigma \) and \( ACQ \) queries.

The problem to address is that our completion process to satisfy \( \Sigma_{UID} \) was defined with fact-thrifty chase steps, which reuse elements from the same facts at the same positions multiple times. This may violate \( \Sigma_{FD} \), and we can show that is the only point where we do so in the construction.

The goal of this section is to define a new version of thrifty chase steps that preserves \( \Sigma_{FD} \), rather than just \( \Sigma_{UFD} \); we call them envelope-thrifty chase steps. We first describe the new saturation process designed for them. Second, we define how they work, redefine the completion process of the previous section to use them, and use this new completion process to prove the Acyclic Universal Models Theorem above.

**A. Envelopes and saturation**

We start by defining a new notion of saturated instances. Recall the notions of fact classes (Definition V.4) and thrifty chase steps (Definition V.8). When a thrifty chase step wants to create a fact \( F_n \) whose chase witness \( F_n \) has fact class \( (R^0, C) \), it needs elements to reuse in \( F_n \) at positions of \( NDng(R^0) \). They must have the right sim-image and must already occur at the positions where they are reused.

Fact-thrifty chase steps reuse a tuple of elements from one fact \( F_i \), and thus apply to fact-saturated instances with one fact for each class. Our new notion of envelope-thrifty chase steps will need saturated instances that have multiple reusable tuples. A set of such tuples is called an envelope for \( (R^0, C) \):

**Definition VII.2.** Consider \( D = (R^0, C) \) in AFactCl, and write \( O := NDng(R^0) \). An envelope \( E \) for \( D \) and for an aligned superinstance \( J = (I, \sim) \) of \( I_0 \) is a non-empty set of \(|O|\) tuples indexed by \( O \), with domain \( \text{dom}(I) \), such that:

- for every FD \( \phi : R^k \rightarrow R^j \) of \( \Sigma_{FD} \) with \( R^k \subseteq O \) and \( R^j \in O \), \( E \) satisfies \( \phi \) (seeing its tuples as facts on \( O \));
- for every FD \( \phi : R^k \rightarrow R^j \) of \( \Sigma_{FD} \) with \( R^k \subseteq O \) and \( R^j \notin O \), for all \( t, t' \in E \), \( \pi_R(t) = \pi_R(t') \) implies \( t = t' \);
- for every \( a \in \text{dom}(E) \), there is exactly one position \( R^j \) in \( O \) such that \( a \in \pi_R(E) \); and then we also have \( a \in \pi_R(J) \);
- if any fact \( F = \mathcal{R}(a) \) of \( J \) and \( R^j \in O \), if \( a_q \in \pi_R(E) \), then \( F \) achieves \( D \) in \( J \) and \( \pi_R(a) \in E \).

Intuitively, the tuples in the envelope \( E \) satisfy the UFDs of \( \Sigma_{UFD} \) within NDng(\( R^0 \)), and never overlap on positions that determine a position out of NDng(\( R^0 \)). Further, their elements already occur at the positions where they will be reused, and have the right sim-image for the fact class \( D \). To simplify the reasoning, we also impose that each element of \( E \) is used at only one position, and occurs at that position only in facts which achieve \( D \) and whose projection to NDng(\( R^0 \)) is in \( E \).

Depending on \( O \), it may be possible to use a singleton tuple as the envelope, like fact-thrifty chase steps, and not violate \( \Sigma_{FD} \). The class is then safe. Otherwise, we focus on the envelope tuples which do not appear in the instance yet.

**Definition VII.3.** We call \( (R^0, C) \) in AFactCl safe if there is no FD \( R^k \rightarrow R^j \) in \( \Sigma_{FD} \) with \( R^k \subseteq NDng(R^0) \) and \( R^j \notin NDng(R^0) \).

Letting \( E \) be an envelope for \( (R^0, C) \) and \( J \) be an aligned superinstance, the remaining tuples of \( E \) are \( E \setminus \pi_{NDng(R^0)}(J) \) if \( (R^0, C) \) is unsafe, and \( E \) if it is safe.

We now introduce the notion of global envelopes, that give us one envelope per class of AFactCl. This leads to our new notion of saturation: a saturated instance has a global envelope with many remaining tuples in the unsafe classes. Note that this implies fact-saturation.

**Definition VII.4.** A global envelope \( E \) for an aligned superinstance \( J = (I, \sim) \) of \( I_0 \) is a mapping from each \( D \in \text{AFactCl} \)
to an envelope \( E(D) \) for \( D \) and \( J \), such that the envelopes have pairwise disjoint domains.

We call \( J \) a \textit{n-envelope-saturated} if it has a global envelope \( E \) such that \( E(D) \) has \( n \) remaining tuples for all unsafe \( D \in \text{AFactCl} \). \( J \) is \textit{envelope-saturated} if it is \( n \)-envelope-saturated for \( n > 0 \), and \textit{envelope-exhausted} otherwise.

We now justify that we can make arbitrarily saturated superinstances of \( I_0 \) (the switch to \( I_0' \) is a technicality):

**Proposition VII.5** (Sufficiently envelope-saturated solutions). For any \( K \in \mathbb{N} \) and instance \( I_0 \), we can build a superinstance \( I_0' \) of \( I_0 \) that is \( k \)-sound for CQ, and an aligned superinstance \( J \) of \( I_0' \) that satisfies \( \Sigma_{\text{FD}} \) and is \((K|J|)-envelope-saturated.

**Example VII.6.** For simplicity, we work with instances rather than aligned superinstances. Consider \( I_0 := \{S(a), T(z)\} \), the UIDs \( \tau : S \subseteq R^1 \) and \( \tau' : T \subseteq R^1 \) for a 3-ary relation \( R \), and the FD \( \phi : R^2 \rightarrow R^3 \). Consider \( I := I_0 \cup \{R(a,b,c)\} \) obtained by one chase step of \( \tau \) on \( S(a) \). It would violate \( \phi \) to perform a fact-thrifty chase step of \( \tau' \) on \( z \) to create \( R(z,b,c) \), reusing \( (b,c) \) at \( \text{NDng}(R^3) = \{R^2 \cdot R^3\} \).

Now, consider the \( k \)-sound \( I_0' := \{S(a), T(z), S(a'), S(z')\} \), and \( I' := I_0' \cup \{R(a,b,c), R(a',b',c')\} \) obtained by two chase steps. The two facts \( R(a,b,c) \) and \( R(a',b',c') \) would be mapped to the same fact class \( D \), so we can define \( E(D) := \{(b,c), (b',c'), (b',c), (b,c)\} \). We can now satisfy \( \Sigma_{\text{FD}} \) on \( I' \) without violating \( \phi \) with two envelope-thrifty chase steps that reuse the remaining tuples \((b',c)\) and \((b,c)\) of \( E(D) \).

The crucial result needed for the Sufficiently Envelope-Saturated Proposition is the following, which may be of independent interest, and is proved using a combinatorial construction. The fact that unary keys are problematic is the reason why we handle classes differently.

**Theorem VII.7** (Dense interpretations). For any set \( \Sigma_{\text{FD}} \) of FDs over a relation \( R \) with no unary key, and \( K \in \mathbb{N} \), there exists a non-empty instance \( I \) of \( R \) that satisfies \( \Sigma_{\text{FD}} \) and has at least \( K \cdot |\text{dom}(I)| \) facts.

Hence, we have defined the new notion of \( n \)-envelope-saturation, and a saturation process to achieve it: the Sufficiently Envelope-Saturated Solutions Proposition. Unlike the Fact-Saturated Solutions Lemma, where one fact of each class was enough, we have shown that envelope-saturated superinstances may have an arbitrarily high saturation relative to the instance size.

**B. Envelope-thrifty chase steps**

We can now introduce envelope-thrifty chase steps:

**Definition VII.8.** Envelope-thrifty chase steps are thrifty chase steps (Definition V.8) applicable to envelope-saturated aligned superinstances. Let \( S' \) be the exported position of the new fact \( F_w \) let \( F_w = S(b') \) be the chase witness, and let \( D = (S',C) \in \text{AFactCl} \) be the fact class of \( F_w \). We choose some remaining tuple \( t \) of \( E(D) \) and define \( b_r := t_r \) for all \( S' \in \text{NDng}(S') \).

Recall from Lemma V.9 that fact-thrifty chase steps apply to fact-saturated aligned superinstances, and never violate \( \Sigma_{\text{UFD}} \). Similarly, envelope-thrifty chase steps apply to envelope-saturated aligned superinstances, and never violate \( \Sigma_{\text{FD}} \):

**Lemma VII.9.** For \( n > 0 \), for any \( n \)-envelope-saturated aligned superinstance \( J \) that satisfies \( \Sigma_{\text{FD}} \), the result \( J' \) of an envelope-thrifty chase step on \( J \) is an \((n-1)\)-envelope-saturated superinstance that satisfies \( \Sigma_{\text{FD}} \).

We now modify the Fact-Thrifty Completion Proposition (Proposition V.10), generalized without assumption reversible as in the previous section, to use envelope-thrifty chase steps instead of fact-thrifty chase steps. This is possible because the choice of reused elements at non-dangerous positions makes no difference in terms of applicable UIDs, as they already occur at the position where they are reused. Hence, we can perform the exact same process as before (except the non-dangerous reuses), using Lemma VII.9 to justify that \( \Sigma_{\text{FD}} \) is preserved; but we must abort if we reach an envelope-exhausted instance:

**Proposition VII.10** (Envelope-thrifty completion). For any envelope-saturated-aligned superinstance \( J \) of \( I_0 \) that satisfies \( \Sigma_{\text{FD}} \), we can obtain by envelope-thrifty chase steps an aligned superinstance \( J' \) of \( I_0 \), such that \( J' \) is either envelope-exhausted or satisfies \( \Sigma \).

The last problem to address is exhaustion. Unlike fact-saturation, envelope-saturation “runs out”; whenever we use a remaining tuple \( t \) in a chase step to create \( F_s \) and obtain a new aligned superinstance \( J' \), then we cannot use \( t \) again in \( J' \). So we must start with a sufficiently envelope-saturated superinstance, and we must control how many chase steps are applied in the envelope-thrifty completion process. From the details of our construction, we can show the following:

**Lemma VII.11** (Envelope blowup). There exists \( B \in \mathbb{N} \) depending only on \( k \) and \( \Sigma \) such that, for any aligned superinstance \( J' = (I', \text{sim}') \) of some \( k \)-sound \( I'_0 \) such that \( J \) satisfies \( \Sigma_{\text{FD}} \) and is \((B|I|)-envelope-saturated. Now, apply the Envelope-Thrifty Completion Proposition to obtain an aligned superinstance \( J' \) of \( I_0 \). By the Envelope Blowup Lemma, \( J' \) contains \((B|I|) \) new facts, so, by Lemma VII.9, \( J' \) must still be 1-envelope-saturated. Hence, \( J' \) satisfies \( \Sigma \). This concludes the proof, as \( J' \) is an aligned superinstance of \( I_0 \).

**VIII. CYCLIC QUERIES**

We now finally complete our proof of the Universal Models Theorem (Theorem III.5) by moving from acyclic Boolean CQs to arbitrary Boolean CQs. We do so by a generic process which is essentially independent from our previous construction.
Intuitively, the only cyclic CQs that hold in \( \text{Chase}(I_0, \Sigma_{\text{UID}}) \) either have an acyclic self-homomorphic match (so they are implied by an acyclic CQ that also holds) or have all cycles matched to elements of \( I_0 \). Hence, in a k-sound instance for CQ, no other cyclic queries must be true. We ensure this by a cycle blowup process that takes the product of our \( I \) with a group of high girth, following Otto [11]. However, we need to adjust this construction to avoid creating FD violations.

We let \( I_1 = (I, \text{sim}) \) be the aligned superinstance obtained from the Acyclic Universal Models Theorem (Theorem VII.1). Its underlying instance \( I_1 \) is a finite superinstance of \( I_0 \) that satisfies \( \Sigma \), and the k-bounded simulation sim guarantees that \( I_1 \) is k-sound for ACQ. Our goal in this section is to make \( I_1 \) k-sound for CQ while still satisfying \( \Sigma \), so that it is k-universal. This will conclude the proof of the Universal Models Theorem (Theorem III.5).

A. Simple product

Let us first introduce preliminary notions:

**Definition VIII.1.** A group \( G = (S, \cdot) \) over a finite set \( S \) consists of an associate product law \( \cdot : S^2 \to S \), a neutral element \( e \in S \), and an inverse law \( \cdot^{-1} : S \to S \) such that \( x \cdot x^{-1} = x^{-1} \cdot x = e \) for all \( x \in S \). We say that \( G \) is generated by \( X \subseteq S \) if all elements of \( S \) can be written as a product of elements of \( X \) and \( X^{-1} := \{ x^{-1} : x \in X \} \).

Given a group \( G \) generated by \( X \), the girth of \( G \) under \( X \) is the length of the shortest non-empty word \( w \) of elements of \( X \) and \( X^{-1} \) such that \( w_1 \cdots w_n = e \) and \( w_i \neq w_i^{-1} \) for all \( 1 \leq i < n \). (If \( X = \{ g \} \) with \( g = g^{-1} \), the girth is 1.)

**Lemma VIII.2 (9)).** For all \( n \in \mathbb{N} \) and finite non-empty set \( X \), there is a finite group \( G = (S, \cdot) \) generated by \( X \) with girth \( \geq n \) under \( X \). We call \( G \) an \( n \)-acyclic group generated by \( X \).

In other words, in an \( n \)-acyclic group generated by \( X \), there is no short product of elements of \( X \) and their inverses which evaluates to \( e \), except those that include a factor \( x^{-1} \).

We now take the product of \( I_1 \) with such a finite group \( G \). This ensures that any cycles in the product instance are large, because they project to cycles in \( G \). We use a specific generator:

**Definition VIII.3.** The fact labels of a superinstance \( I_0 \) are \( \Lambda(I) := \{ [f]_0 \mid F \in I_0, 1 \leq i \leq |F| \} \).

Now, we define the product of a superinstance \( I_0 \) with a group generated by \( \Lambda(I) \). We make sure not to blow up cycles in \( I_0 \), so the result remains a superinstance of \( I_0 \):

**Definition VIII.4.** Let \( I \) be a finite superinstance of \( I_0 \) and \( G \) be a finite group generated by \( \Lambda(I) \). The product of \( I \) by \( G \) preserving \( I_0 \) is the finite instance \( (I, I_0) \otimes G \) with domain \( \text{dom}(I) \times G \) consisting of the following facts, for all \( g \in G \):

- For every fact \( R(a) \) of \( I_0 \), the fact \( R((a_1, g), \ldots, (a_r, g)) \).
- For every fact \( F = R(a) \) of \( I_0 \), the following fact:
  \[ R((a_1, g), \ldots, (a_r, g), [F]_0) \]

We identify \( (a, e) \) to \( a \) for \( a \in \text{dom}(I_0) \), so \( (I, I_0) \otimes G \) is still a superinstance of \( I_0 \).

We say a superinstance \( I \) of \( I_0 \) is \( k \)-instance-sound (for \( k \)) if for any CQ \( q \) such that \( |q| \leq k \), if \( q \) has a match in \( I \) involving an element of \( I_0 \), then \( \text{Chase}(I_0, \Sigma_{\text{UID}}) \models q \). We can ensure that \( I_1 \) is \( k \)-instance-sound, up to having performed \( k \) chase rounds on \( I_0 \) initially. We can then state the following property:

**Lemma VIII.5** (Simple product). Let \( I \) be a finite superinstance of \( I_0 \) and \( G \) a finite \( (2k+1) \)-acyclic group generated by \( \Lambda(I) \). If \( I \) is \( k \)-sound for ACQ and \( k \)-instance-sound, then \( (I, I_0) \otimes G \) is \( k \)-sound for CQ.

**Example VIII.6.** Consider \( F_0 := R(a, b), I_0 := \{ F_0 \} \), and \( \Sigma_{\text{UID}} \) consisting of \( \tau : R^2 \subseteq S^1, \tau' : S^2 \subseteq R^1 \), and \( (\tau')^{-1} \). Let \( F := S(b, a), \) and \( I := I_0 \cup \{ F \} \). I satisfies \( \Sigma_{\text{UID}} \) and is sound for ACQ, but not for CQ: take for instance \( q : \exists y.R(x, y) \cup S(y, x) \), which is cyclic and holds in \( I \) while \( (I_0, \Sigma_{\text{UID}}) \models \lnot q \).

We have \( \Lambda(I) = \{ [1]^1, [2]^1 \} \). Identify \( [1]^1 \) and \( [2]^1 \) to 1 and 2 and consider the group \( G := \{ (0, 1, 2) \} \times \{ 2 \} \), which is addition modulo 3. \( G \) has girth 2 under \( \Lambda(I) \).

The product \( I_0 :=(I, I_0) \otimes G \), writing pairs as subscripts for brevity, is \( \{ R(a_0, b_0), R(a_1, b_1), R(a_2, b_2), S(b_1, a_2), S(b_2, a_0), S(b, a_3) \} \). In this case, \( I_0 \) happens to be 5-sound for CQ.

We cannot conclude directly with the simple product, because \( I_0 :=(I, I_0) \otimes G \) may violate \( \Sigma_{\text{FD}} \) even though \( I \mid \Sigma_{\text{FD}} \). Indeed, there may be a relation \( R, \) a UFDF \( \phi : R^p \to R^q \in \Sigma_{\text{FD}}, \) and two \( R \)-facts \( F \) and \( F' \) in \( I_0 \) with \( \pi_{R^p}(F) \neq \pi_{R^p}(F') \). In \( I_0 \), the images of \( F \) and \( F' \) may overlap only on \( R^p \), so they could violate \( \phi \).

B. Mixed product

What we need is a more refined notion of product, that does not attempt to blow up cycles within fact overlaps. To define it, we need to consider a quotient of \( I_0 \):

**Definition VIII.7.** The quotient \( I / \sim \) of an instance \( I \) by an equivalence relation \( \sim \) on \( \text{dom}(I) \) is defined as follows:

- \( \text{dom}(I / \sim) \) is the equivalence classes of \( \sim \) on \( \text{dom}(I) \).
- \( I / \sim \) contains one fact \( R(a) \) for every fact \( R(a) \) of \( I \) where \( A_i \) is the \( i \)-class of \( a_i \) for all \( R^i \in \text{Pos}(R) \).

The quotient homomorphism \( \chi_{\sim} \) is the homomorphism from \( I \) to \( I / \sim \) defined accordingly.

We quotient \( I_0 \) by the equivalence relation \( \sim_k \) (recall Definition V.1), yielding \( I'_0 = I_0 / \sim_k \). The resulting \( I'_0 \) may no longer satisfy \( \Sigma \). However, it is still k-sound for ACQ, for the following reason:

**Lemma VIII.8.** Any \( k \)-bounded simulation from an instance \( I \) to an instance \( I' \) defines a \( k \)-bounded simulation from \( I / \sim_k \) to \( I' \).

We then consider the homomorphism \( \chi_{\sim_k} \) from \( I_0 \) to \( I'_0 \), and blow up cycles in \( I_0 \) by a mixed product that only distinguishes facts with a different image in \( I'_0 \) by \( \chi_{\sim_k} \). The point is that, as we show from our construction, facts of \( I_0 \) that have the same elements at the same positions always have the same \( \sim_k \)-class. Hence, they are mapped to the same fact by \( \chi_{\sim_k} \) and will not be distinguished by the mixed product. Let us formalize this:
Definition VIII.9. Let $I$ be a superinstance of $I_0$ and $h$ be a homomorphism from $I$ to some instance $I'$. We say $I$ is cautious for $h$ if for any relation $R$, for any two $R$-facts $F$ and $F'$ such that $\pi_R(F) = \pi_R(F')$ for some $R^0 \in \text{Pos}(R)$, either $F, F' \in I_0$, or $h(F) = h(F')$.

Lemma VIII.10 (Cautiousness). The superinstance $I_1$ of $I_0$ constructed by the Acyclic Universal Models Theorem (Theorem VII.1) is cautious for $\chi_{\Sigma_1}$.

The reason why $I_1$ is cautious is that, except for facts of $I_0$, overlaps between facts only occur when reusing envelope elements at non-dangerous positions, in which case the sim-images of both facts are $\sim_{\Sigma}$-equivalent in $\text{Chase}(I_0, \Sigma_{\text{UID}})$.

We can then show that, from our construction, such elements are actually $\sim_{\Sigma}$-equivalent in $I_1$.

We now define the notion of mixed product, which uses the same fact label for facts of the same image by $h$.

Definition VIII.11. Let $I$ be a finite superinstance of $I_0$ with a homomorphism $h$ to another finite superinstance $I'$ of $I_0$ such that $h_{I_0}$ is the identity and $h_{I'}(I_0)$ maps to $I' \setminus I_0$. Let $G$ be a finite group generated by $\Lambda(I')$.

The mixed product of $I$ by $G$ via $h$ preserving $I_0$, written $(I, I_0) \circ^G h$, is the finite superinstance of $I_0$ with domain $\text{dom}(I) \times G$ consisting of the following facts, for every $g \in G$:

- For every fact $R(a)$ of $I_0$, the fact $R((a, g), \ldots, (a, g))$.
- For every fact $R(a)$ of $I' \setminus I_0$, the following fact:
  $R((a, g, h_{I_0}^{-1}(F)), \ldots, (a, g, h_{I_0}^{-1}(F)))$.

We now show that the mixed product preserves UID$s$ and FD$\text{e}s$ when cautiousness is assumed.

Lemma VIII.12 (Mixed product preservation). For any UID or FD $\tau$, if $I \models \tau$ and $I$ is cautious for $h$, then $(I, I_0) \circ^G h \models \tau$.

Second, we show that $h : I \rightarrow I'$ lifts to a homomorphism from the homomorphism $h$ to the simple product.

Lemma VIII.13 (Mixed product homomorphism). There is a homomorphism from $(I, I_0) \circ^G h$ to $(I', I_0) \circ G$ which is the identity on $I_0 \times G$.

We can now conclude our proof of the Universal Models Theorem (Theorem III.5). We construct $I_t = (I_t, \text{sim})$ by the Acyclic Universal Models Theorem (Theorem VII.1) and consider $I_0$. It is a finite superinstance of $I_0$ which is $k$-universal for $\Sigma$ and $\text{ACQ}$. Further, up to having distinguished the elements of $I_0$ with fresh predicates and having performed initial chasing, we can ensure that $I' := I_t \setminus I_0$ is $k$-instance-sound and that the homomorphism $\chi_{\Sigma_1} : I_t \rightarrow I'$ satisfies the hypotheses of the mixed product.

Let $G$ be a $(2k + 1)$-acyclic group generated by $\Lambda(I'_t)$, and consider $I_p := (I'_t, I_0) \circ G$. As $I_t$ was $k$-sound for $\text{ACQ}$, so is $I'_t$ by Lemma VIII.8, and as $I'_t$ is also $k$-instance-sound, $I_p$ is $k$-sound for $\text{CQ}$ by the Simple Product Lemma (Lemma VIII.5). However, as we explained, in general $I_p \not\models \Sigma$. We thus construct $I_\text{m} := (I_t, I_0) \circ^G h$, with $h := \chi_{\Sigma_1}$. By the Mixed Product Homomorphism Lemma, $I_\text{m}$ has a homomorphism to $I_0$, so it is also $k$-sound for $\text{CQ}$. Further, $I_t$ is cautious for $\chi_{\Sigma_1}$ by the Cautiousness Lemma, so, by the Mixed Product Preservation Lemma, we have $I_\text{m} \models \Sigma$ because $I_t \models \Sigma$.

Hence, the mixed product $I_\text{m}$ is a finite $k$-universal instance for $\Sigma$ and $\text{CQ}$. This concludes the proof of the Universal Models Theorem, and hence of our main theorem (Theorem III.2).

IX. Conclusion

In this work we have developed the first techniques on arbitrary arity schemas to build finite models that satisfy both referential constraints and number restrictions, while controlling which CQs are satisfied. We have used this to prove that finite open-world query answering for CQs, UID$s$ and FD$\text{e}s$ is finitely controllable up to finite closure of the dependencies. Using this, we have isolated the complexity of FQA for UID$s$ and FD$\text{e}s$.

As presented the constructions are quite specific to dependencies, but in future work we will look to extend them to constraint languages containing disjunction, with the goal of generalizing to higher arity the rich arity-2 constraint languages of, e.g., [7], [12], while maintaining the decidability of finite open-world query answering.

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