# Path Constraints in Semistructured Databases

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## Abstract

We investigate a class of path constraints that is of interest in connection with both semistructured and structured data. In standard database systems, constraints are typically expressed as part of the schema, but in semistructured data there is no explicit schema and path constraints provide a natural alternative. As with structured data, path constraints on semistructured data express integrity constraints associated with the semantics of data and are important in query optimization. We show that in semistructured databases, despite the simple syntax of the constraints, their associated implication problem is r.e. complete and finite implication problem is co-r.e. complete. However, we establish the decidability of the implication and finite implication problems for several fragments of the path constraint language, and demonstrate that these fragments suffice to express important semantic information such as extent constraints, inverse relationships and local database constraints commonly found in object-oriented databases.

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## 1 INTRODUCTION

Path inclusion constraints have been studied by Abiteboul and Vianu in [5] for semistructured databases. In semistructured databases, the data is unconstrained by any type system or schema and typically has an irregular structure [2, 12]. The study of semistructured data has generated the development of new data models and query languages (e.g., [4, 14, 23, 33, 34]) appropriate to this form of data representation, which already exists in certain scientific data formats. Recently, XML (eXtensible Markup Language [11]) has emerged as a standard for data exchange on the World Wide Web. While a schema may be imposed on an XML document, it is not required, and XML data is usefully treated as semistructured data [20]. Certain kinds of integrity constraints found in object-oriented databases are also common in semistructured databases. Some of these can be expressed as path constraints introduced in [5].

To illustrate the kinds of constraints that we want to capture, let us first investigate the constraints that are commonly placed on object-oriented databases. Con-

sider the following object-oriented schema (expressed in $O_2$ [6]):

```
class student{
      Name:     string;
      Taking:   set(course);
}

class course{
      CName:     string;
      Enrolled:  set(student);
}

Students:  set(student);
Courses:   set(course);
```

in which we assume that the declarations `Students` and `Courses` define (persistent) entry points into the database. As it stands, this declaration does not provide full information about the intended structure. Given such a database one would often expect the following informally stated constraints to hold:

(a) $\forall\, s \in Students\ \ \forall\, c \in s.Taking\ \ (c \in Courses)$

(b) $\forall\, c \in Courses\ \ \forall\, s \in c.Enrolled\ \ (s \in Students)$

That is, any course taken by a student must be a course that occurs in the database extent of courses, and any student enrolled in a course must be a student that similarly occurs in the database. We shall call such constraints *extent* constraints. It should be noted that there is a natural analogy between extent constraints and (unary) inclusion dependencies developed for relational databases.

We might also expect an *inverse relationship* to hold between `Taking` and `Enrolled`. Object-oriented databases differ in the ways they enable one to state and enforce extent constraints and inverse relationships. Compare, for example, $O_2$ [6] and ObjectStore [30].

Let us develop a more formal notation for describing such constraints. In our object-oriented database there are two sets of objects, `Students` and `Courses`. We express this in semistructured data by building a graph with a root node $r$ and a node for each object. Edges connect the root to these object nodes, and these edges are labeled either `Students` or `Courses`. Edges emanating from these nodes indicate attributes or relationships with other objects and are appropriately labeled. For example, a node representing a student object has a single `Name` edge connected to a string node, and multiple `Taking` edges connected to course nodes. See Figure 1 for an example of such a graph.

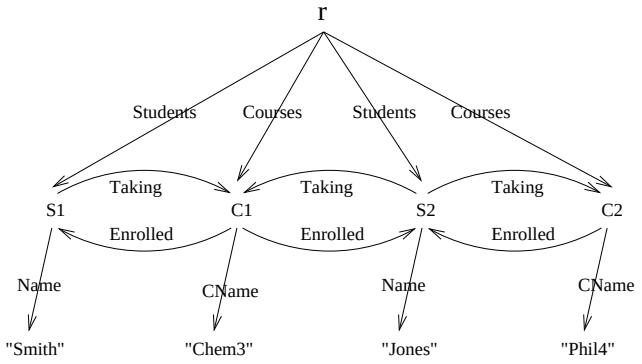


**Figure 1**: Representation of a student/course database

Using this representation of data we can examine certain kinds of constraints.

**Extent Constraints**. By taking edge labels as binary predicates, constraints of the form (a) and (b) above can be stated as:

$$\forall\, c\ (\exists\, s\ (Students(r,s) \wedge Taking(s,c)) \rightarrow Courses(r,c))$$

$$\forall\, s\ (\exists\, c\ (Courses(r,c) \wedge Enrolled(c,s)) \rightarrow Students(r,s))$$

Here $r$ is a constant denoting the root node, and variables $c$, $s$ range over vertices. The first constraint above states that any vertex that is reached from the root by following a `Students` edge followed by a `Taking` edge can also be reached from the root by following a `Courses` edge. Similarly, the second asserts that any vertex that is reached from the root by following a `Courses` edge followed by an `Enrolled` edge can also be reached from the root by following a `Students` edge.

These constraints are examples of "word constraints" studied in [5]; the implication problems for word constraints were shown to be decidable in semistructured databases there. Also studied in [5] was a form of constraints in which paths are represented by regular expressions. We do not consider this general form of constraints here.

**Inverse Constraints**. These are common in object-oriented databases [17]. With respect to our student/course schema, the inverse relationship between `Taking` and `Enrolled` is expressed as:

$$\forall\, s\ (Students(r,s) \rightarrow \forall\, c\ (Taking(s,c) \rightarrow Enrolled(c,s)))$$

$$\forall\, c\ (Courses(r,c) \rightarrow \forall\, s\ (Enrolled(c,s) \rightarrow Taking(s,c)))$$

The first constraint above states that for any student $s$

and any $c$, if $c$ is reachable from $s$ by following a `Taking` edge, then $s$ is also reachable from $c$ by following an `Enrolled` edge. Similarly, the second constraint asserts that for any course $c$ and any $s$, if $s$ is reachable from $c$ by following an `Enrolled` edge, then $c$ is also reachable from $s$ by following a `Taking` edge. Such constraints cannot be expressed as word constraints or even by the more general path constraints given in [5].

**Local Database Constraints**. In database integration it is sometimes desirable to make one database a component of another database, or to build a "database of databases". Suppose, for example, we want to bring together a number of student/course databases as described above. We might write something like:

```
class School-DB{
   DB-identifier:  string;
   Students:set(student); // as defined above
   Courses: set(course);  // as defined above
}

Schools:  set(School-DB);
```

Now we may want certain constraints to hold on components of this database. For example, the "extent constraints" and "inverse constraints" described above now hold on each member of the `Schools` set. Here we refer to a component database such as a member of the set `Schools` as a *local database* and its constraints as *local database constraints*. Extending our graph representation by adding `Schools` edges from a new root node to the roots of local databases, the local extent and inverse constraints are:

$$\forall\, d\,(Schools(r,d) \rightarrow \forall c\,(\exists\, s\,(Students(d,s) \wedge Taking(s,c)) \rightarrow Courses(d,c)))$$

$$\forall\, d\,(Schools(r,d) \rightarrow \forall\, s\,(\exists\, c\,(Courses(d,c) \wedge Enrolled(c,s)) \rightarrow Students(d,s)))$$

$$\forall\, s\,(\exists\, d\,(Schools(r,d) \wedge Students(d,s)) \rightarrow \forall c\,(Taking(s,c) \rightarrow Enrolled(c,s)))$$

$$\forall\, c\,(\exists\, d\,(Schools(r,d) \wedge Courses(d,c)) \rightarrow \forall s\,(Enrolled(c,s) \rightarrow Taking(s,c)))$$

Again, these cannot be stated as word constraints or by the more general constraints of [5].

These considerations give rise to the question whether there is a natural generalization of the constraints of [5] which will capture these slightly more complicated forms. Here we consider a class of path constraints, $P_c$, of either the form

$$\forall\, x\,(\alpha(r,x) \rightarrow \forall\, y\,(\beta(x,y) \rightarrow \gamma(x,y))),$$

or the form

$$\forall\, x\,(\alpha(r,x) \rightarrow \forall\, y\,(\beta(x,y) \rightarrow \gamma(y,x))),$$

where $\alpha(x,y)$ ($\beta(x,y)$, $\gamma(x,y)$) represents a path, i.e., a sequence of edge labels, from node $x$ to node $y$. As demonstrated above, $\alpha(x,y)$ can be expressed as a first-order logic formula with two free variables $x$ and $y$ by treating edge labels as binary predicates. The path constraint language $P_c$ is a mild generalization of the class of word constraints studied in [5].

This class of path constraints can be used to express all the integrity constraints we have so far encountered. These constraints are not only a fundamental part of the semantics of the data, but are also important in query optimization. They have proven useful in a variety of database contexts, ranging from semistructured data such as data on the World Wide Web and in XML documents, to structured data as found in object-oriented databases. In particular, among the numerous proposals for adding structure or semantics to XML documents, several [10, 26, 31, 32] advocate the need for these integrity constraints. In standard database systems, integrity constraints are typically expressed as part of the schema, but in semistructured data there is no explicit schema and path constraints provide a natural alternative.

To illustrate how these constraints might be used in query optimization, consider again the student/course database given in Figure 1. Suppose, for example, we want to find the names of all the courses enrolled by students who are taking the course "Chem3". Without the inverse and extent constraints described above, one would write the query as $Q_1$ (in OQL syntax [17]):

```
Q1      select distinct c.CName
        from   Courses c,
               c.Enrolled s,
               s.Taking c'
        where  c'.CName = "Chem3"
```

Given these inverse and extent constraints, one can show that $Q_1$ is equivalent to $Q_2$ given below:

```
Q2      select distinct c.CName
        from   Courses c',
               c'.Enrolled s,
               s.Taking c
        where  c'.CName = "Chem3"
```

In other words, given these constraints, one can rewrite $Q_1$ to $Q_2$. In most cases, $Q_2$ is more efficient than $Q_1$. Indeed, $Q_2$ complies with the familiar optimization principle originating in relational database theory: performing selections as early as possible.

To take advantage of path constraints, it is important to be able to reason about them. This gives rise to the question of logical implication, the most important theoretical question in connection with path constraints. In general, we may know that a set of path constraints is satisfied by a database. The question of logical implication is: what other path constraints are necessarily satisfied by the database? To see why logical implication is important, consider the queries $Q_1$ and $Q_2$ against the student/course database given above. To show that $Q_1$ can be rewritten to $Q_2$, the following constraints of $P_c$ are also needed in addition to the given inverse and extent constraints:

$$\forall s\ (\exists c'\ (Courses(r,\ c') \wedge Enrolled(c',\ s)) \rightarrow \forall c\ (Taking(s,\ c) \rightarrow Enrolled(c,\ s)))$$

$$\forall c\ (\exists c'\ (Courses(r,\ c') \wedge \exists s\ (Enrolled(c',\ s) \wedge Taking(s,\ c))) \rightarrow Courses(r,\ c))$$

To use these constraints, we need to show that they necessarily hold if the given extent and inverse constraints hold. That is, they are implied by the given path constraints.

There are two forms of implication problems associated with path constraints. Databases are usually considered to be finite. Logical implication is called *finite implication* for the case in which only finite database instances are permitted. It is also interesting to consider logical implication in the traditional logic framework in which infinite instances are also allowed. Logical implication is called *unrestricted implication*, or simply *implication*, for the case in which both finite database instances and infinite instances are permitted.

In the remainder of the paper, we investigate the implication and finite implication problems associated with path constraints of $P_c$ in the context of semistructured data. Surprisingly, the implication problems for this mild generalization of word constraints are undecidable, whereas the implication problems for word constraints are decidable in PTIME [5]. However, certain restricted cases are decidable, and these cases are sufficient to express at least the constraints we have described above.

**Related work.** There is a natural analogy between the work on path constraints and inclusion dependency theory developed for relational databases (see, e.g., [3] for an in-depth presentation of inclusion dependency theory). Path constraints specify inclusions among certain sets of objects, and can be viewed as a generalization of inclusion dependencies. Inclusion dependencies have proven useful in semantic specification and query optimization for relational databases. In the same way, path constraints are important in a variety of database contexts, ranging from semistructured data to object-oriented databases.

Another form of constraints defined in terms of navigation paths, called *path functional dependencies*, has been studied by Weddell, et al. [8, 29]. These constraints differ significantly from the path constraints investigated here because they are a generalization of functional dependencies for a restricted type system, while $P_c$ constraints can be viewed as a generalization of inclusion dependencies for both semistructured and structured databases.

Closer to the work reported here is the path inclusion constraint language introduced and investigated by Abiteboul and Vianu in [5]. A constraint in this language is an expression of the form $p \subseteq q$ or $p = q$, where $p$ and $q$ are regular expressions representing paths. In particular, if $p$ and $q$ are simply paths, i.e., sequences of edge labels, the constraint is called a *word constraint*. Such a constraint expresses the inclusion or equality relation between the two sets of nodes reachable along $p$ and $q$. The decidability of the implication problems for this language was established for semistructured data in [5]. In addition, it was also shown there that word constraint implication is decidable in PTIME. This constraint language differs from the constraint language $P_c$ in expressive power. On the one hand, the language of [5] allows a more general form of path expressions than $P_c$. On the other hand, it cannot express inverse and local database constraints, whereas these constraints are expressible in $P_c$.

Recently, the application of integrity constraints to query optimization was also studied by Popa and Tannen in [35]. Among other things, [35] developed an equational theory for query rewriting by using a certain form of constraints. Semantic optimization has also been investigated for semistructured databases in [13, 24] and for structured databases in [18, 19, 25].

Another issue is the interaction between path constraints and types. Structured data, e.g., data in object-oriented databases, is constrained by a schema, in which both types and integrity constraints are specified. In addition, although the XML standard itself does not require any type system, a number of proposals [10, 26, 32] have been developed that roughly correspond to data definition languages. These allow one to constrain the structure of XML data by imposing a type on it. These and other proposals (e.g., [31]) also advocate the need for integrity constraints, which can be expressed as path constraints. The type system or schema definition may also be viewed as imposing a constraint on the data. It is a constraint of a different form. That is, type con-

straints cannot be expressed as path constraints and *vice versa*. In structured data and possibly in XML documents both forms of constraints are present, and therefore, we need to understand the interaction between them. In general we can no longer expect results developed for semistructured data to hold when a type is imposed on the data. In other words, the imposition of a type can alter the computational complexity of the path constraint implication problem in unexpected ways. Indeed, in [16] we have shown that adding a type system may in some cases simplify the analysis of path constraint implication, and in other cases make it harder. More specifically, some decidability results on path constraint implication developed for semistructured data break down when some type system is added, and on the other hand, some undecidability results on untyped data also collapse when some type constraint is imposed. This issue was first addressed in [15] and then treated in detail in [16].

**Organization.** The remainder of the paper is organized as follows. Section 2 formally presents our path constraint language $P_c$. Section 3 establishes the undecidability of the implication and finite implication problems associated with $P_c$ in the context of semistructured databases. Section 4 identifies several fragments of $P_c$, and shows that the implication and finite implication problems for each of these fragments are decidable in semistructured databases. It also demonstrates that these fragments suffice to express many important integrity constraints such as extent, inverse and local database constraints. Finally, Section 5 summarizes our results.

## 2 PATH CONSTRAINTS

In this section, we first present an abstraction of semistructured databases in terms of first-order logic, and then define paths and path constraints of $P_c$.

### 2.1 Semistructured Databases

Semistructured data is usually represented as an edge-labeled (rooted) directed graph, e.g., in UnQL [14] and in OEM [4, 34]. See [2, 12] for surveys of semistructured data models. Along the same lines, here we use an abstraction of semistructured databases as (finite) first-order logic structures of a relational signature

$$\sigma = (r,\ E),$$

where $r$ is a constant denoting the root and $E$ is a finite set of binary relation symbols denoting the edge labels.

We specify a *$\sigma$-structure* $G$ by giving $(|G|,\ r^G,\ E^G)$, where

- $|G|$ is a set called the *universe* (*domain*) of $G$, and elements of $|G|$ are called the *nodes* (*vertices*) of $G$;
- $r^G$ is a distinguished element of $|G|$, called the *root node* of $G$;
- $E^G$ is a finite set of binary relations on $|G|$, each of which is named by a relation symbol of $E$. For any $K \in E$, we write $K^G$ for the relation in $G$ named by $K$.

Structure $G$ can be naturally depicted as a rooted edge-labeled directed graph with $|G|$ as the set of vertices, $E^G$ the set of labeled edges and $r^G$ the root. For any $K \in E$ and $a, b \in |G|$, there is an edge labeled $K$ from $a$ to $b$ in the graph if and only if $(a, b) \in K^G$.

It should be mentioned that we do not assume the reachability of all nodes from the root in a $\sigma$-structure (graph). However, none of our results or proofs are affected if reachability is enforced.

### 2.2 Paths

A path, i.e., a sequence of labels, can be represented as a logic formula with two free variables. More specifically, a path is a first-order logic formula $\alpha(x, y)$ of one of the following forms:

- $x = y$, denoted by $\epsilon(x, y)$ and called an *empty path*;
- $K(x, y)$, where $K \in E$; or
- $\exists z(K(x, z) \wedge \beta(z, y))$, where $K \in E$ and $\beta(z, y)$ is a path.

Here the free variables $x$ and $y$ denote the tail and head nodes of the path, respectively. We write $\alpha(x,\ y)$ as $\alpha$ when the parameters $x$ and $y$ are clear from the context. In particular, we may replace free variable $x$ or $y$ by $r$, where $r$ is the constant denoting the root given in signature $\sigma$. That is, we use $\alpha(r,\ y)$ or $\alpha(x,\ r)$ to denote a path from or to the root.

We have seen many examples of paths in Section 1. Among them are:

$$\exists\, z\, (Students(x,\ z) \wedge Taking(z,\ y))$$

$$\exists\, z\, (Courses(x,\ z) \wedge \exists\, w\, (Enrolled(z,\ w) \wedge Taking(w,\ y)))$$

The *concatenation* of paths $\alpha(x,z)$ and $\beta(z,y)$, denoted by $\alpha(x,z)\cdot\beta(z,y)$ or simply $\alpha\cdot\beta(x,y)$, is the path

- $\beta(x,y)$, if $\alpha=\epsilon$;
- $\exists\, z\,(K(x,z)\wedge\beta(z,y))$, if $\alpha=K$ for some $K\in E$;
- $\exists\, u\,(K(x,u)\wedge(\alpha'(u,z)\cdot\beta(z,y)))$, if $\alpha(x,z)$ is of the form $\exists\, u\,(K(x,u)\wedge\alpha'(u,z))$, where $K\in E$ and $\alpha'$ is a path.

For example, the paths above can be written as:

$$Students\cdot Taking(x,y)$$
$$Courses\cdot Enrolled\cdot Taking(x,y)$$

We use $(\alpha)^m$ to denote the $m$-time concatenations of $\alpha$, defined by:

$$(\alpha)^m \;=\; \begin{cases} \epsilon & \text{if } m=0 \\ \alpha\cdot(\alpha)^{m-1} & \text{otherwise} \end{cases}$$

A path $\rho$ is said to be a *proper prefix* of $\varrho$, denoted by $\rho\prec_p\varrho$, iff there exists a path $\lambda$ such that $\lambda\neq\epsilon$ and $\varrho=\rho\cdot\lambda$. A path $\rho$ is said to be a *prefix* of $\varrho$, denoted by $\rho\preceq_p\varrho$, iff $\rho\prec_p\varrho$ or $\rho=\varrho$. Similarly, $\rho$ is said to be a *suffix* of $\varrho$, denoted by $\rho\preceq_s\varrho$, iff there exists $\lambda$ such that $\varrho=\lambda\cdot\rho$.

For example, the path $Courses\cdot Enrolled\cdot Taking$ has the following prefixes: the empty path $\epsilon$, $Courses$, $Courses\cdot Enrolled$ and itself. Its suffixes include $\epsilon$, $Taking$, $Enrolled\cdot Taking$ and itself.

The *length* of path $\alpha$, $|\alpha|$, is defined by:

$$|\alpha| \;=\; \begin{cases} 0 & \text{if } \alpha=\epsilon \\ 1 & \text{if } \alpha=K \\ 1+|\beta| & \text{if } \alpha=K\cdot\beta \end{cases}$$

For example, $|Courses\cdot Enrolled\cdot Taking|=3$ and $|Students\cdot Taking|=2$.

In particular, a path of the form $\alpha(r,x)$ or $\alpha(x,r)$, i.e., a path from or to the root, can be expressed as a first-order logic formula with at most two *distinct* variables. For example, the path

$$Students\cdot Taking\cdot Enrolled\cdot Taking(r,\,x)$$

can be expressed as:

$$\exists\, y\;(Taking(y,\,x)\wedge\exists\, x\;(Enrolled(x,\,y)\wedge \exists\, y\;(Taking(y,\,x)\wedge Students(r,\,y))))$$

Observe that this logic formula uses only two distinct variables. In general, a path $\alpha(x,\,y)$ can be expressed as a first-order logic formula with at most three distinct variables.

### 2.3 Path Constraint Language $P_c$

By using path formulas, the path constraint language $P_c$ is formalized as follows.

**Definition 2.1:** A *path constraint* $\varphi$ is an expression of either the *forward* form

$$\forall\, x\,(\alpha(r,\,x)\rightarrow\forall\, y\,(\beta(x,\,y)\rightarrow\gamma(x,\,y))),$$

or the *backward* form

$$\forall\, x\,(\alpha(r,\,x)\rightarrow\forall\, y\,(\beta(x,\,y)\rightarrow\gamma(y,\,x))),$$

where $\alpha,\beta,\gamma$ are paths, called the *prefix*, *left tail* and *right tail* of $\varphi$, and denoted by $pf(\varphi)$, $lt(\varphi)$ and $rt(\varphi)$, respectively.

A path constraint is called a *forward constraint* if it is of the forward form, and is called a *backward constraint* if it is of the backward form.

The set of all path constraints is denoted by $P_c$. ∎

For example, all the path constraints we have seen in Section 1 are $P_c$ constraints. Among these, the extent and local extent constraints are examples of forward constraints, while the inverse and local inverse constraints are backward constraints. By using path concatenation "·", we may represent these constraints in a simpler form. For example, the extent constraints given in Section 1 can be rewritten as:

$$\forall\, c\,(Students\cdot Taking(r,\,c)\rightarrow Courses(r,\,c))$$
$$\forall\, s\,(Courses\cdot Enrolled(r,\,s)\rightarrow Students(r,\,s))$$

A forward constraint of $P_c$ asserts that for any vertex $x$ that is reached from the root $r$ by following path $\alpha$ and for any vertex $y$ that is reached from $x$ by following path $\beta$, $y$ is also reachable from $x$ by following path $\gamma$. Similarly, a backward $P_c$ constraint states that for any $x$ that is reached from $r$ by following $\alpha$ and for any $y$ that is reached from $x$ by following $\beta$, $x$ is also reachable from $y$ by following $\gamma$.

As demonstrated in Section 1, path constraints of $P_c$ are capable of expressing, among other things, extent, inverse and local database constraints.

Next, we identify several special subclasses of $P_c$.

We call a path constraint $\varphi$ of $P_c$ a *simple (path) constraint* if $pf(\varphi)=\epsilon$. That is, the prefix of $\varphi$ is an empty path. More specifically, $\varphi$ is of either the form

$$\forall\, y\,(\beta(r,y)\rightarrow\gamma(r,y)),$$

or the form

$$\forall\, y\,(\beta(r,y)\rightarrow\gamma(y,r)).$$

The set of all simple path constraints is denoted by $P_s$.

A proper subclass of simple path constraints, called *word constraints*, was introduced and investigated in [5]. A word constraint can be represented as

$$\forall\, y\, (\beta(r, y) \rightarrow \gamma(r, y)),$$

where $\beta$ and $\gamma$ are paths. The set of all word constraints is denoted by $P_w$.

In other words, a word constraint is a simple forward path constraint of $P_c$. As demonstrated in Section 1, extent constraints can be expressed as word constraints. However, inverse and local database constraints are not expressible in $P_w$.

We borrow the standard notions of model and implication from first-order logic [22].

Let $G$ be a $\sigma$-structure and $\varphi$ a $P_c$ constraint. We use $G \models \varphi$ to denote that $G$ *satisfies* $\varphi$ (i.e., $G$ *is a model of* $\varphi$). Let $\Sigma$ be a set of $P_c$ constraints. We use $G \models \Sigma$ to denote that $G$ *satisfies* $\Sigma$ (i.e., $G$ *is a model of* $\Sigma$). That is, for every $\phi \in \Sigma$, $G \models \phi$.

Let $\Sigma \cup \{\varphi\}$ be a finite subset of $P_c$. We use $\Sigma \models \varphi$ to denote that $\Sigma$ *implies* $\varphi$. That is, for every $\sigma$-structure $G$, if $G \models \Sigma$, then $G \models \varphi$. Similarly, we use $\Sigma \models_f \varphi$ to denote that $\Sigma$ *finitely implies* $\varphi$. That is, for every finite $\sigma$-structure $G$, if $G \models \Sigma$, then $G \models \varphi$.

In the context of semistructured databases, the *implication problem for* $P_c$ is the problem of determining, given any finite subset $\Sigma \cup \{\varphi\}$ of $P_c$, whether $\Sigma \models \varphi$. Similarly, the *finite implication problem for* $P_c$ is the problem of determining, given any finite subset $\Sigma \cup \{\varphi\}$ of $P_c$, whether $\Sigma \models_f \varphi$.

As observed by [5], every word constraint (in fact, every simple path constraint) can be expressed by a sentence in two-variable first-order logic ($FO^2$), the fragment of first-order logic consisting of all relational sentences with at most two distinct variables. Recently, Grädel, Kolaitis and Vardi [27] have shown that the satisfiability problem for $FO^2$ is NEXPTIME-complete by establishing that any satisfiable $FO^2$ sentence has a model of size exponential in the length of the sentence. The decidability of the implication and finite implication problems for word constraints follows immediately. In fact, [5] directly established (without reference to the embedding into $FO^2$) that the implication and finite implication problems for word constraints are in PTIME.

In contrast to word constraints, many path constraints of $P_c$ are not expressible in $FO^2$.

**Example 2.1:** Consider the structures $G$ and $G'$ given in Figure 2. It is easy to verify, using the 2-pebble

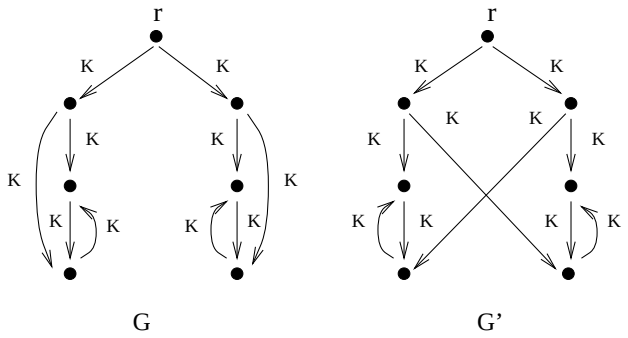


**Figure 2**: Structures distinguishable by $P_c$

Ehrenfeucht-Fraïssé style game [7, 21, 28], that $G$ and $G'$ are equivalent in $FO^2$. However, $G$ and $G'$ are distinguished by the path constraint

$$\varphi = \forall\, x\, (K(r, x) \rightarrow \forall\, y\, (K(x, y) \rightarrow K \cdot K(x, y))),$$

because $G \models \varphi$ but $G' \not\models \varphi$. This shows that $\varphi$ is not expressible in $FO^2$. ∎

The central technical problems investigated in this paper are the implication and finite implication problems for $P_c$, and fragments thereof, in the context of semistructured databases.

## 3 UNDECIDABLE IMPLICATION PROBLEMS

In this section, we show that despite the simple syntax of $P_c$, the implication and finite implication problems for $P_c$ are undecidable in the context of semistructured databases.

**Theorem 3.1:** The implication problem for $P_c$ is r.e. complete, and the finite implication problem for $P_c$ is co-r.e. complete. ∎

In fact, these undecidability results also hold for two proper subclasses of $P_c$. One of the subclasses, $P_f$, is the set of all the constraints of $P_c$ having the forward form. The other, $P_+$, is the set

$$\{\varphi \mid \varphi \in P_c,\ lt(\varphi) \neq \epsilon,\ rt(\varphi) \neq \epsilon\},$$

where $lt(\varphi)$ and $rt(\varphi)$ are described in Definition 2.1. The set $P_+$ is the largest subset of $P_c$ without equality.

For $P_+$ and $P_f$ we have the following theorems, from which Theorem 3.1 follows immediately.

**Theorem 3.2:** The implication problem for $P_+$ is r.e. complete, and the finite implication problem for $P_+$ is co-r.e. complete. ∎

**Theorem 3.3:** The implication problem for $P_f$ is r.e.

complete, and the finite implication problem for $P_f$ is co-r.e. complete. ∎

To prove Theorem 3.2, we consider the satisfiability and finite satisfiability problems corresponding to $P_f$ constraint implication. First recall the following.

Let $X$ be a recursive class of logic sentences. The *satisfiability problem* for $X$ is the problem of determining, given any $\psi \in X$, whether $\psi$ has a model. The *finite satisfiability problem* for $X$ is to determine, given any $\psi \in X$, whether $\psi$ has a finite model.

The (finite) implication problem for $P_f$ corresponds to the (finite) satisfiability problem for the following set:

$$S(P_+) = \{\bigwedge \Sigma \wedge \neg\varphi \mid \varphi \in P_+,\ \Sigma \subset P_+,\ \Sigma \text{ is finite}\}.$$

More specifically, to prove Theorem 3.2, it suffices to show that the satisfiability problem for $S(P_+)$ is co-r.e. complete and the finite satisfiability problem for $S(P_+)$ is r.e. complete. The idea of the proof is to show that there exists a conservative reduction from the set of all first-order logic sentences to $S(P_+)$. To do this, we establish a reduction from the halting problem for two-register machines.

Along the same lines, to prove Theorem 3.3 we consider the set

$$S(P_f) = \{\bigwedge \Sigma \wedge \neg\varphi \mid \varphi \in P_f,\ \Sigma \subset P_f,\ \Sigma \text{ is finite}\}.$$

We show that there exists a conservative reduction from the set of all first-order logic sentences to $S(P_f)$. Again, this is established by reduction from the halting problem for two-register machines.

We prove Theorems 3.2 and 3.3 in Sections 3.2 and 3.3, respectively. Before we present these proofs, we first recall the definitions of conservative reductions and two-register machines (2-RMs. See, e.g., [1, 9]).

### 3.1 Conservative Reduction and 2-RM

We first review the notion of conservative reductions. To do so, we borrow the following notations from [1, 9].

Let $X$ be a class of sentences. We write $N(X)$ for the set of all *unsatisfiable* sentences in $X$, i.e.,

$$N(X) = \{\psi \mid \psi \in X,\ \psi \text{ does not have a model}\},$$

and $F(X)$ for the set of all *finitely satisfiable* sentences in $X$, i.e.,

$$F(X) = \{\psi \mid \psi \in X,\ \psi \text{ has a finite model}\}.$$

We write $FO$ for the set of all first-order sentences.

Conservative reductions are defined as follows.

**Definition 3.1 [9]:** Let $X$ and $Y$ be recursive classes of sentences. A *conservative reduction* from $X$ to $Y$ is a recursive function $f : X \to Y$ such that for any $\psi \in X$,

- $\psi$ is satisfiable iff $f(\psi)$ is satisfiable; and
- $\psi$ is finitely satisfiable iff $f(\psi)$ is finitely satisfiable.

A recursive class of sentences $X$ is said to be a *conservative reduction class* if there exists a conservative reduction from $FO$ to $X$. ∎

Recall that the satisfiability problem for $FO$ is well known to be co-r.e. complete, and the finite satisfiability problem for $FO$ is r.e. complete. Hence, if a recursive class of sentences $X$ is a conservative reduction class, then,

- the satisfiability problem for $X$ is co-r.e. complete; and
- the finite satisfiability problem for $X$ is r.e. complete.

As a result, to show Theorems 3.2 and 3.3, it suffices to show that $S(P_+)$ and $S(P_f)$ are conservative reduction classes.

To show that a recursive subset $X$ of $FO$ is a conservative reduction class, it suffices to reduce $N(FO)$ and $F(FO)$ to $N(X)$ and $F(X)$, respectively. This is described by the notion of semi-conservative reductions.

**Definition 3.2 [9]:** Let $X$ and $Y$ be recursive classes of sentences. A *semi-conservative reduction* from $X$ to $Y$ is a recursive function $f : X \to Y$ such that

- $f(N(X)) \subseteq N(Y)$; and
- $f(F(X)) \subseteq F(Y)$. ∎

**Lemma 3.4 [9]:** If there exists a semi-conservative reduction from $FO$ to a recursive subset $X$ of $FO$, then $X$ is a conservative reduction class. ∎

Hence, to show Theorems 3.2 and 3.3, it suffices to establish the existence of semi-conservative reductions from $FO$ to $S(P_+)$ and $S(P_f)$.

We shall proceed to construct the semi-conservative reductions by making use of the halting problem for two-register machines. Before we present the construction, we first review the notion of two-register machines.

A two-register machine (2-RM) $M$ has two registers $register_1, register_2$, and is programmed by a numbered sequence $I_0, I_1, ..., I_l$ of instructions. Each register contains a natural number. An *instantaneous description*

($ID$) of $M$ is $(i, m, n)$, where $i \in [0, l]$, $m$ and $n$ are natural numbers. It indicates that $M$ is ready to execute instruction $I_i$ (or at "state $i$") with $register_1$ and $register_2$ containing $m$ and $n$, respectively.

An instruction $I_i$ of $M$ can be either an *addition* or a *subtraction*, which defines a relation $\rightarrow_M$ between IDs, described as follows:

- *addition*: $(i, rg, j)$, where $rg$ is either $register_1$ or $register_2$, and $0 \leq i, j \leq l$. Its semantics is: at state $i$, $M$ adds 1 to the content of $rg$, and then goes to state $j$. Accordingly:

$$(i, m, n) \rightarrow_M \begin{cases} (j, m+1, n) & \text{if } rg = register_1 \\ (j, m, n+1) & \text{otherwise} \end{cases}$$

- *subtraction*: $(i, rg, j, k)$, here $rg$ is either $register_1$ or $register_2$, and $0 \leq i, j, k \leq l$. Its semantics is: at state $i$, $M$ tests whether the content of $rg$ is 0, and if it is, then goes to state $j$; otherwise $M$ subtracts 1 from the content of $rg$ and goes to the state $k$. Accordingly:

$$(i, m, n) \rightarrow_M \begin{cases} (j, 0, n) & \text{if } rg = register_1 \text{ and } m = 0 \\ (k, m-1, n) & \text{if } rg = register_1 \text{ and } m \neq 0 \\ (j, m, 0) & \text{if } rg = register_2 \text{ and } n = 0 \\ (k, m, n-1) & \text{if } rg = register_2 \text{ and } n \neq 0 \end{cases}$$

The relation $\rightarrow_M$ can be understood as a set of rewrite rules for IDs. We use $\Rightarrow_M$ to denote the reflexive and transitive closure of $\rightarrow_M$. The relation of *M-reachability* $C \Rightarrow_M D$ holds just in case $M$, started from ID $C$, reaches ID $D$ by application of zero or more $\rightarrow_M$ rules.

A two-register machine may halt at some states. Without loss of generality, one can assume that a halting state has zeros in both registers. That is, halting IDs have the form $(i, 0, 0)$, where $i$ is a halting state and $0 \leq i \leq l$.

Recall the following well-known result.

**Lemma 3.5 [36]:** There exists an effective partial procedure by which, given a sentence in $FO$, we can test whether it has no model, a finite model, or only infinite models. The procedure terminates in the first two cases, but does not terminate in the last case. ■

We fix $M_L$ to be a 2-RM with the following behavior (the existence of such a machine follows from the result just quoted. See [1, 9] for further discussion). The 2-RM $M_L$ has two halting states: $(1, 0, 0)$ and $(2, 0, 0)$. For each $\psi \in FO$, let $m(\psi)$ be an appropriate encoding of $\psi$ (a natural number) and $C(\psi)$ be the ID $(0, m(\psi), 0)$ of $M_L$. Started from $C(\psi)$,

- $M_L$ halts at (1, 0, 0) iff $\psi$ is not satisfiable; and
- $M_L$ halts at (2, 0, 0) iff $\psi$ has a finite model.

In other words, $M_L$ has the following property: for $i = 1, 2$, let

$$H_{M_L,i} = \{\psi \mid \psi \in FO,\ C(\psi) \Rightarrow_{M_L} (i, 0, 0)\}.$$

Then $H_{M_L,1}$ is $N(FO)$ and $H_{M_L,2}$ is $F(FO)$.

If we can encode the description and computations of this 2-RM in terms of path constraints, we can transform certain decision problems regarding $FO$ sentences to the problems for path constraints. More specifically, the idea of the proof of Theorem 3.2 is to encode the description and computations of $M_L$ in terms of $P_+$ constraints. Using this encoding, we are able to define a recursive function $f : FO \rightarrow S(P_+)$ such that for each $\psi \in FO$,

1. if $\psi \in H_{M_L,1}$, then $f(\psi)$ is not satisfiable; and
2. if $\psi \in H_{M_L,2}$, then $f(\psi)$ has a finite model.

That is, $f$ is a semi-conservative reduction from $FO$ to $S(P_+)$.

We can prove Theorem 3.3 along the same lines.

### 3.2 Implication Problems for $P_+$

Next, we prove Theorem 3.2. It suffices to show that $S(P_+)$ is a conservative reduction class. By Lemma 3.4, to establish the conservative reduction class property for $S(P_+)$, it is sufficient to show that there is a semi-conservative reduction from $FO$ to $S(P_+)$.

We establish the existence of the semi-conservative reduction by reduction from the halting problem for 2-RMs. To do this, we first present an encoding of 2-RMs in terms of constraints in $P_+$, and then prove a reduction property of the encoding. Using this reduction property, we define a semi-conservative reduction from $FO$ to $S(P_+)$.

#### 3.2.1 Encoding

We encode the IDs, the contents of the registers and the instructions of a 2-RM in terms of $P_+$ constraints.

Let $M$ be a 2-RM. Assume that $M$ is programmed by

$$I_0,\ I_1,\ \ldots,\ I_l.$$

Without loss of generality, we also assume that the set $E$ of binary relation symbols in signature $\sigma$ includes:

- predicates encoding the states of $M$:
  - $K_0, K_1, ..., K_l$,
  - $K_0^-, K_1^-, ..., K_l^-$;
- predicates encoding the contents of the registers:
  - $R_1^+, R_1^-$: to encode the successor and predecessor of the content of $register_1$;
  - $R_2^+, R_2^-$: to encode the successor and predecessor of the content of $register_2$;
  - $E_{01}, E_{01}^-$: to indicate that $register_1$ is 0;
  - $E_{02}, E_{02}^-$: to indicate that $register_2$ is 0;
- predicates distinguishing $register_1$ from $register_2$ and identifying the root $r$:
  - $L_1, L_1^-$: to identify $register_1$;
  - $L_2, L_2^-$: to identify $register_2$; and
  - $L_r$: to identify the root $r$.

We should remark that all these predicates are binary. Using these predicates, we intend to construct structures of the form shown in Figure 3 ($E_{01}^-$, $E_{02}^-$, $L_1^-$, $L_2^-$, $R_1^-$, $R_2^-$, $K_i^-$ edges are omitted in the graph). Figure 3 illustrates the encoding of the 2-RM $M$. It has (at least) two chains from the root node $rt$. One starts with an edge labeled $E_{01}$ followed by a sequence of $R_1^+$ edges. The nodes in the chain are denoted by natural numbers and intend to represent the contents of $register_1$ of $M$. The $R_1^+$ edges can be viewed as the successor relation on the contents of $register_1$. In addition, there are $R_1^-$ edges (not shown in the graph), which form the inverse relation of $R_1^+$ edges and can be viewed as the predecessor relation on the contents of $register_1$. The $E_{01}$ edge indicates that $register_1$ has 0. There is also an $E_{01}^-$ edge (not shown in the graph), which is the inverse of $E_{01}$. To each node in the chain there is an edge labeled $L_1$ from the root $rt$. These $L_1$ edges are used to identify $register_1$. There are also $L_1^-$ edges (not shown in the graph), which are the inverse of $L_1$ edges. Similarly, the other chain starts with an edge labeled $E_{02}$ followed by a sequence of $R_2^+$ edges. It encodes the contents of $register_2$. Moreover, for each $i \in [0, l]$, there are $K_i$ edges from the nodes in the chain encoding $register_1$ to the nodes in the chain representing $register_2$. For example, as shown in Figure 3, there is a $K_i$ edge from $m$ to $n'$. This indicates that an ID of $M$ is ($i$, $m$, $n$). For the ease of encoding, we also have $K_i^-$ edges (not shown in the graph), which form the inverse relation of

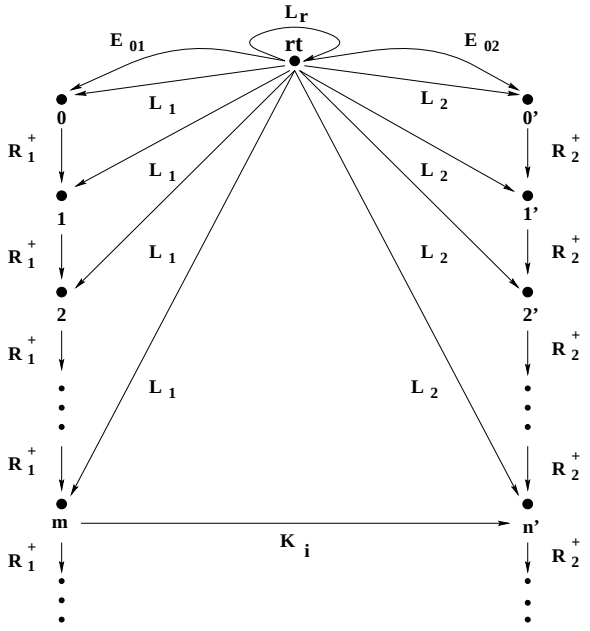


**Figure 3**: A structure depicting 2-RM encoding

$K_i$ edges. Finally, there is an edge labeled $L_r$ from $rt$ to $rt$, which is used to identify the root.

The above requirements on the structure encoding the computations of the 2-RM $M$ can be expressed by $P_+$ constraints. We should remark here that we need not require the structure to consist of only these two chains. Indeed, the structure may have many such chains and others. To prove our results, it suffices that our structure has at least two chains with the properties mentioned above.

We now present the encoding of $M$ in terms of $P_+$ constraints.

**IDs.** We encode each ID $C = (i, m, n)$ of $M$ by $\varphi_C$:

$$\forall x\,(L_1(r,x) \rightarrow \\ \forall y\,((R_1^-)^m \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^n(x,y) \rightarrow K_i(x,y))),$$

where $(\alpha)^m$ stands for the $m$-time concatenations of $\alpha$, as defined in Section 2. It should be noted that $\varphi_C$ is a forward constraint in $P_+$ with $pf(\varphi_C) = L_1$, $lt(\varphi_C) = (R_1^-)^m \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^n$, and $rt(\varphi_C) = K_i$, where $pf$, $lt$ and $rt$ are described in Definition 2.1.

Observe that we require the contents of $register_1$ and $register_2$ to be encoded in a single path $lt(\varphi_C)$. This leads to a lack of symmetry in the treatment of the two registers in the encoding. In particular, the content of $register_1$, encoded as $(R_1^-)^m$, is a prefix of $lt(\varphi_C)$, and the content of $register_2$, encoded as $(R_2^+)^n$, is a suffix of $lt(\varphi_C)$.

**Registers.** We encode the contents of the registers by $\Phi_N$, which is the conjunction of the constraints of $P_+$ given below.

- Successor, predecessor:

$$\begin{aligned}
\phi_1 &= \forall\, x\,(L_1(r,x) \rightarrow \forall\, y\,(R_1^+(x,y) \rightarrow R_1^-(y,x)))\\
\phi_2 &= \forall\, x\,(L_1(r,x) \rightarrow \forall\, y\,(R_1^-(x,y) \rightarrow R_1^+(y,x)))\\
\phi_3 &= \forall\, x\,(L_2(r,x) \rightarrow \forall\, y\,(R_2^+(x,y) \rightarrow R_2^-(y,x)))\\
\phi_4 &= \forall\, x\,(L_2(r,x) \rightarrow \forall\, y\,(R_2^-(x,y) \rightarrow R_2^+(y,x)))\\
\phi_5 &= \forall\, x\,(L_1(r,x) \rightarrow R_1^+ \cdot L_1^-(x,r))\\
\phi_6 &= \forall\, x\,(L_2(r,x) \rightarrow R_2^+ \cdot L_2^-(x,r))
\end{aligned}$$

  These are backward constraints. Constraints $\phi_1$ and $\phi_2$ (resp. $\phi_3$ and $\phi_4$) specify that $R_1^+$ and $R_1^-$ (resp. $R_2^+$ and $R_2^-$) are inverse to each other. Constraints $\phi_5$ and $\phi_6$ assert that the contents of $register_1$ and $register_2$ always have successors.

- Register identification:

$$\begin{aligned}
\phi_7 &= \forall\, x\,(L_1 \cdot R_1^+(r,x) \rightarrow L_1(r,x))\\
\phi_8 &= \forall\, x\,(L_1 \cdot R_1^-(r,x) \rightarrow L_1(r,x))\\
\phi_9 &= \forall\, x\,(L_2 \cdot R_2^+(r,x) \rightarrow L_2(r,x))\\
\phi_{10} &= \forall\, x\,(L_2 \cdot R_2^-(r,x) \rightarrow L_2(r,x))
\end{aligned}$$

  These are simple forward constraints. They ensure that for each node coding a content of $register_1$, there is always an edge labeled $L_1$ from the root to it. Similarly, for any node representing a content of $register_2$, there is an edge labeled $L_2$ from the root to it.

- States: for $i \in [0,l]$,

$$\begin{aligned}
\phi_{11}^i &= \forall\, x\,(L_1(r,x) \rightarrow \forall\, y\,(K_i(x,y) \rightarrow K_i^-(y,x)))\\
\phi_{12}^i &= \forall\, x\,(L_2(r,x) \rightarrow \forall\, y\,(K_i^-(x,y) \rightarrow K_i(y,x)))
\end{aligned}$$

  These are backward constraints. They assert that there is an inverse relationship between $K_i$ and $K_i^-$ for each $i \in [0,l]$.

- Zeros:

$$\begin{aligned}
\phi_{13} &= \forall\, x\,(L_1(r,x) \rightarrow \forall\, y\,(E_{01}^-(x,y) \rightarrow E_{01}(y,x)))\\
\phi_{14} &= \forall\, x\,(L_1 \cdot E_{01}^-(r,x) \rightarrow L_r(r,x))\\
\phi_{15} &= \forall\, x\,(L_r \cdot E_{01}(r,x) \rightarrow E_{01}(r,x))\\
\phi_{16} &= \forall\, x\,(L_1 \cdot E_{01}^- \cdot E_{02}(r,x) \rightarrow E_{02}(r,x))\\
\phi_{17} &= \forall\, x\,(E_{01}(r,x) \rightarrow L_1(r,x))\\
\phi_{18} &= \forall\, x\,(E_{02}(r,x) \rightarrow L_2(r,x))
\end{aligned}$$

  Constraints $\phi_{13}$, $\phi_{14}$ and $\phi_{15}$ assert that if there is an edge labeled $L_1$ from the root to a node $a$ and $a$ has an outgoing edge labeled $E_{01}^-$, then there is an edge labeled $E_{01}$ from the root to $a$. Constraint $\phi_{16}$ ensures that if there exists a path $L_1 \cdot E_{01}^- \cdot E_{02}$ from the root to a node $b$, then there is an $E_{02}$ edge from the root to $b$. Constraint $\phi_{17}$ states that there is an edge labeled $L_1$ from the root to a node coding 0 in $register_1$. Similarly, $\phi_{18}$ states that there is an edge labeled $L_2$ from the root to a node coding 0 in $register_2$.

It should be mentioned that the constraints given above enforce stronger properties than necessary. Some of these constraints are not used in the proofs of our results. We retain these constraints to simply the constructions below.

**Instructions.** For each $i \in [0,l]$, we encode the instruction $I_i$ by $\phi_{I_i}$ given below. Constraint $\phi_{I_i}$ describes the relation $\rightarrow_M$ presented in Section 3.1.

- Addition:

  For $(i, register_1, j)$, $\phi_{I_i}$ is

$$\begin{aligned}
\phi_{a_1}^i = \forall\, x\,(&L_1(r,x) \rightarrow\\
&\forall\, y\,(R_1^- \cdot K_i(x,y) \rightarrow K_j(x,y))).
\end{aligned}$$

  For $(i, register_2, j)$, $\phi_{I_i}$ is

$$\begin{aligned}
\phi_{a_2}^i = \forall\, x\,(&L_1(r,x) \rightarrow\\
&\forall\, y\,(K_i \cdot\ R_2^+(x,y) \rightarrow K_j(x,y))).
\end{aligned}$$

  Note that $\phi_{a_1}^i$ and $\phi_{a_2}^i$ are forward constraints.

- Subtraction:

  For $(i, register_1, j, k)$, $\phi_{I_i}$ is $\phi_{s_1}^i = \phi_{s_{1,0}}^i \wedge \phi_{s_{1,n}}^i$, where

$$\begin{aligned}
\phi_{s_{1,0}}^i &= \forall\, x\,(E_{01}(r,x) \rightarrow \forall\, y\,(K_i(x,y) \rightarrow K_j(x,y))),\\
\phi_{s_{1,n}}^i &= \forall\, x\,(L_1(r,x) \rightarrow\\
&\qquad \forall\, y\,(R_1^+ \cdot K_i(x,y) \rightarrow K_k(x,y))).
\end{aligned}$$

  Note that $\phi_{s_{1,0}}^i$ and $\phi_{s_{1,n}}^i$ are forward constraints.

  For $(i, register_2, j, k)$, $\phi_{I_i}$ is $\phi_{s_2}^i = \phi_{s_{2,0}}^i \wedge \phi_{s_{2,n}}^i$, where

$$\begin{aligned}
\phi_{s_{2,0}}^i &= \forall\, x\,(E_{02}(r,x) \rightarrow \forall\, y\,(K_i^-(x,y) \rightarrow K_j(y,x))),\\
\phi_{s_{2,n}}^i &= \forall\, x\,(L_1(r,x) \rightarrow\\
&\qquad \forall\, y\,(K_i \cdot R_2^-(x,y) \rightarrow K_k(x,y))).
\end{aligned}$$

  Here $\phi_{s_{2,0}}^i$ is a backward constraint and $\phi_{s_{2,n}}^i$ is a forward constraint.

The encoding of the program of $M$ is $\Phi_M = \bigwedge_{i=0}^{l} \phi_{I_i}$. Clearly, $\Phi_M$ is a conjunction of path constraints in $P_+$.

Using the encoding given above, we are able to express the $M$-reachability problem $C \Rightarrow_M D$ as a logical implication problem for $P_+$ constraints. More specifically, we show that the encoding above has the following reduction property.

**Proposition 3.6:** For all IDs $C$ and $D$ of $M$,

$$C \Rightarrow_M D \quad \text{iff} \quad \Phi_N \wedge \Phi_M \wedge \varphi_C \rightarrow \varphi_D \text{ is valid.}$$

■

**Proof:** The proof consists of two parts.

(1) Assume $C \Rightarrow_M D$. We show that for each model $G$ of $\Phi_N \wedge \Phi_M \wedge \varphi_C$, $G \models \varphi_D$. To show this, it suffices to show that for each natural number $t$ and each ID $C'$ of $M$, if $C'$ is reached by $M$ in $t$ steps starting from $C$ (denoted by $C \Rightarrow_M^t C'$), then $G \models \varphi_{C'}$. We prove this claim by induction on $t$.

*Base case:* If $t = 0$, then the claim holds since $G \models \varphi_C$.

*Inductive step:* Assume the claim for $t$.

Suppose $C \Rightarrow_M^t C_1 \rightarrow_M^{I_i} C'$, where $C_1 = (i, m, n)$, and $C_1 \rightarrow_M^{I_i} C'$ means that $C'$ is reached by executing instruction $I_i$ at $C_1$. Then by the induction hypothesis, we have $G \models \varphi_{C_1}$. That is

$$G \models \forall\, x\,(L_1(r,x) \rightarrow \forall\, y\,((R_1^-)^m \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^n(x,y) \rightarrow K_i(x,y))).$$

We argue by contradiction that the claim holds for $t+1$. Suppose $G \not\models \varphi_{C'}$. We show that this assumption leads to a contradiction in each case of $I_i$, which has six cases in total.

*Case 1*: $I_i = (i, register_1, j)$. In this case, $C'$ must be $(j, m+1, n)$. By the assumption, there are $a, b \in |G|$ such that

$$G \models L_1(r,a) \wedge (R_1^-)^{m+1} \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^n(a,b) \wedge \neg K_j(a,b).$$

Thus there exists $c \in |G|$, such that

$$G \models R_1^-(a,c) \wedge (R_1^-)^m \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^n(c,b).$$

By $\phi_8$ in $\Phi_N$, $G \models L_1(r,c)$. Therefore, by $G \models \varphi_{C_1}$, $G \models K_i(c,b)$. Hence $G \models L_1(r,a) \wedge R_1^-(a,c) \wedge K_i(c,b)$. Thus by $\phi_{a_1}^i$ in $\Phi_M$, we have that $G \models K_j(a,b)$. This contradicts the assumption.

*Case 2*: $I_i = (i, register_2, j)$. In this case, $C'$ must be $(j, m, n+1)$. By the assumption, there are $a, b \in |G|$ such that

$$G \models L_1(r,a) \wedge (R_1^-)^m \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^{n+1}(a,b) \wedge \neg K_j(a,b).$$

Hence there exists $c \in |G|$, such that

$$G \models (R_1^-)^m \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^n(a,c) \wedge R_2^+(c,b).$$

By $G \models \varphi_{C_1}$, we have $G \models K_i(a,c)$. As a result, we have $G \models L_1(r,a) \wedge K_i(a,c) \wedge R_2^+(c,b)$. Thus by $\phi_{a_2}^i$ in $\Phi_M$, $G \models K_j(a,b)$. This contradicts the assumption.

*Case 3*: $I_i = (i, register_1, j, k)$ and $m = 0$. In this case, $C'$ must be $(j, 0, n)$. By the assumption, there exist $a, b \in |G|$, such that

$$G \models L_1(r,a) \wedge E_{01}^- \cdot E_{02} \cdot (R_2^+)^n(a,b) \wedge \neg K_j(a,b).$$

Thus by $G \models \varphi_{C_1}$, we have $G \models K_i(a,b)$. In addition, there exists $c \in |G|$, such that $G \models L_1(r,a) \wedge E_{01}^-(a,c)$. By $\phi_{13}, \phi_{14}$ and $\phi_{15}$ in $\Phi_N$, we have $G \models E_{01}(r,a)$. Hence $G \models E_{01}(r,a) \wedge K_i(a,b)$. Thus by $\phi_{s_{1,0}}^i$ in $\Phi_M$, we have $G \models K_j(a,b)$. This contradicts the assumption.

*Case 4*: $I_i = (i, register_1, j, k)$ and $m = p+1$. In this case, $C'$ must be $(k, p, n)$. By the assumption, there exist $a, b \in |G|$, such that

$$G \models L_1(r,a) \wedge (R_1^-)^p \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^n(a,b) \wedge \neg K_k(a,b).$$

Hence by $\phi_5$ in $\Phi_N$, there exists $c \in |G|$, such that

$$G \models L_1(r,a) \wedge R_1^+(a,c).$$

By $\phi_7, \phi_1$ in $\Phi_N$, we have that $G \models L_1(r,c) \wedge R_1^-(c,a)$. Hence $G \models L_1(r,c) \wedge (R_1^-)^{p+1} \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^n(c,b)$. Thus by $G \models \varphi_{C_1}$, we have $G \models K_i(c,b)$. As a result, $G \models L_1(r,a) \wedge R_1^+(a,c) \wedge K_i(c,b)$. Thus by $\phi_{s_{1,n}}^i$ in $\Phi_M$, $G \models K_k(a,b)$. This contradicts the assumption.

*Case 5*: $I_i = (i, register_2, j, k)$ and $n = 0$. In this case, $C'$ must be $(j, m, 0)$. By the assumption, there exist $a, b \in |G|$, such that

$$G \models L_1(r,a) \wedge (R_1^-)^m \cdot E_{01}^- \cdot E_{02}(a,b) \wedge \neg K_j(a,b).$$

Thus by $G \models \varphi_{C_1}$, we have $G \models K_i(a,b)$. By $\phi_{11}^i$ in $\Phi_N$, $G \models K_i^-(b,a)$. Moreover, there exist $c, d \in |G|$, such that $G \models (R_1^-)^m(a,d) \wedge E_{01}^-(d,c) \wedge E_{02}(c,b)$. By $G \models L_1(r,a)$ and $\phi_8$ in $\Phi_N$, we have $G \models L_1(r,d)$. Thus by $\phi_{16}$ in $\Phi_N$, we have $G \models E_{02}(r,b)$. As a result, $G \models E_{02}(r,b) \wedge K_i^-(b,a)$. Thus by $\phi_{s_{2,0}}^i$ in $\Phi_M$, we have $G \models K_j(a,b)$. This contradicts the assumption.

*Case 6*: $I_i = (i, register_2, j, k)$ and $n = p+1$. In this case, $C'$ must be $(k, m, p)$. By the assumption, there exist $a, b \in |G|$, such that

$$G \models L_1(r,a) \wedge (R_1^-)^m \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^p(a,b) \wedge \neg K_k(a,b).$$

Hence there exist $c, d \in |G|$, such that

$$G \models (R_1^-)^m(a,c) \wedge E_{01}^- \cdot E_{02}(c,d) \wedge (R_2^+)^p(d,b).$$

By $\phi_8$ in $\Phi_N$, we have $G \models L_1(r,c)$. By $\phi_{16}$ in $\Phi_N$, $G \models E_{02}(r,d)$. By $\phi_{18}$ in $\Phi_N$, $G \models L_2(r,d)$. By $\phi_9$ in

$\Phi_N$, $G \models L_2(r,b)$. Therefore, by $\phi_6$ in $\Phi_N$, there exists $e \in |G|$, such that $G \models R_2^+(b,e)$. Hence

$$G \models L_1(r,a) \wedge (R_1^-)^m \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^{p+1}(a,e).$$

By $G \models \varphi_{C_1}$, we have $G \models K_i(a,e)$. By $\phi_3$ in $\Phi_N$ and $G \models R_2^+(b,e)$, we have $G \models R_2^-(e,b)$. As a result, we have $G \models L_1(r,a) \wedge K_i(a,e) \wedge R_2^-(e,b)$. Thus by $\phi^i_{s_{2,n}}$ in $\Phi_M$, we have $G \models K_k(a,b)$. This contradicts the assumption.

Hence the claim holds for $t+1$ for all the cases of $I_i$.

(2) Conversely, assume that $C \not\Rightarrow_M D$. We show that $\Phi_N \wedge \Phi_M \wedge \varphi_C \rightarrow \varphi_D$ is not valid. To show this, we construct a $\sigma$-structure $G$ such that $G \models \Phi_N \wedge \Phi_M \wedge \varphi_C$ and $G \models \neg\varphi_D$.

The structure $G$ has the form shown in Figure 3. It is defined as follows. The universe of $G$ consists of a distinguished node $rt$, which is the interpretation of the constant $r$ in $G$, and two distinct infinite chains of natural numbers. More specifically, let $\mathbb{N}$ denote the set of all natural numbers, then

$$|G| = \{rt\} \cup \mathbb{N} \cup \{i' \mid i \in \mathbb{N}\}.$$

The binary relations in $G$ are populated as follows (the superscript $G$ is omitted in the relation names):

$$\begin{aligned}
L_r &= \{(rt, rt)\} \\
E_{01} &= \{(rt, 0)\} \\
E_{01}^- &= \{(0, rt)\} \\
E_{02} &= \{(rt, 0')\} \\
E_{02}^- &= \{(0', rt)\} \\
L_1 &= \{(rt, i) \mid i \in \mathbb{N}\} \\
L_1^- &= \{(i, rt) \mid i \in \mathbb{N}\} \\
L_2 &= \{(rt, i') \mid i \in \mathbb{N}\} \\
L_2^- &= \{(i', rt) \mid i \in \mathbb{N}\} \\
R_1^+ &= \{(i, i+1) \mid i \in \mathbb{N}\} \\
R_1^- &= \{(i+1, i) \mid i \in \mathbb{N}\} \\
R_2^+ &= \{(i', (i+1)') \mid i \in \mathbb{N}\} \\
R_2^- &= \{((i+1)', i') \mid i \in \mathbb{N}\} \\
K_i &= \{(m, n') \mid C \Rightarrow_M (i, m, n)\} \\
K_i^- &= \{(n', m) \mid (m, n') \in K_i\}
\end{aligned}$$

It is easy to verify the following. First, $G \models \Phi_N$. This is immediate from the construction of $G$. Second, $G \models \varphi_C \wedge \neg\varphi_D$, because $C \Rightarrow_M C$, $C \not\Rightarrow_M D$ and by the definition of $K_i$. Finally, $G \models \Phi_M$. To see this, first observe the following simple facts.

*Fact 1*: $G \models K_i(m,n')$ iff $C \Rightarrow_M (i,m,n)$.

*Fact 2*: If $C \Rightarrow_M (i,m,n) \rightarrow_M^{I_i} C'$, then $C \Rightarrow_M C'$. Moreover, $C'$ is determined by the relation $\rightarrow_M$ described in Section 3.1.

Using these facts, we can verify that $G \models \Phi_M$ by contradiction. More specifically, suppose $G \not\models \Phi_M$. Then there is $i \in [0,l]$ such that $G \not\models \phi_{I_i}$. Here $I_i$ has six cases. For each of these cases, the assumption contradicts the facts above. As an example, consider the case in which $I_i$ is $(i, register_1, j)$. Then there must be $m, n' \in |G|$, such that $G \models K_i(m,n') \wedge \neg K_j(m+1,n')$. By Fact 1, $C \Rightarrow_M (i,m,n')$. In addition, by Fact 2, we have $C \Rightarrow_M (j, m+1, n')$. Thus again by Fact 1, $G \models K_j(m+1,n')$. This contradicts the assumption. The proofs for the other cases are similar.

Therefore, if $C \not\Rightarrow_M D$, then $\Phi_N \wedge \Phi_M \wedge \varphi_C \wedge \neg\varphi_D$ is satisfiable. ∎

### 3.2.2 Semi-conservative reduction

Taking advantage of the reduction property established above, we define a recursive function $f : FO \rightarrow S(P_+)$ by:

$$f(\psi) \quad \mapsto \quad \Phi_N \wedge \Phi_M \wedge \varphi_{C(\psi)} \wedge \neg\varphi_{(1,0,0)},$$

where $C(\psi)$ is the ID $(0, m(\psi), 0)$ of the 2-RM $M_L$ with an appropriate encoding $m(\psi)$ of $\psi$, as described in Section 3.1.

The proposition below shows that $f$ is indeed a semi-conservative reduction from $FO$ to $S(P_+)$.

**Proposition 3.7:** Let $M_L$ be the 2-RM described in Section 3.1. For each $\psi \in FO$,

1. $\psi \in H_{M_L,1}$ iff $f(\psi)$ is not satisfiable; and
2. if $\psi \in H_{M_L,2}$, then $f(\psi)$ has a finite model.

∎

**Proof:** Recall $H_{M_L,1} = N(FO)$ and $H_{M_L,2} = F(FO)$ from Section 3.1.

(1) By Proposition 3.6, we have $C(\psi) \Rightarrow_{M_L} (1,0,0)$ iff $\Phi_N \wedge \Phi_M \wedge \varphi_{C(\psi)} \rightarrow \varphi_{(1,0,0)}$ is valid. In other words, $C(\psi) \Rightarrow_{M_L} (1,0,0)$ iff $\Phi_N \wedge \Phi_M \wedge \varphi_{C(\psi)} \wedge \neg\varphi_{(1,0,0)}$ is not satisfiable. Since $\psi \in H_{M_L,1}$ iff $C(\psi) \Rightarrow_{M_L} (1,0,0)$, we have that $\psi \in H_{M_L,1}$ iff $f(\psi)$ is not satisfiable.

(2) We show that if $\psi \in H_{M_L,2}$, then $f(\psi)$ has a finite model.

First note that if $\psi \in H_{M_L,2}$, then the computation of $M_L$ with initial ID $C(\psi)$ is finite. Therefore, the set

$$SID_{C(\psi)} \;=\; \{(i,m,n) \mid C(\psi) \Rightarrow_{M_L} (i,m,n)\}$$

is finite. Hence there is a natural number $p$, such that for each $(i,m,n) \in SID_{C(\psi)}$, $m+2 \leq p$ and $n+2 \leq p$.

Now we construct a finite $\sigma$-structure $H$ satisfying $\Phi_N \wedge \Phi_M \wedge \varphi_{C(\psi)} \wedge \neg\varphi_{(1,0,0)}$. The universe of $H$ has

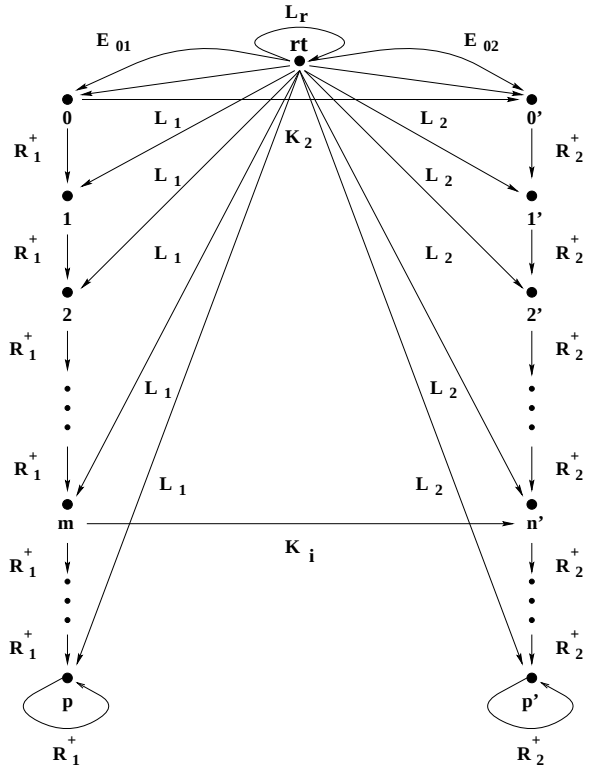


**Figure 4**: The structure $H$ in Proposition 3.7

$2p+1$ nodes. More specifically,

$$|H| \;=\; \{rt, 1, 2, ..., p\} \;\cup\; \{1', 2', ..., p'\},$$

where $rt$ is the interpretation of the constant $r$ in $H$.

The binary relations $L_r, E_{01}, E_{02}, E_{01}^-, E_{02}^-, K_i$ and $K_i^-$ in $H$ are exactly the same as those in the $\sigma$-structure $G$ given in the proof of Proposition 3.6. The binary relations $L_1$, $L_1^-$, $L_2$, $L_2^-$, $R_1^+$, $R_1^-$, $R_2^+$ and $R_2^-$ are populated in $H$ as follows (the superscript $H$ is omitted in the relation names):

$$\begin{array}{lcl}
R_1^+ & = & \{(i, i+1) \mid 0 \le i < p\} \cup \{(p,p)\} \\
R_1^- & = & \{(i+1, i) \mid 0 \le i < p\} \cup \{(p,p)\} \\
R_2^+ & = & \{(i', (i+1)') \mid 0 \le i < p\} \cup \{(p',p')\} \\
R_2^- & = & \{((i+1)', i') \mid 0 \le i < p\} \cup \{(p',p')\} \\
L_1 & = & \{(rt, i) \mid 0 \le i \le p\} \\
L_1^- & = & \{(i, rt) \mid 0 \le i \le p\} \\
L_2 & = & \{(rt, i') \mid 0 \le i \le p\} \\
L_2^- & = & \{(i', rt) \mid 0 \le i \le p\}
\end{array}$$

See Figure 4 for the structure $H$ ($E_{01}^-$, $E_{02}^-$, $L_1^-$, $L_2^-$, $R_1^-$, $R_2^-$, $K_i^-$ edges are omitted in the graph). Note that the relations $K_i$ and $K_i^-$ in $H$ are well-defined, since if $C(\psi) \Rightarrow_{M_L} (i,m,n)$, then $m < p-1$ and $n < p-1$.

We now show that $H \models \Phi_N \wedge \Phi_M \wedge \varphi_{C(\psi)} \wedge \neg\varphi_{(1,0,0)}$.

First, by $C(\psi) \Rightarrow_{M_L} C(\psi)$ and $C(\psi) \not\Rightarrow_{M_L} (1,0,0)$, we have that $H \models \varphi_{C(\psi)} \wedge \neg\varphi_{(1,0,0)}$.

Second, it is easy to verify that $H \models \Phi_N$. It should be mentioned that it is to ensure $H \models \phi_5 \wedge \phi_6$ that we require $H \models R_1^+(p,p) \wedge R_2^+(p',p')$.

Finally, we show that $H \models \Phi_M$. Since $\psi \in H_{M_L,2}$, it is straightforward to verify the following simple fact.

*Fact 3:* If $C(\psi) \Rightarrow_{M_L} (i,m,n)$, then $m < p-1$ and $n < p-1$.

In addition, Facts 1 and 2 given in the proof of Proposition 3.6 also hold here. Therefore, the argument for showing $G \models \Phi_M$ in the proof of Proposition 3.6, together with Fact 3 given above, proves $H \models \Phi_M$. This verifies that the structure $H$ is indeed a finite model of $\Phi_N \wedge \Phi_M \wedge \varphi_{C(\psi)} \wedge \neg\varphi_{(1,0,0)}$. ∎

As an immediate result of Lemma 3.4 and Proposition 3.7, we have the following corollary, from which Theorem 3.2 follows immediately.

**Corollary 3.8:** The set $S(P_+)$ is a conservative reduction class. ∎

### 3.3 Implication Problems for $P_f$

We next establish Theorem 3.3. As in the proof of Theorem 3.2, we show that the set $S(P_f)$ is a conservative reduction class. To do this, we first present an encoding of 2-RMs with constraints in $P_f$, and then define a semi-conservative reduction from $FO$ to $S(P_f)$.

#### 3.3.1 Encoding

We encode 2-RMs in terms of $P_f$ constraints. Recall that $P_f$ allows the left tail and right tail of a constraint to be empty path $\epsilon$. In other words, equality is allowed in $P_f$.

Let $M$ be a 2-RM. Assume that the set $E$ of binary relation symbols in signature $\sigma$ is the same as the one described in Section 3.2.1, except that the predicates $L_r$ and $K_i^-$ for $i \in [0,l]$ are no longer required here. We define the encoding as follows.

**IDs.** The encoding of each ID $C$ of $M$, $\varphi_C$, is the same as the one given in Section 3.2.1. Note that $\varphi_C$ is in $P_f$.

**Registers.** We encode the contents of the registers by $\Phi_N^f$, which is the conjunction of the constraints of $P_f$ given below.

- Successor, predecessor:

$\phi_1 = \forall\, x\,(L_1(r,x) \rightarrow \forall\, y\,(R_1^+ \cdot R_1^-(x,y) \rightarrow \epsilon(x,y)))$
$\phi_2 = \forall\, x\,(L_1(r,x) \rightarrow \forall\, y\,(R_1^- \cdot R_1^+(x,y) \rightarrow \epsilon(x,y)))$
$\phi_3 = \forall\, x\,(L_2(r,x) \rightarrow \forall\, y\,(R_2^+ \cdot R_2^-(x,y) \rightarrow \epsilon(x,y)))$
$\phi_4 = \forall\, x\,(L_2(r,x) \rightarrow \forall\, y\,(R_2^- \cdot R_2^+(x,y) \rightarrow \epsilon(x,y)))$
$\phi_5 = \forall\, x\,(L_1(r,x) \rightarrow \forall\, y\,(\epsilon(x,y) \rightarrow R_1^+ \cdot R_1^-(x,y)))$
$\phi_6 = \forall\, x\,(L_2(r,x) \rightarrow \forall\, y\,(\epsilon(x,y) \rightarrow R_2^+ \cdot R_2^-(x,y)))$

  Constraints $\phi_1$ and $\phi_2$ (resp. $\phi_3$ and $\phi_4$) assert an inverse relationship between $R_1^+$ and $R_1^-$ (resp. $R_2^+$ and $R_2^-$). It should be noted that since equality is allowed in $P_f$, $\phi_1$ and $\phi_2$ (resp. $\phi_3$ and $\phi_4$) enforce a node representing a content of $register_1$ (resp. $register_2$) to be unique. Constraints $\phi_5$ and $\phi_6$ state that $R_1^+$ and $R_2^+$ edges form "infinite" chains.

- Register identification: $\phi_7, \phi_8, \phi_9$ and $\phi_{10}$ are the same as given in Section 3.2.1.

- Zeros:

$\phi_{11} = \forall\, x\,(L_1 \cdot E_{01}^-(r,x) \rightarrow \epsilon(r,x))$
$\phi_{12} = \forall\, x\,(L_1(r,x) \rightarrow$
$\qquad \forall\, y\,(E_{01}^-(x,y) \rightarrow E_{01}^- \cdot E_{01} \cdot E_{01}^-(x,y)))$
$\phi_{13} = \forall\, x\,(L_1(r,x) \rightarrow \forall\, y\,(E_{01}^- \cdot E_{01}(x,y) \rightarrow \epsilon(x,y)))$
$\phi_{14} = \forall\, x\,(L_1 \cdot E_{01}^- \cdot E_{02}(r,x) \rightarrow E_{02}(r,x))$
$\phi_{15} = \forall\, x\,(E_{02}(r,x) \rightarrow \forall\, y\,(\epsilon(x,y) \rightarrow E_{02}^- \cdot E_{02}(x,y)))$
$\phi_{16} = \forall\, x\,(E_{02}(r,x) \rightarrow L_2(r,x))$

  Constraints $\phi_{11}$, $\phi_{12}$ and $\phi_{13}$ assert that if there is an edge labeled $L_1$ from the root to a node $a$ and $a$ has an outgoing $E_{01}^-$ edge, then there is an $E_{01}$ edge from the root to $a$. Constraint $\phi_{14}$ states that if there exists a path $L_1 \cdot E_{01}^- \cdot E_{02}$ from the root to a node $b$, then there is an $E_{02}$ edge from the root to $b$. Constraint $\phi_{15}$ asserts that if there is an $E_{02}$ edge from the root to a node $c$, then there exists a node $d$ such that there is an $E_{02}^-$ edge from $c$ to $d$ and there is an $E_{02}$ edge from $d$ to $c$. Finally, $\phi_{16}$ states that there is an edge labeled $L_2$ from the root to a node representing 0 in $register_2$.

**Instructions.** The encoding of instruction $I_i$, $\phi_{I_i}$, is the same as the one given in Section 3.2.1, except that here $\phi^i_{s_{2,0}}$ is

$$\forall\, x\,(L_1(r,x) \rightarrow \forall\, y\,(K_i \cdot E_{02}^- \cdot E_{02}(x,y) \rightarrow K_j(x,y))).$$

The encoding of the program of $M$ is $\Phi_M^f = \bigwedge_{i=0}^{l} \phi_{I_i}$.

It is clear that $\Phi_M^f$ is a conjunction of constraints in $P_f$.

Analogous to Proposition 3.6, we show that the encoding above has the following reduction property.

**Proposition 3.9:** For all IDs $C$ and $D$ of $M$,

$$C \Rightarrow_M D \quad \text{iff} \quad \Phi_N^f \wedge \Phi_M^f \wedge \varphi_C \rightarrow \varphi_D \text{ is valid.}$$

■

**Proof:** The proof is similar to that of Proposition 3.6.

(1) Assume that $C \Rightarrow_M D$. We prove by induction on step $t$ that for each ID $C'$ of $M$ and each model $G$ of $\Phi_N^f \wedge \Phi_M^f \wedge \varphi_C$, if $C \Rightarrow_M^t C'$ then $G \models \varphi_{C'}$. This can be shown in basically the same way as for Proposition 3.6, except for the following cases in the inductive step.

*Case 3*: $I_i = (i, register_1, j, k)$ and $m = 0$. In this case, $C'$ must be $(j, 0, n)$. Suppose, for a contradiction, that there are $a, b \in |G|$, such that

$$G \models L_1(r,a) \wedge E_{01}^- \cdot E_{02} \cdot (R_2^+)^n(a,b) \wedge \neg K_j(a,b).$$

Then by $G \models \varphi_{C_1}$, we have $G \models K_i(a,b)$. In addition, there exists $e \in |G|$, such that $G \models L_1(r,a) \wedge E_{01}^-(a,e)$. By $\phi_{12}$ in $\Phi_N^f$, there exist $c, d \in |G|$, such that

$$G \models L_1(r,a) \wedge E_{01}^-(a,c) \wedge E_{01}(c,d).$$

Thus by $\phi_{13}$ in $\Phi_N^f$, we have $G \models \epsilon(a,d)$. As a result, $G \models L_1(r,a) \wedge E_{01}^-(a,c) \wedge E_{01}(c,a)$. By $\phi_{11}$ in $\Phi_N^f$ and $G \models L_1(r,a) \wedge E_{01}^-(a,c)$, we have $G \models \epsilon(r,c)$. Thus $G \models E_{01}(r,a)$. Hence $G \models E_{01}(r,a) \wedge K_i(a,b)$. Thus by $\phi^i_{s_{1,0}}$ in $\Phi_M^f$, we have $G \models K_j(a,b)$. This contradicts the assumption.

*Case 4*: $I_i = (i, register_1, j, k)$ and $m = p + 1$. In this case, $C'$ must be $(k, p, n)$. Suppose, for a contradiction, that there exist $a, b \in |G|$, such that

$$G \models L_1(r,a) \wedge (R_1^-)^p \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^n(a,b) \wedge \neg K_k(a,b).$$

Then by $\phi_5$ in $\Phi_N^f$, there exists node $c \in |G|$, such that $G \models L_1(r,a) \wedge R_1^+(a,c) \wedge R_1^-(c,a)$. By $\phi_7$ in $\Phi_N^f$, we have $G \models L_1(r,c) \wedge R_1^-(c,a)$. As a result,

$$G \models L_1(r,c) \wedge (R_1^-)^{p+1} \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^n(c,b).$$

Thus by $G \models \varphi_{C_1}$, $G \models K_i(c,b)$. Therefore, we have that $G \models L_1(r,a) \wedge R_1^+(a,c) \wedge K_i(c,b)$. Thus by $\phi^i_{s_{1,n}}$ in $\Phi_M^f$, we have $G \models K_k(a,b)$. This contradicts the assumption.

*Case 5*: $I_i = (i, register_2, j, k)$ and $n = 0$. In this case, $C'$ must be $(j, m, 0)$. Suppose, for a contradiction, that there exist $a, b \in |G|$, such that

$$G \models L_1(r,a) \wedge (R_1^-)^m \cdot E_{01}^- \cdot E_{02}(a,b) \wedge \neg K_j(a,b).$$

Then by $G \models \varphi_{C_1}$, we have $G \models K_i(a,b)$. Moreover, there exist $c, d \in |G|$, such that

$$G \models (R_1^-)^m(a,d) \wedge E_{01}^-(d,c) \wedge E_{02}(c,b).$$

By $G \models L_1(r,a)$ and $\phi_8$ in $\Phi_N^f$, we have $G \models L_1(r,d)$. Thus by $\phi_{14}$ in $\Phi_N^f$, we have $G \models E_{02}(r,b)$. By $\phi_{15}$ in $\Phi_N^f$, there is $e \in |G|$, such that $G \models E_{02}^-(b,e) \wedge E_{02}(e,b)$. Hence $G \models L_1(r,a) \wedge K_i(a,b) \wedge E_{02}^-(b,e) \wedge E_{02}(e,b)$. Thus by $\phi^i_{s_{2,0}}$ in $\Phi_M^f$, we have $G \models K_j(a,b)$. This contradicts the assumption.

*Case 6*: $I_i = (i, register_2, j, k)$ and $n = p+1$. In this case, $C'$ must be $(k, m, p)$. Suppose, for a contradiction, that there exist $a, b \in |G|$, such that

$$G \models L_1(r,a) \wedge (R_1^-)^m \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^p(a,b) \wedge \neg K_k(a,b).$$

Then there exist $c, d \in |G|$, such that

$$G \models (R_1^-)^m(a,c) \wedge E_{01}^- \cdot E_{02}(c,d) \wedge (R_2^+)^p(d,b).$$

By $\phi_8$ in $\Phi_N^f$, we have $G \models L_1(r,c)$. By $\phi_{14}$ in $\Phi_N^f$, $G \models E_{02}(r,d)$. By $\phi_{16}$ in $\Phi_N^f$, $G \models L_2(r,d)$. By $\phi_9$ in $\Phi_N^f$, $G \models L_2(r,b)$. Therefore, by $\phi_6$ in $\Phi_N^f$, there exists $e \in |G|$, such that $G \models R_2^+(b,e) \wedge R_2^-(e,b)$. Therefore,

$$G \models L_1(r,a) \wedge (R_1^-)^m \cdot E_{01}^- \cdot E_{02} \cdot (R_2^+)^{p+1}(a,e).$$

By $G \models \varphi_{C_1}$, $G \models K_i(a,e)$. As a result, we have that $G \models L_1(r,a) \wedge K_i(a,e) \wedge R_2^-(e,b)$. Thus by $\phi^i_{s_{2,n}}$ in $\Phi_M^f$, $G \models K_k(a,b)$. This contradicts the assumption.

(2) Conversely, assume that $C \not\Rightarrow_M D$. It is easy to verify that the $\sigma$-structure $G$ (without $L_r$ and $K_i^-$ edges) constructed in the proof of Proposition 3.6 is a model of $\Phi_N^f \wedge \Phi_M^f \wedge \varphi_C \wedge \neg\varphi_D$. ∎

### 3.3.2 Semi-conservative reduction

We define a recursive function $g: \ FO \to S(P_f)$ by:

$$g(\psi) \quad \mapsto \quad \Phi_N^f \wedge \Phi_M^f \wedge \varphi_{C(\psi)} \wedge \neg\varphi_{(1,0,0)},$$

where $C(\psi)$ is the ID $(0, m(\psi), 0)$ of the 2-RM $M_L$ with an appropriate encoding $m(\psi)$ of $\psi$, as described in Section 3.1.

Proposition 3.10 below shows that the function $g$ is indeed a semi-conservative reduction from $FO$ to $S(P_f)$.

**Proposition 3.10:** Let $M_L$ be the 2-RM described in Section 3.1. For each $\psi \in FO$,

1. $\psi \in H_{M_L,1}$ iff $g(\psi)$ is not satisfiable; and
2. if $\psi \in H_{M_L,2}$, then $g(\psi)$ has a finite model.

∎

**Proof:** The proof is similar to the proof of Proposition 3.7, except that here in the structure $H$ shown in Figure 4, there are no $L_r$ and $K_i^-$ edges. ∎

From Proposition 3.10 and Lemma 3.4 follows the corollary below. As a result, Theorem 3.3 follows.

**Corollary 3.11:** The set $S(P_f)$ is a conservative reduction class. ∎

## 4 DECIDABLE RESTRICTED IMPLICATION

The undecidability results established in the last section suggest that we search for fragments of $P_c$ which possess decidable implication problems, and yet retain sufficient expressive power of the full language. This section identifies several fragments of $P_c$ which share the following properties. First, they each properly contain the set of word constraints. Second, each of them fails to be included in two-variable first-order logic. Third, they allow the formulation of many interesting semantic relations. And finally, the implication and finite implication problems for each of them are decidable in the context of semistructured databases.

We begin by introducing these fragments of $P_c$, and then establish the decidability of their associated implication and finite implication problems. Finally, we investigate a mild generalization of $P_c$, $P_c^\wedge$.

### 4.1 Decidable Fragments of $P_c$

We describe three fragments of $P_c$ and demonstrate their expressive power.

#### 4.1.1 Prefix restricted implication for $P_c$

The implication problems for simple path constraints, which are known to be decidable, can be viewed as a restricted form of the implication problems for $P_c$. More specifically, the implication problems for $P_s$ are the implication problems for $P_c$ under the following restriction: in any finite subset of $P_c$ in the implication problems, the prefix of each constraint is the empty path.

By replacing this prefix restriction with a weaker one, we define the prefix restricted implication problems for $P_c$ as follows.

**Definition 4.1:** A *prefix restricted subset of* $P_c$ is a finite subset of $P_c$ in which the prefixes of all the constraints have the same length.

The *prefix restricted (finite) implication problem for* $P_c$ is the problem to determine, given any prefix restricted subset $\Sigma \cup \{\varphi\}$ of $P_c$, whether $\Sigma \models \varphi$ ($\Sigma \models_f \varphi$).

∎

Obviously, the (finite) implication problem for word constraints is a special case of the prefix restricted (finite) implication problem for $P_c$. Moreover, in contrast to word constraint implication, prefix restricted implication cannot be stated in two-variable first-order logic ($FO^2$). A convenient argument for this is that $\{\varphi\}$, where $\varphi$ is the constraint given in Example 2.1, is a prefix restricted subset of $P_c$. However, $\varphi$ is not expressible in $FO^2$.

Many cases of integrity constraint implication commonly found in databases are instances of the prefix restricted implication problem for $P_c$. Among these are implications for inverse constraints and local database constraints. As an example, consider the set $\Sigma$ consisting of the following local inverse constraints in the school databases described in Section 1:

$$\forall s\,(Schools \cdot Students(r,s) \rightarrow \forall c\,(Taking(s,c) \rightarrow Enrolled(c,s)))$$
$$\forall c\,(Schools \cdot Courses(r,c) \rightarrow \forall s\,(Enrolled(c,s) \rightarrow Taking(s,c)))$$

and the constraint $\varphi$:

$$\forall s_1\,(Schools \cdot Students(r,s_1) \rightarrow \forall s_2\,(\epsilon(s_1,s_2) \rightarrow Taking \cdot Enrolled(s_1,s_2))).$$

The question whether $\Sigma \models \varphi$ ($\Sigma \models_f \varphi$) is an instance of the prefix restricted (finite) implication problem for $P_c$.

### 4.1.2 Sublanguage $P_\beta$

Some cases of path constraint implication canvassed earlier are not instances of the prefix restricted implication. For example, recall the two extent constraints and the two inverse constraints for student/course databases given in Section 1:

$$\forall c\,(Students \cdot Taking(r,c) \rightarrow Courses(r,c))$$
$$\forall s\,(Courses \cdot Enrolled(r,s) \rightarrow Students(r,s))$$
$$\forall s\,(Students(r,s) \rightarrow \forall c\,(Taking(s,c) \rightarrow Enrolled(c,s)))$$
$$\forall c\,(Courses(r,c) \rightarrow \forall s\,(Enrolled(c,s) \rightarrow Taking(s,c)))$$

The set consisting of these constraints is not a prefix restricted subset of $P_c$.

The constraints in the last example, however, are in the sublanguage $P_\beta$ of $P_c$ defined below. Recall the notations $lt(\varphi)$ and $pf(\varphi)$ for a $P_c$ constraint $\varphi$ described in Definition 2.1.

**Definition 4.2:** A *$\beta$-restricted path constraint* $\varphi$ is a constraint in $P_c$ with $|lt(\varphi)| \leq 1$. That is, either $lt(\varphi)$ is $\epsilon$, or $lt(\varphi) = K$ for some $K \in E$.

The sublanguage $P_\beta$ is defined to be the class of $P_c$ constraints $\varphi$ such that either $|pf(\varphi)| = 0$ or $|lt(\varphi)| \leq 1$. In other words, $P_\beta$ consists of all simple path constraints and all $\beta$-restricted path constraints.

The *(finite) implication problem for $P_\beta$* is the problem of determining, given any finite subset $\Sigma \cup \{\varphi\}$ of $P_\beta$, whether $\Sigma \models \varphi$ ($\Sigma \models_f \varphi$). ∎

Note that the class of word constraints is a proper subset of $P_\beta$. In addition, not all constraints in $P_\beta$ are expressible in $FO^2$. Indeed, the constraint $\varphi$ given in Example 2.1 is in $P_\beta$, but is not in $FO^2$.

### 4.1.3 Extended implication for $P_\beta$

Recall the local extent constraints given in Section 1:

$$\forall d\,(Schools(r,d) \rightarrow \forall c\,(Students \cdot Taking(d,c) \rightarrow Courses(d,c)))$$
$$\forall d\,(Schools(r,d) \rightarrow \forall s\,(Courses \cdot Enrolled(d,s) \rightarrow Students(d,s)))$$

Consider the set consisting of these local extent constraints and the local inverse constraints given in Section 4.1.1. This set is neither a prefix restricted subset of $P_c$ nor a subset of $P_\beta$. However, the constraints in this set share the following property: all of them are constraints in student/course databases as shown in Figure 1 augmented with a common prefix `Schools`. In general, when represented in a global environment, path constraints in a local database are augmented with a common prefix. This example motivates the following extension of $P_\beta$.

**Definition 4.3:** Let $\alpha$ be a path and $\varphi$ be a constraint in $P_\beta$. The *extension of $\varphi$ with prefix $\alpha$*, denoted by $\delta(\varphi,\alpha)$, is the constraint defined either by

$$\forall x\,(\alpha \cdot pf(\varphi)(r,x) \rightarrow \forall y\,(lt(\varphi)(x,y) \rightarrow rt(\varphi)(x,y)))$$

when $\varphi$ is of the forward form, or by

$$\forall x\,(\alpha \cdot pf(\varphi)(r,x) \rightarrow \forall y\,(lt(\varphi)(x,y) \rightarrow rt(\varphi)(y,x)))$$

when $\varphi$ is of the backward form. Here $\cdot$ is the path concatenation operator, and $pf$, $lt$ and $rt$ are defined in Definition 2.1.

Let $\alpha$ be a path and $\Sigma$ be a finite subset of $P_\beta$. The *extension of $\Sigma$ with prefix $\alpha$* is the subset of $P_c$ defined by $\{\delta(\varphi,\alpha) \mid \varphi \in \Sigma\}$. Such a set is called a *prefix extended subset of $P_\beta$*.

The *extended (finite) implication problem for* $P_\beta$ is the problem of determining, given any prefix extended subset $\Sigma \cup \{\varphi\}$ of $P_\beta$, whether $\Sigma \models \varphi$ ($\Sigma \models_f \varphi$). ■

For instance, the set described in the last example is a prefix extended subset of $P_\beta$.

Note that the (finite) implication problem for $P_\beta$ is a special case of the extended (finite) implication problem for $P_\beta$, namely, when the prefix $\alpha$ described in Definition 4.3 is the empty path $\epsilon$. As an immediate result, implications of word constraints are special cases of extended implications of $P_\beta$ constraints. In addition, extended implications of $P_\beta$ constraints cannot be stated in $FO^2$.

## 4.2 Decidability of Prefix Restricted Implication

In this section, we show the following:

**Theorem 4.1:** The prefix restricted implication and finite implication problems for $P_c$ are decidable. ■

The idea of the proof is to show that the satisfiability and finite satisfiability problems for the set $S_p$:

$$\{\bigwedge \Sigma \wedge \neg\varphi \mid \Sigma \cup \{\varphi\} \text{ is a prefix restricted subset of } P_c\}$$

are decidable. That is, we show that it is decidable to determine, given any $\psi \in S_p$, whether there is a (finite) $\sigma$-structure such that $G \models \psi$.

To show that $S_p$ possesses decidable satisfiability problems, let us recall the following notion from [9].

**Definition 4.4 [9]:** A class $X$ of logic sentences has the *small model property* for satisfiability iff there exists a recursive function $s$ such that for each $\psi \in X$, if $\psi$ is satisfiable, then $\psi$ has a finite model of size at most $s(|\psi|)$, where $|\psi|$ stands for the length of $\psi$. ■

If a class $X$ of logic sentences has the small model property, then the satisfiability and finite satisfiability problems for $X$ coincide and are decidable. In fact, for any $\psi \in X$, one can determine whether $\psi$ is satisfiable in $s(|\psi|)$-space, where $s$ is the recursive function described in Definition 4.4. Therefore, to show the decidability of the satisfiability and finite satisfiability problems for $S_p$, it suffices to establish the small model property for $S_p$. To do this, we use a path label criterion to characterize whether a $\sigma$-structure satisfies a sentence of $S_p$. More specifically, given a structure $G$ and a sentence $\psi$ of $S_p$, we label each node of $G$ with paths in $\psi$. The path label of $G$, $LB(G, \psi)$, is the collection of the labels of all the nodes in $G$. This path label has the following properties:

- for any $\sigma$-structure $H$, if $LB(H, \psi) = LB(G, \psi)$, then $H \models \psi$ iff $G \models \psi$; and
- there is a $\sigma$-structure $H$ of size at most $2^{2^{2|\psi|}}$, such that $LB(H, \psi) = LB(G, \psi)$.

As a result, if $\psi$ is satisfiable, then it has a model of size at most $2^{2^{2|\psi|}}$.

We next define the path labels and show that they have the properties described above.

### 4.2.1 Path labels

Let $G = (|G|, r^G, E^G)$ and $\psi \in S_p$, where $\psi = \bigwedge \Sigma \wedge \neg\varphi$. To define path labels, we need the following notations:

$$Paths_\alpha(\psi) = \{pf(\phi) \mid \phi \in \Sigma \cup \{\varphi\}\}$$
$$Paths_\beta(\psi) = \{lt(\phi) \mid \phi \in \Sigma \cup \{\varphi\}\}$$
$$Paths^+_\gamma(\psi) = \{rt(\phi) \mid \phi \in \Sigma \cup \{\varphi\}, \ \phi \text{ has the forward form}\}$$
$$Paths^-_\gamma(\psi) = \{-rt(\phi) \mid \phi \in \Sigma \cup \{\varphi\}, \ \phi \text{ has the backward form}\}$$
$$Paths_{(\beta,\gamma)}(\psi) = Paths_\beta(\psi) \cup Paths^+_\gamma(\psi) \cup Paths^-_\gamma(\psi)$$

Here the notation $-\rho$ denotes the pair $(-, \rho)$. We use this notation merely to distinguish the occurrence of a path as the right tail of a backward constraint as opposed to a forward constraint. The notations $pf$, $lt$ and $rt$ are described in Definition 2.1.

For each node $a$ in $|G|$, we define a path label using paths in $Paths_\alpha(\psi)$ and $Paths_{(\beta,\gamma)}(\psi)$. This label consists of a pair of sets. Its first component is the set of paths in $Paths_\alpha(\psi)$ from $r^G$ to $a$. That is,

$$lb_\alpha(a, G, \psi) = \{\rho \mid \rho \in Paths_\alpha(\psi), \ G \models \rho(r^G, a)\}.$$

The second component is a collection of sets of paths in $Paths_{(\beta,\gamma)}(\psi)$. Each set consists of the paths between the node $a$ and some node in $|G|$. More specifically, for each $b \in |G|$, let:

$$lbs_\beta(a, b, G, \psi) = \{\rho \mid \rho \in Paths_\beta(\psi), \ G \models \rho(a, b)\}$$
$$lbs_\gamma(a, b, G, \psi) = \{\rho \mid \rho \in Paths^+_\gamma(\psi), \ G \models \rho(a, b)\} \cup \{-\rho \mid -\rho \in Paths^-_\gamma(\psi), \ G \models \rho(b, a)\}$$

We define $lbs_{(\beta,\gamma)}(a, b, G, \psi)$ to be

$$lbs_\beta(a, b, G, \psi) \ \cup \ lbs_\gamma(a, b, G, \psi).$$

The second component of the label is defined by:

$$lb_{(\beta,\gamma)}(a, G, \psi) = \{lbs_{(\beta,\gamma)}(a, b, G, \psi) \mid b \in |G|\}$$

More precisely, we define the *label of node $a$ in $G$ w.r.t. $\psi$*, denoted by $lb(a, G, \psi)$ to be

- $(\emptyset,\ \emptyset)$, if $lb_\alpha(a, G, \psi) = \emptyset$; or
- $(lb_\alpha(a, G, \psi),\ lb_{(\beta,\gamma)}(a, G, \psi))$, otherwise.

The *label of* $G$ *w.r.t.* $\psi$ is defined by

$$LB(G, \psi) \ = \ \{lb(a, G, \psi) \mid a \in |G|\}.$$

Every label $l \in LB(G, \psi)$ is a pair of sets. We refer to the first component of $l$ as $lb_\alpha(l)$, and the second as $lb_{(\beta,\gamma)}(l)$. In addition, we use the following notations:

$$\begin{aligned} LB_\alpha(G, \psi) &= \{lb_\alpha(l) \mid l \in LB(G, \psi)\} \\ LB_{(\beta,\gamma)}(G, \psi) &= \{lb_{(\beta,\gamma)}(l) \mid l \in LB(G, \psi)\} \end{aligned}$$

Let us examine the cardinality of $LB(G, \psi)$. We use the notation $card(S)$ to denote the cardinality of a set $S$. It is easy to verify that

$$\begin{aligned} card(Paths_\alpha(\psi)) &\leq |\psi|, \\ card(Paths_{(\beta,\gamma)}(\psi)) &\leq |\psi|. \end{aligned}$$

Note that for any $l \in LB(G, \psi)$, $lb_\alpha(l)$ is a subset of $Paths_\alpha(\psi)$ and $lb_{(\beta,\gamma)}(l)$ is a subset of the power set of $Paths_{(\beta,\gamma)}(\psi)$. Therefore,

$$card(LB(G, \psi)) \ \leq \ 2^{|\psi| + 2^{|\psi|}}.$$

In particular, if $\psi$ involves simple constraints only, i.e., $\Sigma \cup \{\varphi\}$ is a subset of $P_s$, then $Paths_\alpha(\psi) = \{\epsilon\}$. In this case, it is easy to verify that $card(LB(G, \psi))$ is at most 2. More specifically, $LB(G, \psi) \subseteq \{(\emptyset, \emptyset),\ lb(r^G, G, \psi)\}$.

We shall use $s_\alpha(\psi)$ to denote the prefix length of $\varphi$. That is, $s_\alpha(\psi) = |pf(\varphi)|$. Note that the prefixes of all the constraints in $\Sigma \cup \{\varphi\}$ have the same length.

The lemma below shows that $LB(G, \psi)$ characterizes whether $G \models \psi$. This lemma can be easily verified by contradiction.

**Lemma 4.2:** For any $\sigma$-structures $G$, $H$, and any sentence $\psi \in S_p$, if $LB(G, \psi) = LB(H, \psi)$, then $G \models \psi$ iff $H \models \psi$. ∎

### 4.2.2 The small model property

Next, we establish the small model property for $S_p$. By Lemma 4.2, it suffices to show the following.

**Proposition 4.3:** For each $\sigma$-structure $G$ and each sentence $\psi$ in $S_p$, there is a $\sigma$-structure $H$, such that

1. the size of $H$ is at most $2^{2^{2|\psi|}}$; and
2. $LB(H, \psi) = LB(G, \psi)$.

∎

For if the proposition holds, then every satisfiable sentence $\psi$ in $S_p$ has a model of size at most $2^{2^{2|\psi|}}$. That is, $S_p$ has the small model property.

The idea of the proof of Proposition 4.3 is as follows. Let $G$ be a $\sigma$-structure and $\psi$ a sentence in $S_p$. We first construct a graph $G_\alpha$ that includes precisely one node $a_l$ representing $lb_\alpha(l)$ for each $l \in LB(G, \psi)$. We then construct a graph $G_l$ for each $l \in LB(G, \psi)$, such that the root of $G_l$ represents $lb_{(\beta,\gamma)}(l)$. Finally, we glue to each node $a_l$ the root of the corresponding graph $G_l$. This yields the $\sigma$-structure $H$ described in Proposition 4.3.

The implementation of the idea requires two lemmas and the following notation.

**Definition 4.5:** Let $G$ be a $\sigma$-structure, $m$ be a natural number and $a \in |G|$. The *m-neighborhood of a in* $G$ is the structure $G(a) = (|G(a)|, r^{G(a)}, E^{G(a)})$, where

- $|G(a)| \ = \ \{c \mid c \in |G|,$ there is path $\rho$, $|\rho| \leq m$ and either $G \models \rho(a, c)$ or $G \models \rho(c, a)\}$;
- $r^{G(a)} = a$; and
- for all $b, c \in |G(a)|$ and any $K \in E$, $G(a) \models K(b, c)$ iff $G \models K(b, c)$.

That is, $G(a)$ is the restriction of $G$ to $|G(a)|$ with $a$ as the new root. ∎

Given a $\sigma$-structure $G$ and a sentence $\psi$ in $S_p$, the first lemma below proves the existence of a $\sigma$-structure $G_\alpha$ which has the following properties.

- $LB_\alpha(G_\alpha, \psi) = LB_\alpha(G, \psi)$. In addition, for each $l \in LB(G, \psi)$, there is a distinguished node $a_l$ in $|G_\alpha|$ such that $lb_\alpha(a_l, G_\alpha, \psi) = lb_\alpha(l)$.
- For each $a \in |G_\alpha|$, if $lb_\alpha(a, G_\alpha, \psi) \neq \emptyset$, then $a$ does not have any outgoing edge. That is, for each $K \in E$ and $b \in |G_\alpha|$, $G_\alpha \models \neg K(a, b)$.

We shall proceed to construct the $\sigma$-structure $H$ described in Proposition 4.3, such that in $H$, $G_\alpha$ is the $s_\alpha(\psi)$-neighborhood of $r^H$. This will ensure that

$$LB_\alpha(H, \psi) = LB_\alpha(G, \psi).$$

**Lemma 4.4:** For each $\sigma$-structure $G$ and $\psi \in S_p$, there is a $\sigma$-structure $G_\alpha = (|G_\alpha|, r^{G_\alpha}, E^{G_\alpha})$, such that

1. the size of $G_\alpha$ is at most $|\psi| + 2^{|\psi| + 2^{|\psi|}}$;
2. there is a subset $L_\alpha$ of $|G_\alpha|$, such that

(a) there exists a bijection $f : LB(G,\psi) \to L_\alpha$, such that $lb_\alpha(l) = lb_\alpha(f(l), G_\alpha, \psi)$ for each label $l \in LB(G,\psi)$; and in addition, for every $K \in E$ and $b \in |G_\alpha|$, $G_\alpha \models \neg K(f(l), b)$;

(b) for each $b \in |G_\alpha| \setminus L_\alpha$, $lb_\alpha(b, G_\alpha, \psi) = \emptyset$.

■

**Proof:** Let $I_\alpha(\psi) = \{\rho \mid \varrho \in Paths_\alpha(\psi),\ \rho \prec_p \varrho\}$. Here $\rho \prec_p \varrho$ stands for that $\rho$ is a proper prefix of $\varrho$, as defined in Section 2. We construct $G_\alpha$ using $LB(G,\psi)$ and $I_\alpha(\psi)$ as follows. For each $\rho \in I_\alpha(\psi)$, let $a_\rho$ be a distinguished node, and for each $l \in LB(G,\psi)$, let $a_l$ be a distinguished node. Let

- $L_\alpha = \{a_l \mid l \in LB(G,\psi)\}$;
- $|G_\alpha| = L_\alpha \cup \{a_\rho \mid \rho \in I_\alpha(\psi)\}$;
- $r^{G_\alpha} = \begin{cases} a_\epsilon & \text{if } s_\alpha(\psi) \geq 1 \\ a_{lb(r^G, G, \psi)} & \text{otherwise;} \end{cases}$
- for all $a, b \in |G_\alpha|$ and $K \in E$, $G_\alpha \models K(a,b)$ iff there exists $\rho \in I_\alpha(\psi)$, such that $a = a_\rho$ (i.e., $a \notin L_\alpha$), and one of the following conditions is satisfied:
  - there exists $\varrho \in I_\alpha(\psi)$, such that $b = a_\varrho$ (i.e., $b \notin L_\alpha$), and $\varrho = \rho \cdot K$; or
  - there exists $l \in LB(G,\psi)$, such that $b = a_l$ (i.e., $b \in L_\alpha$), and there exists $\varrho \in lb_\alpha(l)$, such that $\varrho = \rho \cdot K$.

It should be noted that when $s_\alpha(\psi) = 0$, i.e., when $\psi$ involves simple constraints only, $I_\alpha(\psi) = \emptyset$ and $|G_\alpha|$ consists of $r^{G_\alpha}$ and at most another node. This is because in this case, $LB(G,\psi) \subseteq \{(\emptyset, \emptyset),\ lb(r^G, G, \psi)\}$. Here $r^{G_\alpha}$ represents the label of the root $r^G$ if $G$, i.e., $r^{G_\alpha} = a_{lb(r^G, G, \psi)}$. The other node, if it exists, is $a_{(\emptyset,\emptyset)}$.

The structure $G_\alpha$ is basically a rooted acyclic directed graph. It has the following properties.

- The restriction of $G_\alpha$ to $\{a_\rho \mid \rho \in I_\alpha(\psi)\}$ is a tree of height $s_\alpha(\psi) - 1$. For each node $a_\rho$ in the tree, there is a single path $\rho$ from the root $r^{G_\alpha}$ to $a_\rho$.
- At level $s_\alpha(\psi)$, there are $card(LB(G,\psi))$ many nodes. Each of these nodes is uniquely marked with a label in $LB(G,\psi)$. In addition, it does not have any outgoing edge, and all its incoming edges are from leaves of the tree mentioned above.

We now verify that $G_\alpha$ indeed meets all the requirements of the lemma.

(1) *The size of* $G_\alpha$. Let $size(A)$ denote the size of a structure $A$. It is easy to verify that

$$\begin{aligned} card(I_\alpha(\psi)) &\leq |\psi|, \\ card(L_\alpha) &= card(LB(G,\psi)). \end{aligned}$$

Therefore, $size(G_\alpha)$ is at most $|\psi| + 2^{|\psi| + 2^{|\psi|}}$. In particular, when $s_\alpha(\psi) = 0$, $size(G_\alpha)$ is at most 2.

(2) *Properties of* $L_\alpha$. The bijection $f$ from $LB(G,\psi)$ to $L_\alpha$ can be defined by: $l \mapsto a_l$. To verify the other properties of $L_\alpha$, first observe the following:

*Claim*: For any $\varrho \in I_\alpha(\psi)$, $|\varrho| < s_\alpha(\psi)$ and

$$\{\rho \mid \rho \text{ is a path, } G_\alpha \models \rho(r^{G_\alpha}, a_\varrho)\} = \{\varrho\}.$$

This claim can be verified by a straightforward induction on $|\varrho|$. By this claim and the definition of $G_\alpha$, it is easy to verify the second statement of the lemma. ■

The next lemma deals with $LB_{(\beta,\gamma)}(G,\psi)$. More specifically, given a label $l$ in $LB(G,\psi)$, it constructs a $\sigma$-structure $G_l = (|G_l|, r^{G_l}, E^{G_l})$ such that

$$lb_{(\beta,\gamma)}(r^{G_l}, G_l, \psi) = lb_{(\beta,\gamma)}(l).$$

We shall construct the structure $H$ described in Proposition 4.3 such that for each $l$ in $LB(G,\psi)$, $G_l$ is part of $H$, and moreover,

$$lb_{(\beta,\gamma)}(r^{G_l}, H, \psi) = lb_{(\beta,\gamma)}(r^{G_l}, G_l, \psi).$$

**Lemma 4.5:** Let G be a $\sigma$-structure and $\psi \in S_p$. For each $l \in LB(G,\psi)$, there is a $\sigma$-structure $G_l$, such that

1. the size of $G_l$ is at most $2^{|\psi|}$; and
2. $lb_{(\beta,\gamma)}(r^{G_l}, G_l, \psi) = lb_{(\beta,\gamma)}(l)$.

■

**Proof:** We give a filtration argument. Since $l$ is in $LB(G,\psi)$, there exists $a \in |G|$ such that $lb(a, G, \psi) = l$. Let

$$\begin{aligned} I^+(\psi) &= \{\rho \mid \varrho \in Paths_\beta(\psi) \cup Paths^+_\gamma(\psi),\ \rho \preceq_p \varrho\}, \\ I^-(\psi) &= \{-\rho \mid -\varrho \in Paths^-_\gamma(\psi),\ \rho \preceq_s \varrho\}, \\ I(\psi) &= I^+(\psi) \cup I^-(\psi). \end{aligned}$$

Here $\rho \preceq_p \varrho$ ($\rho \preceq_s \varrho$) means that $\rho$ is a prefix (suffix) of $\varrho$, as defined in Section 2. It is easy to verify that $card(I(\psi)) \leq |\psi|$.

We define a function $g$ from $|G|$ to the power set of $I(\psi)$ such that for any $b \in |G|$,

$$\begin{aligned} g(b) \mapsto &\{\rho \mid \rho \in I^+(\psi), G \models \rho(a,b)\} \cup \\ &\{-\rho \mid -\rho \in I^-(\psi), G \models \rho(b,a)\}. \end{aligned}$$

Clearly, the action of $g$ induces an equivalence relation$\sim$ on $|G|$:

$$b \sim b' \quad \text{iff} \quad g(b) = g(b').$$

We denote the equivalence class of $b$ with respect to $\sim$ as $[b]$. We proceed to construct a $\sigma$-structure $G_l$ whose nodes are these equivalence classes.

- $|G_l| = \{[b] \mid b \in |G|\}$;
- $r^{G_l} = [a]$;
- for each $K \in E$ and $o_1, o_2 \in |G_l|$, $G_l \models K(o_1, o_2)$ iff there exist $b_1, b_2 \in |G|$, such that $[b_1] = o_1$, $[b_2] = o_2$, and $G \models K(b_1, b_2)$.

Obviously, the size of $G_l$ is no larger than the cardinality of the power set of $I(\psi)$, and therefore, is at most $2^{|\psi|}$. In addition, it can be verified by a straightforward induction on $|\rho|$ and $|\varrho|$ that for any $\rho \in I^+(\psi)$, $-\varrho \in I^-(\psi)$ and $b \in |G|$,

$$G \models \rho(a, b) \quad \text{iff} \quad G_l \models \rho(r^{G_l}, [b]),$$
$$G \models \varrho(b, a) \quad \text{iff} \quad G_l \models \varrho([b], r^{G_l}).$$

From these follows that $lb_{(\beta,\gamma)}(r^{G_l}, G_l, \psi) = lb_{(\beta,\gamma)}(l)$. ∎

Finally, we prove Proposition 4.3. As mentioned earlier, given a $\sigma$-structure $G$ and a sentence $\psi$ in $S_p$, we define the structure $H$ described in Proposition 4.3 such that

- the structure $G_\alpha$ described in Lemma 4.4 is the $s_\alpha(\psi)$-neighborhood of $r^H$ in $H$;
- for each $l \in LB(G, \psi)$, $G_l$ in Lemma 4.5 is part of $H$ such that
  - $r^{G_l} = f(l)$, where $f$ is the function specified in Lemma 4.4,
  - $lb_{(\beta,\gamma)}(r^{G_l}, H, \psi) = lb_{(\beta,\gamma)}(l)$, and
  - $lb_\alpha(r^{G_l}, H, \psi) = lb_\alpha(l)$.

**Proof of Proposition 4.3:** Given a $\sigma$-structure $G$ and $\psi \in S_p$, let $G_\alpha$ be the $\sigma$-structure specified in Lemma 4.4, and for each $l \in LB(G, \psi)$, let $G_l$ be the structure specified in Lemma 4.5. Without loss of generality, assume that $|G_l| \cap |G_\alpha| = \emptyset$ and $|G_l| \cap |G_{l'}| = \emptyset$ if $l \neq l'$. Using these, we now construct a $\sigma$-structure $H = (|H|, r^H, E^H)$, as follows.

- $|H| = |G_\alpha| \cup \bigcup_{l \in LB(G,\psi)} (|G_l| \setminus \{r^{G_l}\})$;
- $r^H = r^{G_\alpha}$;

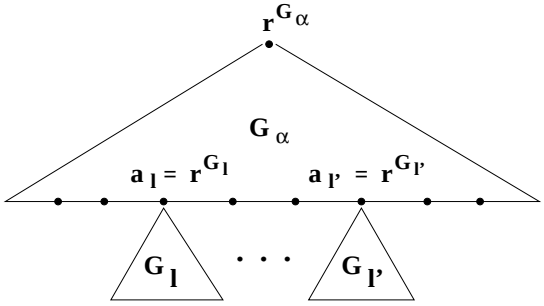


**Figure 5**: The structure $H$ in Proposition 4.3

- For all $a, b \in |H|$ and each $K \in E$, $H \models K(a, b)$ iff one of the following conditions is satisfied:
  - $a, b \in |G_\alpha|$ and $G_\alpha \models K(a, b)$;
  - There are $l \in LB(G, \psi)$, $a, b \in |G_l|$ such that $G_l \models K(a, b)$;
  - Let $L_\alpha$ be the subset of $|G_\alpha|$ and $f$ be the function specified in Lemma 4.4. For some $l \in LB(G, \psi)$,
    - $a = f(l)$, $b \in |G_l|$ and $G_l \models K(r^{G_l}, b)$; or
    - $b = f(l)$, $a \in |G_l|$ and $G_l \models K(a, r^{G_l})$; or
    - $a = b = f(l)$ and $G_l \models K(r^{G_l}, r^{G_l})$.

Intuitively, $H$ is built from $G_\alpha$ and $G_l$'s by identifying $f(l)$ with $r^{G_l}$ for each $l \in LB(G, \psi)$. See Figure 5 for the structure $H$.

We now show that $H$ is indeed the structure desired.

(1) *The size of* $H$. Obviously, $size(H)$ is no larger than

$$size(G_\alpha) + \sum_{l \in LB(G,\psi)} size(G_l) - card(LB(G, \psi)).$$

By Lemmas 4.4 and 4.5, it can be shown that $size(H)$ is no larger than $2^{2^{2|\psi|}}$. Note that when $s_\alpha(\psi) = 0$, $size(H)$ is at most $2^{|\psi|}$.

(2) $LB(H, \psi) = LB(G, \psi)$. By Lemmas 4.4, 4.5 and the definition of $H$, it is easy to verify the following:

*Claim*: Let $L_\alpha$ be the set and $f$ the function specified in Lemma 4.4. They have the following properties.

1. For each $a \in |H| \setminus L_\alpha$, $lb(a, H, \psi) = (\emptyset, \emptyset)$.
2. For each $l \in LB(G, \psi)$, $lb(f(l), H, \psi) = l$.

By the claim, $LB(G, \psi) \subseteq LB(H, \psi)$. In addition, by Lemma 4.4, $f$ is a bijection between $LB(G, \psi)$ and $L_\alpha$. Therefore, $LB(H, \psi) = LB(G, \psi)$. It should be noted that the proof of the claim uses the restriction on prefixes described in Definition 4.1. ∎

### 4.3 Decidability of Implication Problems for $P_\beta$

We now establish the following:

**Theorem 4.6:** The implication and finite implication problems for $P_\beta$ are decidable. ∎

In the same way as in the proof of Theorem 4.1, we show Theorem 4.6 by establishing the small model property for the set:

$$S(P_\beta) = \{\bigwedge \Sigma \wedge \neg\varphi \mid \varphi \in P_\beta,\ \Sigma \subset P_\beta,\ \Sigma \text{ is finite}\}.$$

To do this, we give a filtration argument. Given a satisfiable sentence $\psi$ in $S(P_\beta)$, we find the set of paths in $\psi$ and use a path labeling mechanism similar to the one employed in the proof of Theorem 4.1. More specifically, let $G$ be a model of $\psi$. We use the paths in $\psi$ to label each node of $G$, and therefore, obtain the label of $G$ with respect to $\psi$. The cardinality of this label is determined only by $|\psi|$, the length of $\psi$. We then construct a $\sigma$-structure $H$, such that $H$ and $G$ have the same label with respect to $\psi$, and moreover, $H \models \psi$. In addition, each node of $H$ has a unique path label. The size of $H$ is, therefore, bounded by the cardinality of the label of $G$ with respect to $\psi$, which is at most $2^{|\psi|}$. Thus the small model property is established.

We first define the path labels, called *relative path labels*. Using the path labels, we then establish the small model property for $S(P_\beta)$.

#### 4.3.1 Relative path labels

Let $\psi$ be a satisfiable sentence of $S(P_\beta)$, where $\psi$ is $\bigwedge \Sigma \wedge \neg\varphi$. We use the following to denote paths in $\psi$:

$$\begin{aligned} Paths_{(\alpha,\beta)}(\psi) &= \{pf(\phi) \mid \phi \in \Sigma \cup \{\varphi\}\} \cup \\ &\quad \{lt(\phi) \mid \phi \in \Sigma \cup \{\varphi\},\ \phi \in P_s\} \\ I_{(\alpha,\beta)}(\psi) &= \{\rho \mid \varrho \in Paths_{(\alpha,\beta)}(\psi),\ \rho \preceq_p \varrho\} \\ I(\varphi) &= \begin{cases} \{\rho \mid \rho \preceq_p rt(\varphi)\} & \text{if } \varphi \text{ has forward form} \\ \{\rho \mid \rho \preceq_s rt(\varphi)\} & \text{if } \varphi \text{ has backward form} \end{cases} \end{aligned}$$

Here $\rho \preceq_p \varrho$ ($\rho \preceq_s \varrho$) means that $\rho$ is a prefix (suffix) of $\varrho$, as defined in Section 2.

Let $G$ be a model of $\psi$, $G = (|G|, r^G, E^G)$, and $(a, b)$ be a pair of nodes in $|G|$ such that

$$G \models pf(\varphi)(r, a) \wedge lt(\varphi)(a, b) \wedge \neg rt(\varphi)(a, b)$$

if $\varphi$ is a forward constraint, and

$$G \models pf(\varphi)(r, a) \wedge lt(\varphi)(a, b) \wedge \neg rt(\varphi)(b, a)$$

if $\varphi$ is a backward constraint. This pair is referred to as a *witness of* $\neg\varphi$ *in* $G$.

For each $c \in |G|$, we label $c$ with a pair. The first component of the pair is

$$ls_{(\alpha,\beta)}(c, G, \psi) = \{\rho \mid \rho \in I_{(\alpha,\beta)}(\psi),\ G \models \rho(r^G, c)\}.$$

The second component, $ls_\varphi(c, a, G, \psi)$, is defined to be

- $\{\rho \mid \rho \in I(\varphi),\ G \models \rho(a, c)\}$ if $\varphi$ is a forward constraint, and
- $\{\rho \mid \rho \in I(\varphi),\ G \models \rho(c, a)\}$ if $\varphi$ is a backward constraint.

The *path label of node $c$ in $G$ relative to $\psi$ and $a$* is defined to be:

$$ls(c, G, \psi, a) = (ls_{(\alpha,\beta)}(c, G, \psi),\ ls_\varphi(c, a, G, \psi))$$

The *path label of $G$ relative to $\psi$ and $a$* is defined to be:

$$LS(G, \psi, a) = \{ls(c, G, \psi, a) \mid c \in |G|\}$$

We now examine the cardinality of $LS(G, \psi, a)$. It is easy to verify that $card(I_{(\alpha,\beta)}(\psi)) + card(I(\varphi)) \leq |\psi|$. Note that for each $c \in |G|$, $ls_{(\alpha,\beta)}(c, G, \psi) \subseteq I_{(\alpha,\beta)}(\psi)$ and $ls_\varphi(c, a, G, \psi) \subseteq I(\varphi)$. Hence $card(LS(G, \psi, a))$ is at most $2^{|\psi|}$.

The notion of relative path labels differs from the one described in Section 4.2.1 in the following respects. First, relative path labels are defined for models of satisfiable sentences in $S(P_\beta)$, rather than for arbitrary $\sigma$-structures. Second, the relative path label of a node $a$ in a structure involves only the paths between $a$ and two fixed nodes in the structure, namely, the root node and a node in a witness of $\neg\varphi$, whereas the one given in Section 4.2.1 contains paths connecting all pairs of nodes in the structure. As a result, a relative path label has a much smaller cardinality. Third, a relative path label does not characterize whether a $\sigma$-structure is a model of a sentence in $S(P_\beta)$, but based on it we are able to construct a filtration argument to establish the small model property for $S(P_\beta)$.

#### 4.3.2 The small model property

Using relative path labels we show the following:

**Proposition 4.7:** Every satisfiable sentence $\psi$ of $S(P_\beta)$ has a model of size at most $2^{|\psi|}$. ∎

**Proof:** Let $\psi$ be a satisfiable sentence in $S(P_\beta)$, where $\psi = \bigwedge \Sigma \wedge \neg\varphi$, and $\Sigma \cup \{\varphi\}$ is a finite subset of $P_\beta$. Since $\psi$ is satisfiable, there is a $\sigma$-structure $G = (|G|, r^G, E^G)$ such that $G \models \psi$. It follows that there exist $a$, $b$ in $|G|$ such that $(a, b)$ is a witness of $\neg\varphi$ in $G$. Consider

$LS(G, \psi, a)$. As in the proof of Lemma 4.5, we define an equivalence relation $\sim$ on $|G|$ by:

$$b \sim b' \quad \text{iff} \quad ls(b, G, \psi, a) = ls(b', G, \psi, a).$$

For each $b \in |G|$ we denote the equivalence class of $b$ with respect to $\sim$ as $[b]$. By taking these equivalence classes as nodes, we proceed to construct a $\sigma$-structure $H$ as follows:

- $|H| = \{[b] \mid b \in |G|\}$;
- $r^H = [r^G]$;
- for each $K \in E$ and $o_1, o_2 \in |H|$, $H \models K(o_1, o_2)$ iff there exist $b_1, b_2 \in |G|$, such that $[b_1] = o_1$, $[b_2] = o_2$, and $G \models K(b_1, b_2)$.

We next show that $H \models \psi$, and moreover, the size of $H$ is at most $2^{|\psi|}$.

(1) *The size of H.* Since $size(H) = card(LS(G, \psi, a))$, $size(H)$ is at most $2^{|\psi|}$.

(2) $H \models \psi$. It suffices to show the following claims.

*Claim 1:* For any path $\rho$ and $c, d \in |G|$, if $G \models \rho(c, d)$, then $H \models \rho([c], [d])$.

*Claim 2:* For each $c \in |G|$,

$$ls(c, G, \psi, a) = ls([c], H, \psi, [a]).$$

Claim 1 can be easily verified by induction on $|\rho|$. Similarly, Claim 2 can be verified by showing that for any $\rho \in I_{(\alpha,\beta)}(\psi)$, $\varrho \in I(\varphi)$ and $c \in |G|$,

$$\rho \in ls_{(\alpha,\beta)}(c, G, \psi) \quad \text{iff} \quad \rho \in ls_{(\alpha,\beta)}([c], H, \psi),$$
$$\varrho \in ls_{\varphi}(c, a, G, \psi) \quad \text{iff} \quad \varrho \in ls_{\varphi}([c], [a], H, \psi).$$

Again, these can be shown by induction on $|\rho|$ and $|\varrho|$.

Using these claims, we prove $H \models \psi$ as follows.

We first show that $H \models \Sigma$. Suppose, for a contradiction, that there exists $\phi \in \Sigma$ such that $H \models \neg\phi$. Without loss of generality, assume that $\phi$ is a forward constraint (the argument for the backward case is analogous). Then there exist $c, d \in |H|$, such that

$$H \models pf(\phi)(r^H, c) \wedge lt(\phi)(c, d) \wedge \neg rt(\phi)(c, d).$$

We have two cases to consider.

*Case 1:* $\phi$ is a simple constraint. That is, $pf(\phi) = \epsilon$ and $c = r^H$. In this case, we have $lt(\phi) \in ls_{(\alpha,\beta)}(d, H, \psi)$ and $H \models \neg rt(\phi)(r^H, d)$. By the definition of $H$, there exists $d_1 \in |G|$, such that $[d_1] = d$. By Claim 2, $ls(d_1, G, \psi, a) = ls(d, H, \psi, [a])$. By the definition of $ls$, we have $ls_{(\alpha,\beta)}(d_1, G, \psi) = ls_{(\alpha,\beta)}(d, H, \psi)$. Hence $lt(\phi) \in ls_{(\alpha,\beta)}(d_1, G, \psi)$. That is, $G \models lt(\phi)(r^G, d_1)$. Since $G \models \phi$, we have that $G \models rt(\phi)(r^G, d_1)$. By Claim 1, we have $H \models rt(\phi)(r^H, d)$. This contradicts the assumption.

*Case 2:* $\phi$ is a $\beta$-restricted constraint, i.e., $|lt(\phi)| \leq 1$.

If $|lt(\phi)| = 0$, then $c = d$. Thus by the assumption, $pf(\phi) \in ls_{(\alpha,\beta)}(c, H, \psi)$ and $H \models \neg rt(\phi)(c, c)$. By the definition of $H$, there exists $c_1 \in |G|$, such that $[c_1] = c$. By Claim 2, $ls_{(\alpha,\beta)}(c_1, G, \psi) = ls_{(\alpha,\beta)}(c, H, \psi)$. Thus $pf(\phi) \in ls_{(\alpha,\beta)}(c_1, G, \psi)$. That is, $G \models pf(\phi)(r^G, c_1)$. By $G \models \phi$, $G \models rt(\phi)(c_1, c_1)$. Thus by Claim 1, we have $H \models rt(\phi)(c, c)$. This contradicts the assumption.

If $|lt(\phi)| = 1$, then $lt(\phi) = K$ for some $K \in E$. By the assumption, we have $pf(\phi) \in ls_{(\alpha,\beta)}(c, H, \psi)$ and $H \models K(c, d) \wedge \neg rt(\phi)(c, d)$. By the definition of $H$, there exist $c_1, d_1 \in |G|$, such that $[c_1] = c$, $[d_1] = d$ and moreover, $G \models K(c_1, d_1)$. By Claim 2, we have that $ls_{(\alpha,\beta)}(c_1, G, \psi) = ls_{(\alpha,\beta)}(c, H, \psi)$. As a result, we have $G \models pf(\phi)(r^G, c_1)$. By $G \models \phi$, $G \models rt(\phi)(c_1, d_1)$. Thus by Claim 1, we have $H \models rt(\phi)(c, d)$. Again, this contradicts the assumption.

We next show that $H \models \neg\varphi$. Since $(a, b)$ is a witness of $\neg\varphi$ in $G$, $G \models pf(\varphi)(r^G, a) \wedge lt(\varphi)(a, b)$. By Claim 1,

$$H \models pf(\varphi)(r^H, [a]) \wedge lt(\varphi)([a], [b]).$$

By Claim 2, $ls_{\varphi}(b, a, G, \psi) = ls_{\varphi}([b], [a], H, \psi)$. Hence when $\varphi$ is a forward constraint, by $G \models \neg rt(\varphi)(a, b)$, we have that $H \models \neg rt(\varphi)([a], [b])$; and when $\varphi$ is a backward constraint, by $G \models \neg rt(\varphi)(b, a)$, we have that $H \models \neg rt(\varphi)([b], [a])$. Therefore, $H \models \neg\varphi$. ∎

### 4.4 Decidability of Extended Implication for $P_\beta$

Next, we prove the following:

**Theorem 4.8:** The extended implication and finite implication problems for $P_\beta$ are decidable. ∎

We prove the theorem by reduction to the implication problems for $P_\beta$, whose decidability is established by Theorem 4.6.

Let $Pts$ be the set of all paths, and let $S_e(P_\beta)$ be

$$\{\bigwedge \Sigma \wedge \neg\varphi \mid \Sigma \cup \{\varphi\} \text{ is a prefix extended subset of } P_\beta\}.$$

Recall the set $S(P_\beta)$ defined in Section 4.3. We define the *prefix extension function from* $S(P_\beta)$ *to* $S_e(P_\beta)$ to be the mapping $f : S(P_\beta) \times Pts \to S_e(P_\beta)$, such that

$$f(\bigwedge \Sigma \wedge \neg\varphi, \alpha) \mapsto \bigwedge_{\phi \in \Sigma} \delta(\phi, \alpha) \wedge \neg\delta(\varphi, \alpha),$$

where $\delta$ is described in Definition 4.3.

To prove Theorem 4.8, it suffices to show:

**Proposition 4.9:** Let $\psi$ be a sentence in $S(P_\beta)$, $\alpha$ a path, and $f$ the prefix extension function from $S(P_\beta)$ to $S_e(P_\beta)$. Then

1. $\psi$ is satisfiable iff $f(\psi, \alpha)$ is satisfiable;
2. $\psi$ is finitely satisfiable iff $f(\psi, \alpha)$ is finitely satisfiable. In addition, if $\psi$ has a finite model of size $N$, then $f(\psi, \alpha)$ has a model of size $N + |\alpha|$.

■

For if Proposition 4.9 holds, then $S_e(P_\beta)$ has the small model property for satisfiability. More specifically, given $\phi \in S_e(P_\beta)$, we can determine a path $\alpha$ and $\psi \in S(P_\beta)$ in linear time, such that $\phi = f(\psi, \alpha)$. In addition, $|\phi| \geq |\psi| + |\alpha|$. If $\phi$ is satisfiable, then by Proposition 4.9, so is $\psi$. By Proposition 4.7, $\psi$ has a model of size at most $2^{|\psi|}$. Thus again by Proposition 4.9, $\phi$ has a model of size at most $2^{|\psi|+|\alpha|}$, which is no larger than $2^{|\phi|}$. Therefore, $S_e(P_\beta)$ has the small model property and it follows that the extended implication and finite implication problems for $P_\beta$ are decidable.

**Proof of Proposition 4.9:** We only prove (2) of the proposition. The proof of (1) is similar.

Let $\psi = \bigwedge \Sigma \wedge \neg\varphi$. Note that if $|\alpha| = 0$, then $f(\psi, \alpha) = \psi$. Obviously, the proposition holds in this case. Hence in the sequel, we assume that $|\alpha| \geq 1$.

Assume that $\psi$ has a finite model $G = (|G|, r^G, E^G)$. We show that $f(\psi, \alpha)$ has a model $H = (|H|, r^H, E^H)$, and moreover, the size of $H$, $size(H)$, is $size(G) + |\alpha|$.

Let $R_\alpha = \{\rho \mid \rho \text{ is a path}, \rho \prec_p \alpha\}$, where $\rho \prec_p \alpha$ means that $\rho$ is a proper prefix of $\alpha$. We construct $H$ as follows. For each $\rho \in R_\alpha$, let $c_\rho$ be a distinct node which is not in $|G|$. Let

- $|H| = |G| \cup \{c_\rho \mid \rho \in R_\alpha\}$;
- $r^H = c_\epsilon$;
- For all $a, b \in |H|$ and each $K \in E$, $H \models K(a, b)$ iff one of the following conditions is satisfied:
  - there exists $\rho \in R_\alpha$, such that $a = c_\rho$ and $b = c_{\rho \cdot K}$ and $\rho \cdot K \in R_\alpha$; or
  - there exists $\rho \in R_\alpha$, such that $\alpha = \rho \cdot K$ and $a = c_\rho$ and $b = r^G$; or
  - $a, b \in |G|$ and $G \models K(a, b)$.

Obviously, $size(H) = size(G) + |\alpha|$. In addition, it is straightforward to verify that $H \models f(\psi, \alpha)$.

Conversely, suppose that $f(\psi, \alpha)$ has a finite model $G = (|G|, r^G, E^G)$. We construct a finite model of $\psi$.

Without loss of generality, assume that $\varphi$ is a forward constraint (the proof for the backward case is analogous). Since $G \models \neg\delta(\varphi, \alpha)$, there exist $a, b, c \in |G|$, such that

$$G \models \alpha(r^G, a) \wedge pf(\varphi)(a, b) \wedge lt(\varphi)(b, c) \wedge \neg rt(\varphi)(b, c).$$

Let $m$ be the largest natural number in the following set: $\{|pf(\phi)| + |lt(\phi)| + |rt(\phi)| \mid \phi \in \Sigma \cup \{\varphi\}\}$. Let $G(a)$ be the $m$-neighborhood of $a$ in $G$, as described in Definition 4.5. Clearly, $G(a)$ is a finite $\sigma$-structure. We next prove that $G(a) \models \psi$.

We first show $G(a) \models \neg\varphi$. By $|pf(\varphi)| + |lt(\varphi)| < m$ and $|pf(\varphi)| + |rt(\varphi)| < m$, we have that $b \in |G(a)|$ and $c \in |G(a)|$. Thus by the definition of $G(a)$, we have

$$G(a) \models pf(\varphi)(a, b) \wedge lt(\varphi)(b, c) \wedge \neg rt(\varphi)(b, c).$$

That is, $G(a) \models \neg\varphi$.

Second, we show by contradiction that for any $\phi \in \Sigma$, $G(a) \models \phi$. Suppose that there exists $\phi \in \Sigma$ such that $G(a) \models \neg\phi$. Without loss of generality, assume that $\phi$ is a forward constraint (the proof for the backward case is analogous). Then there exist $d, e \in |G(a)|$ such that

$$G(a) \models pf(\phi)(a, d) \wedge lt(\phi)(d, e) \wedge \neg rt(\phi)(d, e).$$

Thus by the definition of $G(a)$, we have

$$G \models \alpha(r^G, a) \wedge pf(\phi)(a, d) \wedge lt(\phi)(d, e) \wedge \neg rt(\phi)(d, e).$$

That is, $G \models \neg\delta(\phi, \alpha)$. This contradicts the assumption that $G \models f(\psi, \alpha)$. ■

### 4.5 Conjunctive Path Constraints

We next show that the complexity results established above also hold for an extension of path constraints. This extension is defined as follows.

**Definition 4.6:** A *conjunctive path constraint* $\phi$ is an expression of either the *forward* form

$$\forall x \, ( \bigwedge_{\alpha \in A} \alpha(r, x) \rightarrow \forall y \, ( \bigwedge_{\beta \in B} \beta(x, y) \rightarrow \gamma(x, y))),$$

or the *backward* form

$$\forall x \, ( \bigwedge_{\alpha \in A} \alpha(r, x) \rightarrow \forall y \, ( \bigwedge_{\beta \in B} \beta(x, y) \rightarrow \gamma(y, x))),$$

where $A, B$ are non-empty finite sets of paths, and are denoted by $pf(\phi)$ and $lt(\phi)$, respectively. Here $\gamma$ is a path, denoted by $rt(\phi)$. The set of all conjunctive path constraints is denoted by $P_c^\wedge$. ■

As an example, consider the following conjunctive path constraints:

$$\forall x\,(dept(r,x) \rightarrow \forall y\,(ta(x,y) \rightarrow student(x,y)))$$

$$\forall x\,(dept(r,x) \rightarrow \forall y\,(ta(x,y) \rightarrow employee(x,y)))$$

$$\forall x\,(dept(r,x) \rightarrow \forall y\,((student(x,y) \wedge employee(x,y)) \rightarrow ta(x,y)))$$

Abusing object-oriented database terms, these $P_c^\wedge$ constraints assert:

- TA of a department is a "subclass" of both Student and Employee of the department; and
- the "extent" of TA is the intersection of the "extents" of Student and Employee.

Obviously, $P_c$ is a subclass of $P_c^\wedge$. Therefore, the corollary below follows from Theorem 3.1 immediately.

**Corollary 4.10:** The implication problem for $P_c^\wedge$ is r.e. complete, and the finite implication problem for $P_c^\wedge$ is co-r.e. complete. ∎

Below we define fragments of $P_c^\wedge$ analogous to the fragments of $P_c$ discussed above.

**Definition 4.7:** A finite subset $\Sigma$ of $P_c^\wedge$ is called a *prefix restricted subset* of $P_c^\wedge$ iff for all $\phi$, $\psi$ in $\Sigma$, all the paths in $pf(\phi) \cup pf(\psi)$ have the same length.

The *prefix restricted (finite) implication problem for* $P_c^\wedge$ is the problem to determine, given any finite prefix restricted subset $\Sigma \cup \{\phi\}$ of $P_c^\wedge$, whether all the (finite) models of $\Sigma$ are also models of $\phi$. ∎

**Definition 4.8:** A *simple conjunctive path constraint* $\phi$ is a constraint of $P_c^\wedge$ with $pf(\phi) = \{\epsilon\}$.

A *$\beta$-restricted conjunctive path constraint* $\phi$ is a constraint of $P_c^\wedge$ such that for each $\beta \in lt(\phi)$, $|\beta| \leq 1$.

The sublanguage $P_\beta^\wedge$ is defined to be the class of $P_c^\wedge$ constraints $\phi$ such that either for any $\alpha \in pf(\phi)$, $|\alpha| = 0$, or for any $\beta \in lt(\phi)$, $|\beta| \leq 1$. That is, $P_c^\wedge$ is the set of all simple conjunctive path constraints and all $\beta$-restricted conjunctive path constraints. ∎

**Definition 4.9:** Let $\rho$ be a path and $\phi$ be a constraint in $P_\beta^\wedge$. The *extension of $\phi$ with prefix $\rho$*, denoted by $\delta(\phi, \rho)$, is the constraint in $P_c^\wedge$ defined either by

$$\forall x\,(\bigwedge_{\alpha \in pf(\phi)} \rho \cdot \alpha(r,x) \rightarrow \forall y\,(\bigwedge_{\beta \in lt(\phi)} \beta(x,y) \rightarrow rt(\phi)(x,y)))$$

when $\phi$ is of the forward form, or by

$$\forall x\,(\bigwedge_{\alpha \in pf(\phi)} \rho \cdot \alpha(r,x) \rightarrow \forall y\,(\bigwedge_{\beta \in lt(\phi)} \beta(x,y) \rightarrow rt(\phi)(y,x)))$$

when $\phi$ is of the backward form.

Let $\rho$ be a path and $\Sigma$ a finite subset of $P_\beta^\wedge$. The *extension of $\Sigma$ with prefix $\rho$* is the subset of $P_c^\wedge$ defined by $\{\delta(\phi, \rho) \mid \phi \in \Sigma\}$. Such a set is called a *prefix extended subset of $P_\beta^\wedge$*.

The *extended (finite) implication problem for* $P_\beta^\wedge$ is the problem of determining, given any prefix extended subset $\Sigma \cup \{\phi\}$ of $P_\beta^\wedge$, whether all the (finite) models of $\Sigma$ are also models of $\phi$. ∎

On semistructured data we have the following, which are analogous to Theorems 4.1, 4.6 and 4.8.

**Theorem 4.11:** The following problems are decidable:

- The prefix restricted implication and finite implication problems for $P_c^\wedge$.
- The implication and finite implication problems for $P_\beta^\wedge$.
- The extended implication and finite implication problems for $P_\beta^\wedge$. ∎

With slight modification, the proofs of Theorems 4.1, 4.6 and 4.8 are applicable to Theorem 4.11.

With thanks to an anonymous referee, we observe that the arguments for these theorems can even be used to establish the decidability of certain extensions of the decidable fragments of $P_c$ and $P_c^\wedge$. For example, the proof of Theorem 4.1 yields a stronger result: the satisfiability of any Boolean combination of constraints in prefix restricted subsets of $P_c$ is decidable. More specifically, let $\Sigma$ be a a prefix restricted subset of $P_c$. We define a set $B(\Sigma)$ of logic sentences as follows:

- $\Sigma \subseteq B(\Sigma)$;
- if $\varphi \in B(\Sigma)$, then so is $\neg\varphi$;
- if $\varphi$ and $\phi$ are in $B(\Sigma)$, then so are $\varphi \wedge \phi$ and $\varphi \vee \phi$.

The *(finite) satisfiability problem for Boolean combinations of constraints in prefix restricted subsets of* $P_c$ is the problem to determine, given any prefix restricted subset $\Sigma$ of $P_c$ and any $\varphi \in B(\Sigma)$, whether $\varphi$ has a (finite) model.

With slight modification, the argument for Theorem 4.1 can be used to prove the following:

**Proposition 4.12:** The satisfiability and finite satisfiability problems for Boolean combinations of constraints in prefix restricted subsets of $P_c$ are decidable. ∎

## 5 CONCLUSIONS

We have introduced a class of path constraints, $P_c$, and investigated its associated implication and finite implication problems. These path constraints capture many natural integrity constraints that commonly arise in both structured and semistructured databases. They are not only a fundamental part of the semantics of the data; they are also useful in query optimization. The importance of these constraints was also emphasized in several XML proposals (e.g., [10, 26, 31, 32]). Due to the recent popularity of the World Wide Web and the success of the XML standard [11], these constraints have found a wide range of applications.

In the context of semistructured data, we have shown that, despite the simple syntax of the language $P_c$, its associated implication problem is r.e. complete and its finite implication problem is co-r.e. complete. These results are rather surprising since $P_c$ is a mild generalization of word constraints introduced and studied in [5], for which the implication and finite implication problems are in PTIME. In light of these undecidability results, we have also identified several fragments of $P_c$ which suffice to express many interesting semantic relations such as extent, inverse and local database constraints, and properly contain the class of word constraints. We have established the decidability of the implication and finite implication problems associated with each of these fragments.

Another issue of equal importance is the interaction between path and type constraints. Although the XML standard itself does not require any schema or type system, a number of proposals have been developed that allow one to constrain the structure of XML data by imposing a schema or a type constraint on it. These and other proposals also advocate the need for certain integrity constraints, which can be expressed as $P_c$ constraints. It is likely that future XML proposals will involve both forms of constraints, and it is therefore appropriate to understand the interaction between them. It would be tempting to directly apply the complexity results developed for semistructured data to typed data. However, we have shown in [15, 16] that path constraints interact with type constraints. More specifically, a number of decidability and undecidability results have been established there which demonstrate that adding a type system may in some cases simplify reasoning about path constraints, and in other cases make it harder. A full treatment of these results will appear in a future publication.

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