Equivalences of Schema Mappings

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Abstract

The majority of computer science areas nowadays deal extensively with different forms of finite relational structures, usually with some form of constraints attached. In the databases domain, we can view the usual relations (tables) as structures , being constrained by dependencies, which impose relationships on the data that can appear in instances. In graph theory, we can view graphs as structures, and the constraints can generate the problems that concern us, for example k-coloring. In this project, we will try to formalize precisely the relational structures and constraints. We will cover a very researched class of constraints, namely tuple-generating dependencies, examining their behavior with respect to database instances. We will also examine how we can decide equivalence of schemas, by imposing conditions on the form of the dependencies.

Acknowledgements

Many thanks to my supervisor Michael Benedikt for coming up with the idea of the project, for all the help and advice provided, and for constantly bringing up new ideas and methods to solve the problems at hand. His papers and lecture notes constituted the basis for the work of this project, and his weekly meeting notes proved to be essential in progressing with the contributions.

Contents

1. Introduction

Schema mappings are high-level specifications that describe how to map information from a source schema to a target schema. They are a crucial building block in several areas of database research, including data exchange[4] (where we start with data structured under a source schema and we aim to create a target schema that best reflects the input data) and data integration[5] (where we provide a unified view of all the data from different sources).

1.1. Motivation

In order to describe the relationship between source and target schemas, we use sets of constraints. Naturally, there has been a lot of research on manipulating schema mappings (with operations such as inverse and composition), but this project is focused on the optimization aspect. This consists of the removal of redundant constraints, an operation which can speed up drastically the computation of our target instances.

Example 1: Starting with source database $D_0 = \{R(1,2)\}$ and constraints

$C = \{ R(x,y) \rightarrow S(y,x), S(x,y) \rightarrow R(y,x) \}$, we would obtain the target instance $D_0 \cup \{S(2,1)\}$, but we can see that the second constraint in C does not bring any contribution to this, so we can get rid of it.

Using this optimization procedure, we ultimately want to tell if schemas are equivalent (different notions of equivalence will be discussed later). If we possess a repository of schemas which already have some established equivalences between them, this makes querying them more efficient. Consequently, it is important to test any new equivalences that would appear from updating this repository.

1.2. Contributions

The main goal of this project is to prove decidability of redundancy testing for particular (and very used in the literature) classes of constraints. This will be done using automata over trees that encode the source instances. Where this decidability has already been proven, our aim is to obtain a better time/memory complexity. In the cases where undecidability has been established, we wish to restrict the class of constraints until the

problem becomes decidable. Another important goal is to study the behavior of different forms of schema mapping equivalences and how they are related, depending on the source instances.

1.3. Challenges

The first parts of this project involved getting familiar with the already existing related work, most of it treating similar problems with very different approaches. A crucial concept throughout the project will be the chase procedure, which has been defined in many places and in various ways, therefore trying to encode its structure using graph theory and automata was a big stepping stone. Another challenge arose from the introduction of two new types of equivalences between schemas and our attempt to fit them in the already existing picture of schema equivalences.

1.4. Structure of the Report

The rest of the report is structured as follows: an introduction of the notations and concepts that will be constantly used throughout the project is presented in Section 2. In Section 3 we describe the tree model for our structures, and automata that can accept this model as input. In Section 4, we present the relationship between different forms of equivalences for schema mappings into detail. Finally, in Section 5, we present the conclusions, limitations and future directions for this project.

2. Preliminaries

2.1. Relational Database Schema

A *relational schema* Sch consists of a set of distinct relation definitions $(R_1, R_2, ..., R_n)$, each with an associated "arity". A *relation definition* (also called *table*) consists of its relation name R_i and a collection of attribute names paired with their types
$(A_1 : type_1, ..., A_n : type_n)$. Since the type of the attributes is not impactful for this project, and for simplicity of definitions, we will mostly use integer types.
A *tuple* (also called *fact*) for a given relation definition R_i is a function that assigns to each attribute A_i one value from the domain given by its type.
A *primary key* for a table R_i is a set of attributes that uniquely determines a tuple in any relation instance (each attribute in the primary key will be underlined).
A *database instance* I over a schema Sch consists of one relation instance I(R_i) for each relation definition R_i. A *relation instance* for R_i is a set of tuples for R_i such that no two tuples agree on all the attributes from the primary key of the table.
Example 2: Schema Sch contains information about a work environment, with one table *EmployeeInfo(EmployeeID, Name, Job, Salary)* and one table for structural organization *WorksFor(EmployeeID, BossID)*. The presented database instance only consists of a relation instance for *EmployeeInfo* and has three tuples, with primary key {EmployeeID}.

EmployeeID	Name	Job	Salary
81	Gilbert Marshall	Reporter	40000
209	Jane Hunt	Lawyer	45000
333	Neville Barton	Lawyer	40000

2.2. First-order Logic

Throughout the project we will mostly use *function-free first-order logic* for describing our relation instances, constraints and queries. A *signature* (also called *vocabulary*) for this logic consists of a finite collection of constant symbols and a finite collection of *relations* (also called *predicates*), each having a given *arity*. We can therefore view a relational

schema as a signature, and we will use both terms interchangeably.

Syntax : A first-order formula is built from *atomic formulas*, which can either be *relational atoms* $\mathrm{R}(\vec{t})$, where R is a relation and $\vec{t}$ consists of *terms* (constants or variables), or an equality between two terms. From this, we build formulas inductively using boolean operators $(\wedge, \vee, \neg)$ and quantifiers $(\forall, \exists)$.

$$\varphi \ ::= \ R(\vec{t}) \mid t_i = t_j \mid \varphi \wedge \varphi \mid \varphi \vee \varphi \mid \neg\varphi \mid \forall x\, \varphi \mid \exists x\, \varphi$$

A variable x occurring in a formula φ is *bound* if it is in the scope of a quantifier. Otherwise, x is *free*.

Given a signature σ, we define a *structure* over σ to consist of a *domain*, an interpretation for each relation in σ as sets of tuples with values from the domain (must preserve the arities), and also an interpretation for each constant symbol in the domain. Thus, we can view an instance I over schema Sch as a structure (Adom(I), R_1, ..., R_n), where Adom(I) is the set of values that appear in I and is called the *active domain* of I.

Semantics : For a first-order logic formula $\varphi(\vec{x})$, structure M and function σ assigning each variable from $\vec{x}$ to a value in domain(M), we can define inductively on the structure of φ the notion of *satisfiability* $\mathrm{M}, \sigma \vDash \varphi(\vec{x})$:

- $\mathrm{M}, \sigma \vDash R(x_1, ..., x_n)$ iff $\langle \sigma(x_1), ..., \sigma(x_n) \rangle \in \mathrm{M(R)}$;
- $\mathrm{M}, \sigma \vDash x_1 = x_2$ iff $\sigma(x_1) = \sigma(x_2)$;
- $\mathrm{M}, \sigma \vDash \varphi_1 \wedge \varphi_2$ iff $\mathrm{M}, \sigma \vDash \varphi_1$ and $\mathrm{M}, \sigma \vDash \varphi_2$ (analog for $\vee$ and $\neg$);
- $\mathrm{M}, \sigma \vDash \exists x\, \varphi$ iff there is c of type(x) such that $\mathrm{M}, \sigma \cup \{x \mapsto c\} \vDash \varphi$ (analog for $\forall$).

Example 3: Considering the instance from Example 2, the formula
φ(x, y) = EmployeeInfo(81, x, y, 45000) is not satisfiable by any variable binding, but the formula φ'(x, y) = EmployeeInfo(81, x, "Reporter", y) is satisfied by the mapping
$\sigma = \{\mathrm{x} \mapsto$ "Gilbert Marshall", $\mathrm{y} \mapsto 40000\}$.

2.3. Queries

A *query* is a function mapping instances I over relational schemas Sch to relational instances of a fixed relation. If the query has n free variables, then the resulting instance

will be n-ary. A *Boolean query* has no free variables and maps instances to either True or False. We will define queries using the function-free first-order logic from above.

To define the particular class of queries that interests us in the project, we recall the fragment of first-order logic called *positive existential*($\exists^+$) *first-order logic*, which does not allow the $\neg$ and $\forall$ operators.

Conjunctive Queries (CQs) are a fragment of $\exists^+$ first-order logic of the form:

$$Q(\vec{x}) = \exists \vec{y}\, \gamma(\vec{x},\ \vec{y})$$

where $\gamma(\vec{x},\ \vec{y})$ represents a **conjunction** of relational atoms that use free variables from $\vec{x}$ and bound variables from $\vec{y}$. A *union of conjunctive queries* (UCQ) is a disjunction of CQs, where every CQ uses the same free variables.

Given instance I and query $Q(\vec{x})$, a *homomorphism of Q in I* (also called *satisfying assignment* or *match*) is a function mapping variables from $\vec{x}$ to values in the active domain of I that makes Q hold in I.

Example 4: The query Q(x, y) = $\exists z, t_1, t_2$ EmployeeInfo(x, y, z, t_1) $\wedge$ EmployeeInfo(x, y, z, t_2) will return the following table:

209	Jane Hunt
333	Neville Barton

Each tuple in the table is a homomorphism of Q in I. We omit the names of the attributes in this project, as we will only care about their position relative to a particular relation name.

A *homomorphism* h *between two structures* I and I' (over the same signature) is a function from the active domain of I to the active domain of I' such that for every relation R and tuple $(t_1, ..., t_n)$, we have:

$$I \vDash R(t_1, ..., t_n) \Rightarrow I' \vDash R(h(t_1), ..., h(t_n))$$

2.4. Dependencies

Dependencies are integrity constraints over relational database schemas. Intuitively, they are rules to be fulfilled by instances over schemas. Given instance I and set of dependencies C, we say that I is *consistent* with C if it satisfies all constraints in C. All dependencies that we will define will be from fragments of the first-order logic from above.

A *tuple-generating dependency* (TGD) φ has the form:

$$\forall \vec{x}\, \vec{y}\, \rho(\vec{x},\, \vec{y}) \rightarrow \exists \vec{z}\, \gamma(\vec{y},\, \vec{z}) \tag{1}$$

where ρ and γ are conjunctions of atoms with arguments from $\vec{x}$ and $\vec{y}$, respectively $\vec{y}$ and $\vec{z}$. Since $\vec{y}$ appears in both sides, these variables will be called *exported variables*. We will refer to $\rho(\vec{x},\, \vec{y})$ as the *body* of the TGD and to $\gamma(\vec{y},\, \vec{z})$ as the *head*.

The intuition behind the "tuple-generating" aspect is that when we start with a database instance D_0 that does not initially satisfy a TGD φ (say we have $\rho(\vec{x},\, \vec{y})$ satisfied, but no $\vec{z}$ such that $\gamma(\vec{y},\, \vec{z})$), we can extend D_0 with new facts (mentioning new symbols), until we satisfy φ[1].

Example 5: Consider a database instance $D_0 = \{\text{R(0,1), R(1,2), S(0,3)}\}$. The TGD $\varphi_1 = \forall$x, y S(x,y) $\rightarrow \exists$ z R(x,z) holds, but the TGD $\varphi_2 = \forall$x, y R(x,y) $\rightarrow \exists$ z S(x,z) does not, because there is no z for x = 1, y = 2 such that S(1,z).

A *guarded tuple-generating dependency* (GTGD) has the form:

$$\forall \vec{x}\, \vec{y}\, R(\vec{x},\, \vec{y}) \wedge \rho(\vec{x},\, \vec{y}) \rightarrow \exists \vec{z}\, \gamma(\vec{y},\, \vec{z})$$

where R is a relation symbol that mentions all variables from $\vec{x}$ and $\vec{y}$ and is called the *guard* of the constraint. In Example 5, both TGDs are guarded, but for instance the TGD $\varphi = \forall$x, y, z R(x,y) $\wedge$ S(x,z) $\rightarrow \exists$t R(t,x) is not.

A *linear tuple-generating dependency* (LTGD) is a GTGD with only one relation symbol

[1] the semantics for TGDs are inherited from first-order logic

in the body[1]:

$$\forall \vec{x}\, \vec{y}\, R(\vec{x},\, \vec{y}) \rightarrow \exists \vec{z}\, \gamma(\vec{y},\, \vec{z})$$

A *schema mapping* M is defined by a triple $\langle$S, T, $\Sigma\rangle$ where S is the source schema, T is the target schema, and Σ is a set of dependencies. Intuitively, Σ maps instances of S into instances of T.

2.5. Open World Query Answering

As we have seen, a database instance I might not be consistent with respect to a set of dependencies C. A natural goal here is to see how to "extend" I with facts in order for the newly formed instance to satisfy C.

I' is a *super-instance* of I if it contains all the facts from I. Given instance I and set of constraints C, a *world* (also called *model*) of I and C is a super-instance of I that satisfies C. Given a query Q($\vec{x}$), a *certain answer* to Q on I, C is a homomorphism h such that the tuple h($\vec{x}$) is in every world of I and C.

The *Open World Query Answering* problem is to decide, given tuple $\vec{t}$, query Q, instance I and set of constraints C, whether $\vec{t}$ is a certain answer to Q on I, C. There is a distinction between the constrained and unconstrained versions of this problem, depending if we only take into consideration the finite super-instances or not, respectively. A similar problem is to determine all certain answers of Q, given I and C.

We will use the notation I $\wedge$ C $\vDash$ Q to indicate that Q holds in all possible worlds of I and C, where Q is a Boolean CQ.

A useful tool in this project is the correspondence between Boolean CQs and databases:

- **Canonical database**: given CQ Q, the canonical database CanonDB(Q) replaces each existential variable in Q with a constant and has one fact for each fact in the body of Q;
- **Canonical query**: given database D, the canonical query CanonQuery(D) replaces each constant from D with an existential variable and has one atom in the body of the query for each fact in D.

[1] some books call it linear guarded TGD, but we can see that all LTGDs are trivially guarded.

2.6. Forward Chaining: The Chase

One common technique for dealing with the open world query answering problem is to derive, given an initial instance I and set of constraints C, the facts that can be implied in all possible worlds.

Given the TGD φ we defined at (1), a *trigger* for φ is a homomorphism h of $\rho(\vec{x}, \vec{y})$ into I. Intuitively, a trigger is simply an assignment of $\vec{x}$ and $\vec{y}$ to values in the active domain of I such that $\rho(\vec{x}, \vec{y})$ holds in I. We say that the trigger is *active* if there is no witness $\vec{z}$ such that $\gamma(\vec{y}, \vec{z})$ holds in I, which means that the TGD constraint is not yet satisfied by I.

In order to derive a world where φ is satisfied, we create **new** constants (known as *labelled nulls*) for $\vec{z}$ and we append the necessary facts to I, in order to have a witness for $\gamma(\vec{y}, \vec{z})$. We call this process a *chase step*, and the resulting super-instance will no longer have h as an active constraint. In order to obtain a super-instance which satisfies all constraints from C, we start from I and make a chase step until there are no active triggers. This procedure will lead to a sequence of instances $\mathrm{I}_0 = \mathrm{I}$, I_1, ..., I_n, ..., where each I_{i+1} is obtained from I_i by performing a chase step. This is called a *chase sequence* and it can be *terminating* if it is finite and the final instance has no active triggers, otherwise it is *non-terminating*.

For efficiency, we can also act in stages, solving multiple active triggers at once:

- Starting from $\mathrm{I}_0 = \mathrm{I}$, apply (in parallel) a chase step for every active trigger and form a super-instance I_1;
- Apply (in parallel) a chase step for each active trigger in I_k and form a super-instance I_{k+1};
- Continue until there are no active triggers in (say) I_n

This is called a *maximal parallel chase sequence* and we call I_n the *parallel chase model*. In case that our process is infinite, we consider as our chase model the direct limit of the structures in it, in our case I_0, I_1, ..., I_n, ..., and we will denote this model as $\mathrm{chase}_C(\mathrm{I})$.

Types of chase: In the literature, there are multiple ways to define chase sequences, depending on which active triggers are picked. We will mention a few:

- **oblivious chase**: for every pair ($\vec{a}$, $\vec{b}$) and TGD φ of the form from (1) with $\rho(\vec{a}$, $\vec{b}) \subseteq$ I, apply a chase step to φ only if the same pair has not contributed to any previous chase step; therefore, add to I a new set of atoms $\gamma(\vec{b}, \vec{c})$, where $\vec{c}$ is a fresh set of labelled nulls;

- **restricted chase**: (also called **standard**) this is a refinement of the previous chase, where we only apply a chase step if the TGD φ is not already satisfied by I i.e. there is no $\vec{a}'$ such that $\gamma(\vec{b}, \vec{a}') \subseteq$ I;

- **super-oblivious chase**: in this variant, we apply chase steps to all matching bodies, no matter if the pair ($\vec{a}$, $\vec{b}$) has been previously used or not.

All chase methods can create infinite instances, but it is clear that the restricted chase creates the smallest instances out of the three, and the super-oblivious one the largest.

Example 6: Given the database D_0 from Example 4 and TGD φ_2, which is not initially satisfied, we can apply one chase step and add a fresh constant $null_1$ and the fact S(1, $null_1$) to D_0. Now, the new instance satisfies φ_2 and if we use the restricted or oblivious chase, we would stop here. For the super-oblivious chase, we would add facts S(1, $null_i$), for i $\geq$ 1.

Properties: First of all, it is important to notice that the chase procedure will always output a possible world of I and C, no matter if the procedure is terminating or not. This can easily be deduced from the fact that there will always be a chase step for each active constraint that occurs, which will automatically solve it.

Theorem 2.6.1 (Universality Theorem). Given database instance I and set of constraints C, chase_C(I) is a *universal model* for I and C, meaning that for any world I' of I and C, there exists a homomorphism from chase_C(I) to I'.

One issue with the chase procedure is that for general TGDs, the termination of the algorithm is undecidable. However, even though for guarded TGDs the chase might be non-terminating, we can decide when to "cut" the procedure, because after some point we no longer obtain new facts (only renamings of the variables).

This crucial theorem will justify the use of the phrase "the chase model", since it implies that for any two chase models, no matter the chase procedure used, there will be a homomorphism between them. Therefore, the chase model is *unique up to homomorphism.*

The main link to the query answering problem is the following proven result:

Corollary 2.6.2. Consider a set of TGDs C, any database instance I, the chase model $\text{chase}_C(\text{I})$ and a set of values Base from I and C. Then, for any CQ Q using only constants from Base, and any tuple $\vec{t}$ with values in Base:

$$\vec{t} \text{ is a certain answer for Q, I, C iff } \vec{t} \text{ is in Q}(\text{chase}_C(\text{I})).$$

It has been proven that the problem of finding certain answers is undecidable for the general class of TGDs, but for restricted versions (such as the guarded TGDs) this problem, although the chase might not terminate, is decidable.

3. Chase Entailment for LTGDs

From now on, our work will only focus on results about LTGDs, but it might mention known results about more general types of TGDs. In this section we will follow closely the approach from [1] in order to prove the following result:

Let us fix a relational schema Sch and finite database instance I over Sch. Let w be the maximal arity of any relation in Sch and A be the active domain of I.

Theorem 3.0.1. For C a set of single-headed LTGDs and φ a single-headed LTGD, we can decide whether φ holds in $\text{chase}_C(\text{I})$.

The approach from [1] follows the plan:

- Show that each such chase structure can be represented by a tree-like model (a structure that can be "coded" in a tree) - Section 3.1;
- Create an automata that will accept trees that code the given chase structure - Section 3.3;
- Create an automata that will accept only trees that satisfy $\neg\varphi$ - Section 3.5;
- Intersect the two automata and check for non-emptiness - Section 3.6;

3.1. Tree-like Property

The goal of this section is to show that the chase procedure for LTGDs outputs a model that is "tree-like"[1]. Intuitively, we want to show that the model can be "coded" as a tree, which will subsequently be used as input for tree automata.

We will show this property for arbitrary source instances I and arbitrary sets of single-headed LTGD constraints[2] C. Let us fix I and C, let the set of constants from I be A = $\{c_1, ..., c_n\}$ and the relation names (R_1, ..., R_m). Let N = $\{n_1, ..., n_i, ...\}$ be the set of labelled nulls that will be used in the chase procedure. We want to represent the chase model of I and C as a labelled ω-tree over a set of predicates Σ, which will contain all

[1] it has been proven in [1] that the chase is tree-like for GTGDs, but this does not apply for TGDs

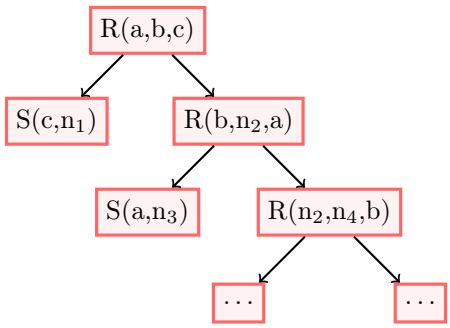
[2] $\varphi = \forall\vec{x}\ \text{R}(\vec{x}) \rightarrow \exists\vec{y}\ \text{S}(\vec{x},\vec{y})$, where R and S are (not necessarily distinct) relational names

possible facts, combining relation names R_i and arguments from A ∪ N.

Example 7: Let I = {R(a,b,c)} and C = {∀x,y,z R(x,y,z) → ∃t R(y,t,x), ∀x,y,z R(x,y,z) → ∃t S(z,t)}. It is clear that the chase procedure here will be non-terminating, since we will always have a new active trigger for each R-fact that is added. Formally, we can represent the structure as an infinite labelled tree using the following procedure:

1. create a root node and label it with all the facts from I and mark it as "unexplored";
2. for each "unexplored" node v, let F(v) be its label (i.e. set of facts), and let C(v) be all the active constraints φ from C such that there exists a fact in F(v) that is a homomorphism for the body of φ;
3. for each such φ, using a chase step we create new facts for each atom in the head of φ, and for each fact we create a single node, which is a child of v and which is labelled only with this fact (using fresh nulls from N each time);
4. mark node v as "explored" (we can imagine that we have a "frontier" of nodes to be expanded, in a BFS fashion;
5. we repeat this process as long as there are "unexplored" nodes; this process might be non-terminating, as we can see below.

Example 8: The labelled tree corresponding to the chase from Example 7 will be:



We can see that N will be infinite as well, therefore in order to create a labelled ω-tree with finite Σ, we need to use a different approach, inspired from [1]:

Observation 1: For every labelled null[1], the subset of vertices that contain it is connected.

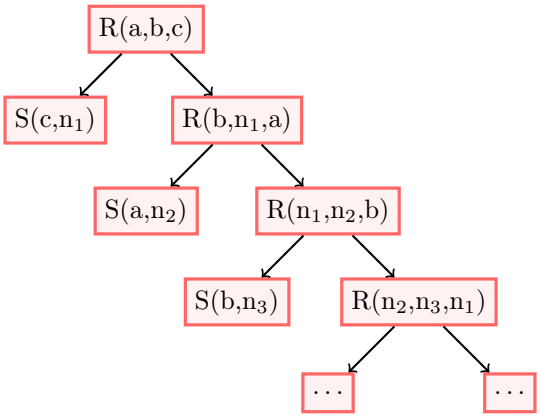
[1] this also holds for constants from I, but we only mention nulls because the set of constants is finite no matter what; for constants introduced in C, it does not hold, but it does not affect any of the following work

Proof: Suppose there exists a labelled null n such that the set of vertices that contain it is not connected. Therefore, there must be two nodes v_1 and v_2 that are labelled with facts that mention n for which no path that connects them exists. For each of the two nodes, we go up the tree as long as the parent of the current node mentions n. We end up with nodes w_1 and w_2 which are the ancestors of v_1 and v_2, respectively, that are the closest to the root and mention n. If $w_1 = w_2$, then there is a path between v_1 and v_2, which leads to a contradiction. If they are distinct nodes, then in both their cases n was introduced by an existential quantifier from a single-headed LTGD applied at their parent (w_1 and w_2 cannot be root since n must be a labelled null, not a constant). This implies that the n introduced at w_1 is distinct from the one introduced at w_2, as we only introduce fresh nulls each time, which leads to a contradiction. □

Following this observation, we could re-use labelled nulls in our representation, at the cost of changing their semantics:

- Let k be a natural number and $L = \{n_1, ..., n_{2k}\}$ be a set of labelled nulls (we will call them *local names* to make a distinction from the previous labelled nulls);
- When we need to create a new node labelled with $S(\vec{x}, \vec{y})$, where $\vec{x}$ are bounded and $\vec{y}$ are fresh (with the size of $\vec{y}$ being q), we use the first "available"[1] q local names;

Example 9: We transform the structure from Example 8 using $k = 3$ and local names in $L = \{n_1, ..., n_6\}$:



The major difference here is that when we have a local name appear in two different nodes that are not connected in the tree, they do not represent the same value.

[1] an "unavailable" local name is one used in the parent node

An important question is what value we should choose for k. Our goal is to minimize its value, since the size of Σ depends on it. As discussed in [1], the optimal value for k is the maximal arity (call it w) of any relation in I or in C.

It is easy to see that we need to have at least $k \geq w$, otherwise, if we encounter two facts $R(x_1, ..., x_w)$ and $R(y_1, ..., y_w)$, where all values mentioned are distinct, we cannot code the values in a consistent way with only 2k local names. In [1] we can see that having $k = w$ is actually sufficient for every instance that we will encounter.

A crucial point now is that every chase structure for source instance I and set of single-headed LTGDs can be represented using this new signature[1].

3.2. Automata over Infinite Trees: 1-way deterministic Buchi

We define the type of automaton that is capable of representing the chase model of I and C described above: let us fix a maximal outdegree r for the trees that will be considered as input from now on.

Definition 3.2.1. A 1-way deterministic Büchi tree automaton is a 5-tuple $\mathcal{A} = <Q, \Sigma, \delta, Init, F>$, where:

- Q is a finite set of *states*;
- Σ is an input *alphabet*;
- $\delta : Q \times \Sigma \to \bigcup_{1 \leq i \leq r} Q^i$ is the *transition function*;
- Init $\subseteq$ Q is the set of *initial* states;
- F $\subseteq$ Q is the set of *final* (also called *accepting*) states.

It takes as input an infinite Σ-tree and processes it top-down. A *run* assigns states from Q to the nodes of the tree. A *successful* (or *accepting*) run must satisfy the following conditions:

- The root of the tree must be assigned to an initial state from Init;
- If a node v labelled with τ and children $v_1, ..., v_n$ is assigned to state q and we have $\delta(q, \tau) = (q_1, ..., q_n)$, then child i must be assigned to state q_i, for $1 \leq i \leq n$;

[1] in [1], we can find the definition of *k tree-code signature*, which is a generalization of what we presented here, which is required for a larger class of FO-formulas, called the *Guarded Fragment*

- for every path π of the tree, there are infinitely many nodes assigned to accepting states.

The language of such an automaton is formed from the trees for which there exist a successful run. An important property that will be needed from these automata is that the emptiness problem is decidable in PTIME, as it is done via reachability analysis. This is also true for the 1-way nondeterministic case.

3.3. Automata for the chase

We will use a 1-way deterministic Büchi tree automaton to input tree structures of the form presented at Section 3.1. We fix I and C, the set of constants A from the active domain of I, and the local names L = {n_1, ..., n_{2k}}, where k is the maximal arity of any relation name from I and C. We define the automaton $\mathcal{A}_{chase}$(I, C) that will accept only structures that are homomorphic to chase$_C$(I):

- Q = {q_0} $\cup$ {$q_{F(t_1,...,t_{arity(F)})}$ | F is a fact from I or C, t_1, ..., $t_{arity(F)} \in$ A $\cup$ L} $\cup$ {q_{Fail}};
- Σ = {I} $\cup$ {$F(t_1, ..., t_{arity(F)})$ | F is a fact from I or C, t_1, ..., $t_{arity(F)} \in$ A $\cup$ L};
- δ : Q $\times$ Σ $\rightarrow$ $\bigcup_{1 \leq i \leq r}$ Q^i presented below;
- Init = {q_0};
- F = Q $\setminus$ {q_{Fail}}.

We created states for each fact that we might see in the coding of a chase structure, and we accept trees based on their structure and labels:
1) At the root, we expect the label to be I, otherwise we go to a sink state q_{Fail}:

$$\delta(q_0, \tau) = \left\{ \begin{array}{ll} (q_{F_1}, ..., q_{F_m}), & \text{if } \tau = I \\ (q_{Fail}), & \text{otherwise} \end{array} \right\}$$

The set of facts F_1, ..., F_m will be all the facts that can be generated from I, by matching the body of a constraint from C. In order to know what local names to expect, we impose

a reasonable **policy** that in choosing a local name for a fresh variable, we always pick the first available local name from L, in the order of the indices. Intuitively, we only allow structures that have at the root the label I, and we then transition to all states that correspond to new facts derived from I and C because this is what we expect to see on the next level.

2) At the "chase states" q_F (the ones that are neither q_0, nor q_{Fail}), we analogously to 1) define the set of new facts that should be generated from matching constraints in C with the body F, call it $C_F = \{F_1, ..., F_k\}$, again using the defined **policy**:

$$\delta(q_F, \tau) = \left\{ \begin{array}{ll} (q_{F_1}, ..., q_{F_k}), & \text{if } \tau = \{F\} \\ (q_{Fail}), & \text{otherwise} \end{array} \right\}$$

3) The final sink state will only transition to itself:

$$\delta(q_{Fail}, \tau) = (q_{Fail})$$

It is easy to see that this automaton accepts structures isomorphic to $\text{chase}_C(I)$, because each state hard-codes the expected labels that we require. However, because of the **policy** that we imposed in order to reduce the transition space, we will not accept all structures that are isomorphic to the chase, but there will exist one that is accepted.

The number of states in Q will be exponential in w (actually it will be $O(w^w)$).

3.4. Automata over Infinite Trees: 2-way alternating Buchi

For the second part of the proof, we will require a more powerful automaton, which will have more flexibility in terms of searching over its input trees.

In order to decide whether a structure satisfies a single-headed LTGD, we will need states where we need to decide that a particular fact holds for at least one tuple, therefore we need existential states, but we also need states that must decide if a particular fact holds for all possible tuples, therefore we need universal states. We will need to make our initial automaton (from Section 3.2.) alternating (a generalization of nondeterminism).

Besides that, in the chase case we only needed to traverse the input tree top-down, since

only the last level of nodes was involved in the creation of new ones. However, in this case we will be interested in traversing nodes in all directions, because we might find facts in other branches that will have an impact in our decision. Therefore, we will make the automaton 2-way (by augmenting it with actions from $\text{Direction}_r = \{\text{Stay, Up}\} \cup \{\text{Down}_i \mid 1 \leq \text{i} \leq \text{r}\}$).

Our transition function will assign pairs of states and labels to **positive boolean combinations of propositions over $\text{Direction}_r \times \mathbf{Q}$**. The intuition is that a transition to

- (dir, q) will tell the automaton to go in direction dir in the input tree and transition to state q (base case);
- $\sigma_1 \wedge \sigma_2$ will mean that we have a universal choice, so both σ_1 and σ_2 need to happen;
- $\sigma_1 \vee \sigma_2$ will mean that we have an existential choice, so at least one of σ_1 and σ_2 need to happen.

As in [1], we denote the set of positive boolean combinations of propositions for a set M with $\text{B}^+(\text{M})$.

Definition 3.4.1. A 2-way alternating Büchi automaton is a 5-tuple
$\mathcal{A} = <\text{Q}, \Sigma, \delta, \text{q}_0, \text{F}>$, where:

- Q is a finite set of *states*;
- Σ is an input *alphabet*;
- $\delta : \text{Q} \times \mathcal{P}(\Sigma) \rightarrow \text{B}^+(\text{Direction}_r \times \text{Q})$ is the *transition function*;
- $\text{q}_0 \in \text{Q}$ is the *initial* state;
- $\text{F} \subseteq \text{Q}$ is the set of *final* states.

The details for a *run* and for an *accepting run* are explained in detail in [1] and are an extension of the conditions from the 1-way deterministic case. The crucial part is that we require the node-child relationship to obey the transition relation, as before. As we did with the 1-way deterministic case, we are interested in the decidability of the non-emptiness problem, and for this type of automaton it has been proven that the problem is decidable in 2EXPTIME.

3.5. Automata for single-headed LTGDs

Our goal is to create an automaton $\mathcal{A}_{\neg\varphi}$ that accepts all tree code chase structures where $\neg\varphi$ holds. For consistency, we will stick to the vocabulary defined at the previous section. Let us fix the single-headed LTGD φ ($\vec{y}$ represents the exported variables):

$$\varphi = \forall\vec{x}\,\vec{y}\,R(\vec{x},\,\vec{y}) \rightarrow \exists\vec{z}\,S(\vec{y},\,\vec{z})$$

$$\neg\varphi = \exists\vec{x}\,\vec{y}\,R(\vec{x},\,\vec{y}) \wedge \forall\vec{z}\,\neg S(\vec{y},\,\vec{z})$$

The automaton $\mathcal{A}_{\neg\varphi}$ will have:

- Q = $\{q_0\} \cup \{q_{\vec{a};\vec{b}} \mid \vec{a}, \vec{b}$ are tuples with elements in A $\cup$ L that we can form for R$\}$ $\cup \{q_{True}, q_{False}\}$;
- Σ is the same as for the chase automaton, without I;
- q_0 is the initial state;
- F = $\{q_{True}\}$.

The transition function will be:

$$\delta(q_0,\tau) = \bigvee_{R(\vec{a};\vec{b})\in\tau} (Stay, q_{\vec{a};\vec{b}}) \vee \bigvee_{d\in Direction_r} (d, q_0)$$

$$\delta(q_{\vec{a};\vec{b}},\tau) = \left\{ \begin{array}{ll} (Stay, q_{True}), & \text{if } \vec{b}\cap\tau = \emptyset \\ (Stay, q_{Fail}), & \text{if } S(\vec{b},\vec{c})\in\tau \\ \bigwedge\limits_{d\in Direction_r} (d, q_{\vec{a};\vec{b}}), & \text{otherwise} \end{array} \right\}$$

$$\delta(q_{True},\tau) = (Stay, q_{True})$$

$$\delta(q_{False},\tau) = (Stay, q_{False})$$

In order for $\neg\varphi$ to be satisfied by one of our coded structures, we will traverse the tree on nodes until we find a node where we can guess that the given pair is $(\vec{a}, \vec{b})$, since the node is labelled with R$(\vec{a}, \vec{b})$. After this guess, we want to show that $\forall\vec{z}\,\neg S(\vec{b},\,\vec{z})$ holds in the tree structure. Starting from the node where we made the guess, we search for $\vec{b}$ in the tree and we have three cases:

1. If $\vec{b}$ is represented by the node and we have the label $S(\vec{b}, \vec{c})$, for some $\vec{c}$, then we fail, and our guess is wrong;

2. If no element from $\vec{b}$ is present in the tuple corresponding to the node, then we can accept, since if we keep searching for $\vec{b}$ from here, we will either go back to already visited nodes, or reach nodes where no element in $\vec{b}$ is represented; this can be explained with **Observation 1** that we made about the *connect subset* property of the tree chase structures;

3. If some elements from $\vec{b}$ are present, we recurse on each direction of the tree.

The number of states will be exponential in the arity of R.

3.6. Time complexity

Intersecting the two automata that we defined, we obtain a 2-way alternating Büchi automaton that only accepts structures isomorphic to $\text{chase}_C(I)$ that do not accept φ. Therefore, we can decide if φ holds in $\text{chase}_C(I)$ by checking if the language of our automaton is $\emptyset$, which we mentioned that it is 2EXPTIME.

Discuss about how to reduce this 2EXPTIME bound to PSPACE: what we have so far - The fact that we can cut off the chase at an exponential level only gives us a 2EXPTIME bound. We can get down to NPSPACE by guessing the branches of the chase that we need, storing information about the last atom we saw in memory (we can also include a counter to be sure we terminate) + Savitch

We want to prove that for single-headed LTGDs the decidability is PSPACE, and to make a contrast to using Courcelle, which would give a worse complexity.

4. Equivalences for Chase and CQs

4.1. Definitions

Let us fix a source schema S and target schema T, and let Σ_1 and Σ_2 be sets of TGD constraints from S to T. We recall three well-studied equivalence types[6] that will be important for the project, together with two more which are newly defined.

1. **Logical equivalence**: $\forall$ instances D_0, $D_0 \vDash \Sigma_1$ iff $D_0 \vDash \Sigma_2$
2. **Chase compatibility**: $\forall$ source instances D_0, $\text{chase}_{\Sigma_1}(D_0) \vDash \Sigma_2$ and $\text{chase}_{\Sigma_2}(D_0) \vDash \Sigma_1$
3. **Chase equivalence**: $\forall$ source instances D_0, $\text{chase}_{\Sigma_1}(D_0)$ and $\text{chase}_{\Sigma_2}(D_0)$ are homomorphically equivalent in both directions (via homomorphisms that preserve the constants in D_0)
4. **CQ-equivalence**: $\forall$ instances D_0, CQ $Q(\vec{x})$, tuple $\vec{t}$ from D_0, $D_0 \wedge \Sigma_1 \vDash Q(\vec{t})$ iff $D_0 \wedge \Sigma_2 \vDash Q(\vec{t})$
5. **DE-equivalence**: $\forall$ source instances D_0, the models of D_0 and Σ_1 and the models of D_0 and Σ_2 coincide.

4.2. Implications

For the already known equivalences, the following results hold:

Logical equivalence $\Rightarrow$ DE-equivalence $\Rightarrow$ CQ-equivalence

We claim the following implications using the new notions:

(A) Logical equivalence $\Rightarrow$ Chase compatibility:

Let D_0 be a source instance. By the Universality theorem for the chase, we know that $\text{chase}_{\Sigma_1}(D_0)$ is a universal model for D_0 and Σ_1, therefore $\text{chase}_{\Sigma_1}(D_0) \vDash \Sigma_1$. Using the assumption, we get that $\text{chase}_{\Sigma_1}(D_0) \vDash \Sigma_2$, too. The other branch is symmetrical.

(B) Chase compatibility $\Rightarrow$ Chase equivalence:

Since $\text{chase}_{\Sigma_1}(D_0) \vDash \Sigma_2$, we have that $\text{chase}_{\Sigma_1}(D_0)$ is a model (world) for Σ_2. Using the Universality of $\text{chase}_{\Sigma_2}(D_0)$ for D_0 and Σ_2, we get that there is a homomorphism from

$\text{chase}_{\Sigma_2}(D_0)$ to $\text{chase}_{\Sigma_1}(D_0)$. The other direction is symmetrical.

(C) Chase equivalence ⇒ CQ-equivalence:

We will do one direction of the iff statement: suppose Σ_1 and Σ_2 are chase equivalent and let instance D_0, CQ $Q(\vec{x})$ and tuple $\vec{t}$. We start with the assumption that $D_0 \wedge \Sigma_1 \vDash Q(\vec{t})$. From this, we know that $Q(\vec{t})$ is a certain answer to D_0 and Σ_1, therefore $Q(\vec{t})$ holds in all possible worlds for D_0 and Σ_1, one of which is $\text{chase}_{\Sigma_1}(D_0)$. By chase equivalence, we have a homomorphism from $\text{chase}_{\Sigma_1}(D_0)$ to $\text{chase}_{\Sigma_2}(D_0)$, which preserves every relation and the constants from D_0. Therefore, it preserves all the CQs, which means that $\text{chase}_{\Sigma_2}(D_0)$ satisfies $Q(\vec{t})$. Using Corollary 2.6.2, we get that $D_0 \wedge \Sigma_2 \vDash Q(\vec{t})$.

(D) CQ-equivalence ⇒ Chase equivalence (in case of terminating[1] chase):

Suppose Σ_1 and Σ_2 are CQ-equivalent and let source instance D_0. We will prove that if the chase procedure for the two sets of constraints terminates, there is a homomorphism from $\text{chase}_{\Sigma_1}(D_0)$ to $\text{chase}_{\Sigma_2}(D_0)$ (the other direction is symmetrical). It is clear that $\text{chase}_{\Sigma_1}(D_0) \vDash \text{CanonQuery}(\text{chase}_{\Sigma_1}(D_0))$. Therefore, by CQ-equivalence, $\text{chase}_{\Sigma_2}(D_0) \vDash \text{CanonQuery}(\text{chase}_{\Sigma_1}(D_0))$. This means that there is a valuation h_{12} from all the existentially quantified variables in the query to values in the domain of $\text{chase}_{\Sigma_2}(D_0)$, such that all the facts from the body of the query are satisfied by $\text{chase}_{\Sigma_2}(D_0)$. Since $\text{CanonQuery}(\text{chase}_{\Sigma_1}(D_0))$ creates an existential variable for each value in $\text{chase}_{\Sigma_1}(D_0)$, we can create a homomorphism based on this correspondence and h_{12}. This homomorphism will be the identity for the constants in D_0, as part of the chase procedure.

The new results are:

Logical equiv. ⇒ Chase compatibility ⇒ Chase equiv. ⇒ CQ-equiv.

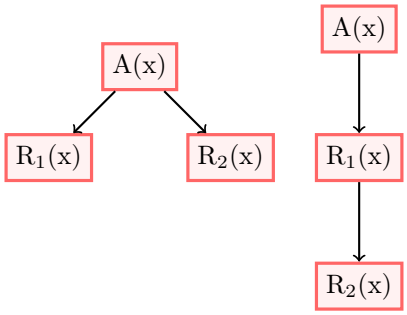
We will further investigate the behavior of the equivalences for the class of LTGDs, by giving counter-examples to the reverse direction of the single implications:

(A') Chase compatibility ⇏ Logical equivalence:

Example 10: Let S consist of unary predicate A(.), and T consist of A(.), and unary predicates $R_1(.)$ and $R_2(.)$. Let:

- $\Sigma_1 = \{A(x) \rightarrow R_1(x);\ A(x) \rightarrow R_2(x)\}$
- $\Sigma_2 = \{A(x) \rightarrow R_1(x);\ R_1(x) \rightarrow R_2(x)\}$

[1] TODO: analyse the case for non-terminating chase



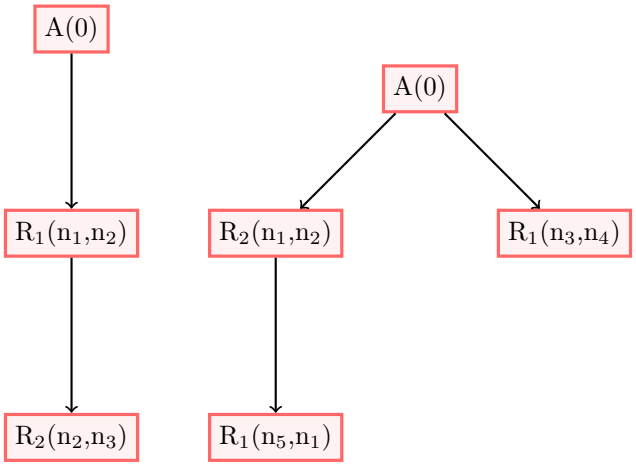
They are chase compatible, as for every source instance D_0 containing facts of type A(x), we will derive the facts $R_1(x)$ and $R_2(x)$. However, they are not logical equivalent, as we have the counter-example $D_0 = \{R_1(0)\}$, which has $D_0 \vDash \Sigma_1$, but $D_0 \nvDash \Sigma_2$.

(B') Chase equivalence $\nRightarrow$ Chase compatibility:

Example 11: Let S consist of unary relation A(.) and T consist of A(.) plus two binary relations $R_1(.\ ,\ .)$ and $R_2(.\ ,\ .)$. Let:

- $\Sigma_1 = \{\forall$ w A(w) $\rightarrow \exists$ x, y R_1(x,y); $\forall$ x, y R_1(x,y) $\rightarrow \exists$ z R_2(y,z)$\}$
- $\Sigma_2 = \{\forall$ w A(w) $\rightarrow \exists$ x, y R_1(x,y); $\forall$ w A(w) $\rightarrow \exists$ y, z R_2(y,z); $\forall$ y, z R_2(y,z) $\rightarrow \exists$ x R_1(x,y)$\}$

They are chase equivalent and it is easy to create homomorphisms between the labelled nulls of the two structures. For chase compatibility, let $D_0 = \{A(0)\}$ and the chases are:



We can clearly see that $\text{chase}_{\Sigma_2}(D_0)$ does not satisfy the second constraint from Σ_1, because of $R_1(n_3,n_4)$.

Q: Under what conditions does CQ-equivalence $\Rightarrow$ Chase compatibility?

Theorem 4.2.1: Let Σ_1 and Σ_2 be two sets of single-headed LTGDs with the following properties:

1. every constraint mentions only binary predicates;
2. the body of each constraint has two universally quantified variables;
3. the head of each constraint contains exactly one exported variable and one existential variable;
4. the set of constraints does not lead to a chase where there exist a value (constant of labelled null) that appears both in a node and in its grandchild;

Then, if Σ_1 and Σ_2 are CQ-equivalent, then they are also chase compatible.

Proof:

Claim 1: In any chase structure based on this class of LTGDs, if the facts from two distinct nodes share a value, then the relationship between them is either parent-child, or they are children of the same node.

Proof 1: Let n_1 and n_2 be such two nodes, sharing value v. Using the **connected subset** property of the chase, we have that all nodes on the path between n_1 and n_2 share v. If the length of the path between them is greater than 2, then there must exist a violation of rule 4. If the distance is 2, then we either have that one node is the grandchild of the other, which is not allowed, or they are the children of the same node. If the distance is 1, we have the parent-child relationship.

From the requirements imposed on the constraints, we can derive their form:

$$\varphi = \forall x\ y\ R(x,\ y) \rightarrow \exists z\ S(y,\ z)$$

$$\varphi = \forall x\ y\ R(x,\ y) \rightarrow \exists z\ S(z,\ y)$$

$$\varphi = \forall x\ y\ R(x,\ y) \rightarrow \exists z\ S(x,\ z)$$

$$\varphi = \forall x\ y\ R(x,\ y) \rightarrow \exists z\ S(z,\ x)$$

We will now argue by contradiction. Suppose that the two sets are CQ-equivalent, but there exists a source instance D_0 such that at least one of the necessary conditions does not hold, say $\text{chase}_{\Sigma_2} \not\models \Sigma_1$. We denote $\text{chase}_{\Sigma_i}(D_0)$ as CH_i, for i $\in \{1,2\}$. Therefore, there

must exist constraint $\varphi \in \Sigma_1$ such that $CH_2 \nvDash \varphi$. We will say that φ is of the form $\forall$x y R(x,y) $\rightarrow \exists$ z S(y,z), but all other cases can be treated the same way. There must exist a witness R(a,b) in CH_2 such that there is no c with $CH_2 \vDash$ S(b,c). Let $F_0 = D_0$, F_1, F_2, ..., F_{k-1}, F_k = R(a,b) be the path (in CH_2) up to this witness.

Claim 2: There must exist a path $F_0^{'} = D_0$, $F_1^{'}$, $F_2^{'}$, ..., $F_{k-1}^{'}$, $F_k^{'}$ in CH_1 that is homomorphic (preserving the constants in D_0) to the given path in CH_2.

Let $R_i(a_i,b_i)$ be the fact corresponding to F_i. We know from the given properties of the constraints that precisely one of a_i and b_i appears in F_{i-1} and the other one is a fresh null. We can form the canonical query Q of the path from CH_2, which will have as free variables all constants from D_0 and k universal variables, one for each fresh null introduced by each fact. The CQ-equivalence between Σ_1 and Σ_2 implies that CH_1 satisfies Q, which in turn implies the existence of facts $F_1^{'}$, $F_2^{'}$, ..., $F_{k-1}^{'}$, $F_k^{'}$ such that $F_i^{'}$ shares exactly one value with $F_{i-1}^{'}$, $1 \leq i \leq k$. We only remain to prove that these facts form a path in CH_1, as the part with the homomorphism is proven by the query satisfaction. We will build this path using strong induction on $0 < i < k$:

Base case: Because of Claim 1, $F_1^{'}$ must be a child of D_0;

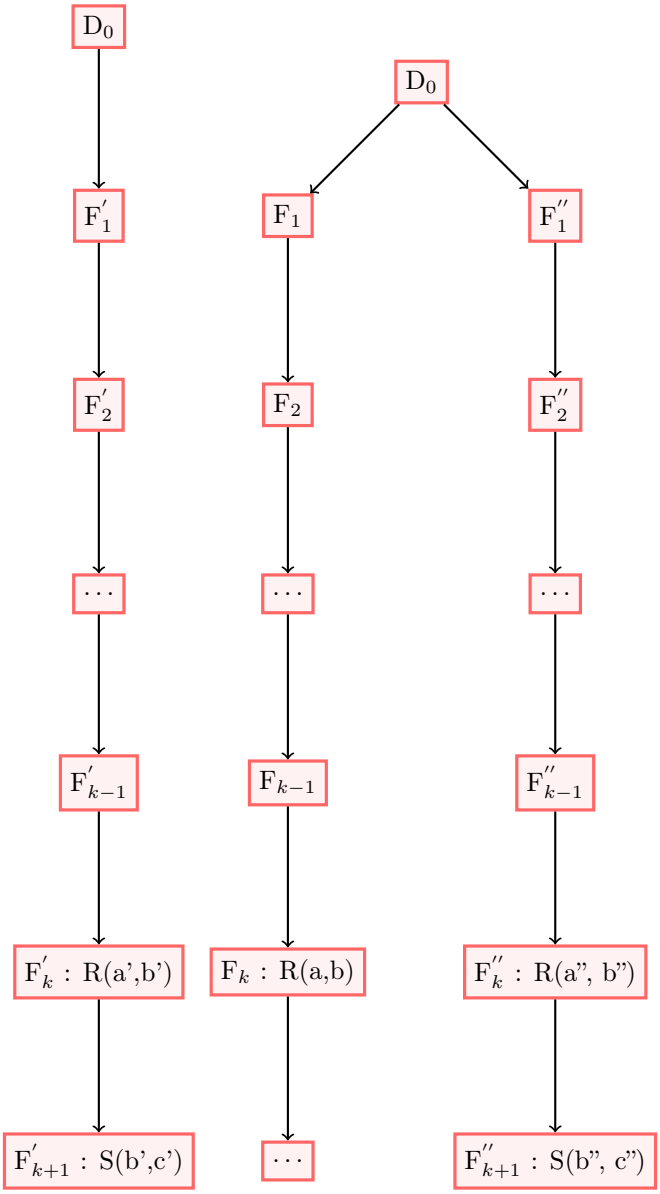
Inductive step: Suppose that $F_0^{'} = D_0$, $F_1^{'}$, $F_2^{'}$, ..., $F_{i-1}^{'}$, $F_i^{'}$ form a path. Because of Claim 1, $F_{i+1}^{'}$ is either a child of $F_i^{'}$, or a child of $F_{i-1}^{'}$, but using the connected subset property for the chase, the latter case will imply that $F_{i-1}^{'}$ contains the value shared between $F_i^{'}$ and $F_{i+1}^{'}$, which violates rule 4.

Therefore, we have that $F_k^{'}$ will have a fact of the form R(a',b'). Because $\varphi \in \Sigma_1$, the chase procedure guarantees that there exist a child $F_{k+1}^{'}$ of $F_k^{'}$ that contains the fact S(b',c'), for a fresh null c'.

Now, we can use a similar approach for the path from CH_1 (augmented with $F_{k+1}^{'}$) to create the canonical query Q', which must be satisfied by CH_2. Analogously to what we did above and using the same reasoning as for Claim 2, there must exist a path $F_0^{''} = D_0$, $F_1^{''}$, $F_2^{''}$, ..., $F_{k-1}^{''}$, $F_k^{''}$, $F_{k+1}^{''}$ in CH_1 that is homomorphic (preserving the constants in D_0) to the path from CH_1.

Because of this last homomorphism, $F_k^{''}$ must have a fact of the form R(a",b") and $F_{k+1}^{''}$ a fact of the form S(b",c"). The chase procedure guarantees that whenever we have a parent-child relationship, the child was created due to a constraint being applied, therefore we

must have a constraint of the same form as φ in Σ_2, but this leads to a contradiction, as F_k could no longer be a witness that φ does not hold in CH_2.



4.3. Decidability for equivalences of LTGD sets

(A) Logical equivalence:

In [1] we are introduced to a fragment of first-order logic called the *Guarded Fragment*, where the formulas are of the form:

$$\varphi(\vec{x}) ::= True | False | R(\vec{t}) \mid t_i = t_j \mid \varphi \wedge \varphi \mid \varphi \vee \varphi \mid \neg\varphi \mid \forall \vec{y}\, R(\vec{x}, \vec{y}) \rightarrow \varphi \mid \exists \vec{y}\, R(\vec{x}, \vec{y}) \wedge \varphi$$

In the existential and universal cases, the free variables of the inner φ are required to be from $\vec{x} \cup \vec{y}$ and the R($\vec{x}$,$\vec{y}$) atom is called the *guard atom*.

It has been proven that we can construct automata for these formulas in order to decide their satisfiability. With this, we can check if two sets of GF formulas are logically equivalent. However, LTGD formulas are not part of GF, for instance

$$\varphi = \forall \text{x, y R(x,y)} \rightarrow \exists \text{ z S(x,z)} \wedge \text{T(y,z)}$$

is not in GF, but we can convert it to GF using a fresh Dummy relation name:

$$\forall \text{x, y R(x,y)} \rightarrow \exists \text{ z Dummy(x,y,z)}$$
$$\forall \text{x, y, z Dummy(x,y,z)} \rightarrow \text{S(x,z)}$$
$$\forall \text{x, y, z Dummy(x,y,z)} \rightarrow \text{T(y,z)}$$

These formulas are all in GF, and it is clear that we can do this for any general LTGD. Therefore, **logical equivalence for LTGDs is decidable**.

(B) Chase compatibility: Using Theorem 2.6.1, we can decide if $\text{chase}_\Sigma(\text{D}_0) \vDash \Sigma$' by checking the entailment for each LTGD $\varphi \in \Sigma$;. Therefore, **chase compatibility for LTGDs is decidable**.

(C) CQ-equivalence: Under the conditions imposed in Theorem 4.2.1, CQ-equivalence is the same as chase compatibility, which would make it decidable.

4.4. Query entailment for the chase

Our goal in this subsection is to: ...

Let us fix a source instance D_0 and a set of LTGDs Σ. Let $\text{M} = \text{chase}_\Sigma(\text{D}_0)$ and we will use the notation M_k to represent the substructure of M such that in the tree representation of M presented at Section 3.1, we chop off the subtrees of M of depth bigger than k.

Definition 4.4.1: Two atoms of the form R(c_1 ... c_n) and R'(c'_1 ... c'_n) are *similar* with respect to D_0 if

- they use the same relation: R = R';
- they have the same equalities between terms: $\text{c}_i = \text{c}_j$ iff $\text{c}'_i = \text{c}'_j$, for $1 \leq \text{i, j} \leq \text{n}$;
- they use the same constants from D_0 in the same positions: $\text{c}_i = \text{d}_0$ iff $\text{c}'_1 = \text{d}_0$, for every $1 \leq \text{i} \leq \text{n}$ and $\text{d}_0 \in \text{Adom}(\text{D}_0)$.

Intuitively, there is a renaming for the non-constant terms in one atom that leads to the other atom. We can extend the notion to sets of facts $\{F_1, ..., F_n\}$ and $\{F'_1, ..., F'_n\}$ to mean that F_i and F'_i are similar, for $1 \leq i \leq n$. Two nodes in the tree representation are similar if their labels are similar.[1]

Observation 4.4.2: If two nodes from M are similar, then their subtrees are isomorphic. This is easy to see, since the isomorphism between the two subtrees is determined by the isomorphism between the two nodes. Additionally, the same rules will be applied to corresponding nodes.

Observation 4.4.3: For a sufficiently large k, every path of size k in M will contain two nodes that are similar with respect to D_0.

The proof of this relies on the fact that there are finitely many "similarity types", meaning that if we start with a set containing an atom $R(c_1, ..., c_n)$ that uses constants from $Adom(D_0)$ and local names (as discussed in Section 3.1), we can only add finitely many new atoms to the set until two of them will be similar. This bound k on the set of dissimilar facts will be exponential in the maximal arity of a relation from D_0 (called it w before). Therefore, if we have a path longer than k in the tree, by the Pigeonhole Principle we will encounter two similar nodes.

Proposition 4.4.4: If a Boolean CQ Q is entailed by M, there there exists an integer k such that Q holds in M_k. This integer k will be exponential in the sizes of Q and of D_0.

Proof: We will begin with the proof for Q constituting of a single atom. We claim that if we choose the k from Observation 4.4.3, we will obtain in M_k all atoms that can be entailed by M. This comes from the fact that if we allow a path longer than k, we will encounter two similar nodes, and by Observation 4.4.2 the subtree coming from the nodes that follows later in the path will be isomorphic to the one from the node that comes earlier, so there will be no new atom in the subtree after this later node. Therefore, we can decide if Q holds in M by checking if the single atom in Q appears in any node from M_k.

For the proof where Q has a number of $q > 1$ atoms, let S_Q be a witness to that i.e. a set of q atoms in M and let h_Q be the corresponding homomorphism of Q into S_Q. We

[1] in the LTGD case we will talk about nodes that are labelled with exactly one fact, excluding the case of the root.

define the closure of S_Q in the tree structure $cl(S_Q)$ to be formed by closing S_Q under least common ancestors. Our goal will be to truncate $cl(S_Q)$ in a similar way as for the single-atom case. We say that two elements in $cl(S_Q)$ are *neighbors* if there is no element from S_Q in the path between them. We will repeat the following process:

1. Find two neighbors n_1 and n_2 (n_1 ancestor of n_2) such that there exists two distinct nodes c_1 and c_2 along their path that are similar with respect to the elements from the fact of n_1;

2. Replace every node from S_Q that comes after c_2 with the corresponding node that comes after c_1 to obtain a set S'_Q with homomorphism h'_Q;

3. Repeat until we cannot find any candidates at 1 anymore.

Claim: After each step 2, we have that h'_Q is also a homomorphism of Q, where the distance between neighbors has decreased.
This is a result of Observation 4.4.2: the function h'_Q will be a homomorphism of Q because the nodes that come after c_2 will have a similar node after c_1, thus by replacing them we still remain with a witness for Q. The distance clearly decreases since c_2 is a node that comes strictly after c_1 in the tree representation.

Using Observation 4.4.3, we can limit the number of nodes between any two facts in the final S_Q, therefore the final size of k will grow proportionally to q, but will still be exponential in w.
Talk about time complexity

4.5. Weaker notions of CQ-equivalence

Let us define new versions of CQ-equivalence for sets of LTGD constraints Σ_1 and Σ_2, which constrain the sizes of the source instances D_0 or the sizes of the CQs Q:

1. **j-CQ-equivalence**: $\forall$ instances D_0, CQ $Q(\vec{x})$ consisting of j atoms, tuple $\vec{t}$ from D_0, $D_0 \wedge \Sigma_1 \vDash Q(\vec{t})$ iff $D_0 \wedge \Sigma_2 \vDash Q(\vec{t})$

2. **CQ-k-instance-equivalence**: $\forall$ instances D_0 containing k atoms, CQ $Q(\vec{x})$, tuple $\vec{t}$ from D_0, $D_0 \wedge \Sigma_1 \vDash Q(\vec{t})$ iff $D_0 \wedge \Sigma_2 \vDash Q(\vec{t})$

3. **j-CQ-k-instance-equivalance**: $\forall$ instances D_0 of k atoms, CQ $Q(\vec{x})$ consisting of j atoms, tuple $\vec{t}$ from D_0, $D_0 \wedge \Sigma_1 \vDash Q(\vec{t})$ iff $D_0 \wedge \Sigma_2 \vDash Q(\vec{t})$

Clearly, we get the following implications, for any j and k:

CQ-equivalence $\Rightarrow$ **j-CQ-equivalence** $\Rightarrow$ **j-CQ-k-instance-equivalence**

CQ-equivalence $\Rightarrow$ **CQ-k-instance-equivalence** $\Rightarrow$ **j-CQ-k-instance-equivalence**

Proposition 4.5.1: For sets of LTGDs Σ_1 and Σ_2, the j-CQ-k-instance-equivalence is decidable.

Proof: Enumerate all possible queries $Q_j(\vec{x})$ of size j and instances D_k of size k, fix a tuple $\vec{t}$ from the fixed source instance, and then we require to decide if the Boolean CQ $Q_j(\vec{t})$ is entailed by D_k and Σ_i, i $\in \{1,2\}$, which by the Universality Theorem of the chase can be reduced to instances of Proposition 4.4.4.

Talk about complexity.

Proposition 4.3.2: The sets of LTGDs Σ_1 and Σ_2 are CQ-equivalent iff they are CQ-1-instance-equivalent.

Proof: We will only prove the non-trivial implication. Suppose that Σ_1 and Σ_2 are CQ-1-instance-equivalent and let D be an arbitrary instance, $Q(\vec{x})$ an arbitrary CQ, and $\vec{t}$ a tuple with constants from D. Suppose $D \wedge \Sigma_1 \vDash Q(\vec{t})$, i.e. $\text{chase}_{\Sigma_1}(D) \vDash Q(\vec{t})$. Our goal is to show that $\text{chase}_{\Sigma_2}(D) \vDash Q(\vec{t})$. Let us write explicitly the form of the query:

$$Q(\vec{t}) = \exists \vec{y}\, R_1(\vec{y_1},\vec{t_1}) \wedge \ldots \wedge R_n(\vec{y_n},\vec{t_n})$$

where $\vec{y_i} \subseteq \vec{y}$ and $\vec{t_i} \subseteq \vec{t}$, $1 \leq i \leq n$. Since $\text{chase}_{\Sigma_1}(D) \vDash Q(\vec{t})$, there must exist valuation $\vec{a}$ for the existential variables in Q such that $\text{chase}_{\Sigma_1}(D)$ contains all facts $R_i(\vec{a_i},\vec{t_i})$. The crucial point here is that each such fact was generated from exactly one fact from D[1], as the bodies of all LTGDs have a single atom. For each such fact $R_i(\vec{a_i},\vec{t_i})$, let D_i be the substructure of D containing just the fact that generated it. Also, for each atom in $Q(\vec{t})$, let

[1] and its creation solely depends on that fact, independently on the other branches created from D

$$\mathrm{Q}_i(\vec{t_i}) = \exists \vec{y_i}\ \mathrm{R}_i(\vec{a_i},\vec{t_i})$$

Then, $\mathrm{chase}_{\Sigma_1}(\mathrm{D}_i) \vDash \mathrm{Q}_i(\vec{t_i})$ and by CQ-1-instance-equivalence, $\mathrm{chase}_{\Sigma_2}(\mathrm{D}_i) \vDash \mathrm{Q}_i(\vec{t_i})$. Thus, since $\mathrm{chase}_{\Sigma_1}(\mathrm{D})$ is formed from all the chases executed on the single-fact instances, we can combine all the homomorphisms for the smaller queries to create a homomorphism for $\mathrm{Q}(\vec{t})$, which proves that $\mathrm{chase}_{\Sigma_2}(\mathrm{D}) \vDash \mathrm{Q}(\vec{t})$.

5. Conclusions

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