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Functional Dependencies for XML

Axiomatisation and Normal Form
in the presence of
Frequencies and Identifiers

A thesis presented in partial fulfilment of the requirements for the degree of
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1 Introduction

XML has gained popularity as a markup language for publishing and exchanging data on the web. Nowadays, there are also ongoing interests in using XML for representing and actually storing data. In particular, much effort has been directed towards turning XML into a real data model by improving the semantics that can be expressed about XML documents. Various works have addressed how to define different classes of integrity constraints and the development of a normalisation theory for XML. One area which received little to no attention from the research community up to five years ago is the study of functional dependencies in the context of XML [37]. Since then, there has been increasingly more research investigating functional dependencies in XML. Nevertheless, a comprehensive dependency theory and normalisation theory for XML have yet to emerge.

Functional dependencies are an integral part of database theory in the relational data model (RDM). In particular, functional dependencies have been vital in the investigation of how to design “good” relational database schemas which avoid or minimise problems relating to data redundancy and data inconsistency. Since the same problems can be shown to exist in poorly designed XML schemas\(^1\), there is a need to investigate how these problems can be eliminated in the context of XML. We believe that the study of an analogy to relational functional dependencies in the context of XML is equally significant towards designing “good” XML schemas.

Researchers have proposed various generalisations of functional dependencies for XML but many do not have direct counterparts in the RDM. One of the main types of storage solutions being proposed for XML is to extend current storage solutions for relational databases to manage XML data (e.g. [9, 13, 24, 25, 27, 39]). A motivation for this approach is that, while technologies for native XML databases are still in the early stages of development, technologies for relational databases are stable and widely available and used. We will limit our study to a definition of functional dependencies which can be readily mapped to the notion of functional dependencies in the RDM.

The main goal of this research is to study functional dependencies for XML in the presence of frequencies and identifiers. Frequencies describe the optionality and cardinality in a DTD which may be associated with elements and attributes, while identifiers refer to attributes whose values are unique within an XML document. Frequencies and identifiers exist naturally in XML, and their existence reflects the much richer (particularly more flexible) structure of XML data. It is therefore surprising that few research into functional dependencies for XML have yet to emerge.

\(^1\)By “XML schemas” we are referring to the structural information of XML data, either implicitly contained in an XML document or explicitly specified using DTDs or other schema specification language.
dependencies for XML has explicitly considered the additional structural information provided by means of frequencies and identifiers.

In this thesis, we continue the study of the subgraph-based approach towards functional dependencies presented in [14, 15]. The thesis covers two issues: axiomatisation for functional dependencies and a normal form which characterises the absence of redundancy. We will present an axiomatisation for functional dependencies on XML schemas with frequencies, and an axiomatisation for functional dependencies on XML schemas with both frequencies and identifiers. In the latter part we propose a normal form which makes use of identifiers. In accordance with other works relating to normal forms in the context of XML, we justify our normal form by proving that it guarantees the absence of redundancy.

1.1 Outline of the Thesis

The rest of the thesis is organised as follows. Section 2 contains some preliminary definitions relating to the XML graph model and a notion of functional dependencies in XML (called XFDs) which we will study. In the next two sections, we discuss inference rules for the derivation of XFDs and present axiomatisations of XFDs which we show to be both sound and complete for the derivation of XFDs. We consider XFDs in the presence of frequencies in Section 3 and XFDs in the presence of frequencies together with identifiers in Section 4. In Section 5, we generalise the notion of redundancy to the context of XML and propose a normal form which is both necessary and sufficient for the absence of redundancy. We also try to highlight the limitation of redundancy as a design quality criteria in the context of XML. Related work is identified in Section 6 and finally we conclude with some possible research directions in Section 7.
2 Preliminary Notations

2.1 XML Graph Model

In this section, we present the XML graph model introduced in [14, 15]. The reader is assumed to be familiar with standard notions from graph theory such as graphs, trees and walks. In accordance with [14, 15], all graphs will be considered to be directed, without parallel arcs and finite unless stated otherwise.

For every graph \( G \), let \( V_G \) denote its set of vertices and \( A_G \) its set of arcs.

2.1.1 Rooted Graphs and Rooted Trees

A rooted graph is a graph with no vertices, or a graph \( G \) with one distinguished vertex \( r_G \), called the root of \( G \), such that there is a directed path from \( r_G \) to every other vertex in \( V_G \). A rooted tree is a rooted graph \( T \) with no non-directed cycles.

A graph \( G \) is called empty, written \( G = \emptyset \), if \( A_G \) is empty and non-empty otherwise. Specifically, \( G \) is an empty rooted graph if it consists of a single vertex \( r_G \) or no vertices.

For every vertex \( v \), let \( \text{Succ}_G(v) \) denote its (possibly empty) set of successors in \( G \). Leaves are those vertices without successors. Let \( L_G \) denote the set of all leaves in \( G \).

**Definition 2.1.** Given a vertex \( v \in V_G \) and a subset \( W \subseteq L_G \) of leaves, a \( v \)-subgraph of \( G \) is the graph union of all directed walks from \( v \) to some \( w \in W \). A \( v \)-walk of \( G \) is a directed walk from \( v \) to a single leaf \( w \in L_G \). Every \( v \)-subgraph/\( v \)-walk of a rooted tree \( T \) is again a rooted tree.

2.1.2 XML Graphs

Let \( ENames \) and \( ANames \) be fixed sets of element names and attribute names respectively. Also let the symbols \( E \), \( A \) and \( S \) reflect whether a vertex represents an element, attribute or text data respectively.

**Definition 2.2.** An XML graph is a rooted graph \( G \) together with the mappings \( \text{name} : V_G \to ENames \cup ANames \) and \( \text{kind} : V_G \to \{E, A, S\} \) assigning every vertex its name and kind respectively. We suppose that every vertex \( v \) of kind \( S \) is mapped to the same name as the name carried by the predecessor of \( v \). If \( G \) is a rooted tree then we can also refer to an XML graph as an XML tree.
In XML no element has two attributes of the same name, therefore no vertex in an XML graph has two successors of kind A carrying the same name. We do not consider mix-content elements, therefore no vertex of kind E may have both a successor of kind S and a successor of kind E. All XML trees are assumed to be unordered trees.

Let $V_E^G$, $V_A^G$ and $V_S^G$ consist of all vertices in $V_G$ of kind E, A and S respectively. We suppose that in a non-empty XML graph, vertices of kind A and S are always leaves and conversely all leaves are either of kind A or S, that is, $L_G = V_A^G \cup V_S^G$. Thus we also do not allow empty elements without attributes, except for the root element.

### 2.1.3 Mappings between XML Graphs

**Definition 2.3.** Let $G'$ and $G$ be two XML graphs, and consider a mapping $\phi : V_G \rightarrow V_{G'}$. $\phi$ is said to be kind-preserving if the image of a vertex is of the same kind as the vertex itself, that is, $\text{kind}(v') = \text{kind}(\phi(v'))$ for all $v' \in V_{G'}$. Further, $\phi$ is name-preserving if the image of a vertex carries the same name as the vertex itself, that is, $\text{name}(v') = \text{name}(\phi(v'))$ for all $v' \in V_{G'}$. The mapping $\phi$ is a homomorphism between $G'$ and $G$ if all of the following conditions hold:

(i) the root of $G'$ is mapped to the root of $G$, that is, $\phi(r_{G'}) = r_G$

(ii) every arc of $G'$ is mapped to an arc of $G$, that is, $(u', v') \in A_{G'}$ implies $(\phi(u'), \phi(v')) \in A_G$

(iii) $\phi$ is kind-preserving and name-preserving.

\[\square\]
Definition 2.4. A homomorphism \( \phi : V_{G'} \rightarrow V_G \) is an isomorphism if \( \phi \) is bijective and \( \phi^{-1} \) is a homomorphism. Whenever such an isomorphism exists, \( G' \) is said to be isomorphic to \( G \), denoted by \( G' \cong G \). Alternatively, we may say that \( G' \) is a copy of \( G \). 

Example 2.1. Let us consider the two XML trees in Figure 2. There is a homomorphism \( \phi : V_{O'} \rightarrow V_O \) between the XML tree \( O' \) and the XML tree \( O \). This is the name-preserving mapping which maps every vertex from \( O' \) to the vertex carrying the same name in \( O \). \( \phi^{-1} \) is clearly root-preserving, name-preserving and kind-preserving. Further, all arcs in \( O \) is mapped to some arc in \( O' \) by \( \phi^{-1} \). Therefore \( \phi^{-1} \) is a homomorphism. However, the homomorphism \( \phi \) is not bijective, therefore \( O' \) is not isomorphic to \( O \). 

Definition 2.5. A subgraph \( H' \) of \( G' \) is a copy of a subgraph \( H \) of \( G \) if the restriction of \( \phi : V_{G'} \rightarrow V_G \) to \( H' \) and \( H \) is an isomorphism between \( H' \) and \( H \). An \( r_G \)-subgraph \( H' \) of \( G' \) is a subcopy of \( G \) if it is a copy of some \( r_G \)-subgraph \( H \) of \( G \). A maximal subcopy of \( G \) is a subcopy of \( G \) which is not an \( r_G \)-subgraph of any other subcopy of \( G \). A maximal subcopy of \( G \) is called an almost copy of \( G \).
It should be noted that all copies of $G$ in $G'$ are almost copies of $G$, but not vice versa. Also we can observe that a homomorphism $\phi : V_{G'} \rightarrow V_G$ is not an isomorphism whenever $G'$ contains more than one copy of $G$ or no copy (but possibly many almost copies) of $G'$.

### 2.1.4 XML Schema Graphs and XML Data Trees

**Definition 2.6.** An XML schema graph is an XML graph $G$ together with a mapping $\text{freq} : A_G \rightarrow \{?, 1, +, *\}$ assigning every arc its frequency. Every arc $a = (v, w)$ where $w$ is of kind $A$ has frequency $\text{freq}(a) = ?$ or $1$. Every arc $a = (v, w)$ where $\text{kind}(v) = E$ and $\text{kind}(w) = S$ has frequency $\text{freq}(a) = 1$. Further, we assume no vertex in $V_G$ has two successors with the same name and the same kind. If $G$ is more specifically an XML tree, then we can talk about an XML schema tree.

![XML tree O (from Figure 2) together with a frequency labels on arcs. From this point on, let O be the XML schema graph shown here.](image)

We re-emphasise, as in [14], that the term “schema graph” is used as an analogy to database schemas in traditional relational database design. There is no intended association between XML schema graphs and the language XML SCHEMA used to describe XML documents.

Unless stated otherwise, whenever the term “schema graph” or “schema tree” is used, we are in fact referring to “XML schema graph” and “XML schema tree” respectively.

An XML schema graph can be generated from a DTD or from an XML document. Refer to [14] for a discussion on how to derive an XML schema graph from a DTD and to [15] for how to generate an XML graph from an XML document.

Several things should be noted in connection with generating XML schema graphs. The first is that, whenever no DTD is available the designer needs to determine a suitable
frequency mapping for the generated XML graph. Secondly, if a DTD is recursive then we only consider a finite number of unfoldings of the recursive expression. Thirdly, we do not consider disjunction. If a DTD contains some disjunctive expression then we simply treat this as a sequential expression with each element in the disjunction being assigned a frequency of * or ?. For example, if \((A|B|C^+)\) is a regular expression in a given DTD, then this is treated as \((A^*, B^*, C^*)\). This is similar to the notion of simplifying DTD [27].

The following are some notations relating to frequencies used throughout the thesis. We use “an f-arc” to refer to an arc of frequency \(f\) and “an \(f/g\)-arc” to refer to an arc of frequency \(f\) or \(g\). For example, a ?-arc refers to an arc of frequency ?, while a */+-arc refers to an arc of frequency * or +. For an XML schema graph \(G\), let \(G_{\leq 1}\) be the graph union of all ?/1-arcs in \(A_G\), and let \(G_{\geq 1}\) be the graph union of all 1/+ -arcs in \(A_G\). Note that \(G_{\leq 1}\) and \(G_{\geq 1}\) may not be r\(_G\)-subgraphs in \(G\).

![Diagram](image)

Figure 5: The subgraphs \(O_{\geq 1}\) and \(O_{\leq 1}\), where \(O\) is the XML schema graph from Figure 4.

**Definition 2.7.** An **XML data tree** is an XML tree \(T'\) together with an evaluation \(val: L_{T'} \rightarrow STRING\) assigning every leaf \(v\) a (possibly empty) string \(val(v)\).

![Diagram](image)

Figure 6: XML tree \(O'\) (from Figure 2) together with an evaluation of all leaves. From this point on, let \(O'\) be the XML data tree shown here.
Definition 2.8. Let $G$ be an XML schema graph. An XML data tree $T'$ is compatible with $G$, denoted by $T' \triangleright G$, if there is a homomorphism $\phi : V_{T'} \rightarrow V_G$ between $T'$ and $G$ such that for every vertex $v'$ of $T'$ and every arc $a = (\phi(v'), w)$ of $G$, the number of arcs $a' = (v', w')$ mapped to $a$ is at most 1 if $freq(a) = \?$, exactly 1 if $freq(a) = 1$, at least 1 if $freq(a) = +$ and arbitrarily many if $freq(a) = *$. In particular, due to Definition 2.6, this homomorphism is unique whenever it exists.

Example 2.2. Recall the homomorphism between $O'$ and $O$ from Example 2.1. It remains to check the frequencies.

Let an $n$-vertex be a vertex carrying the name "n". For the single F-vertex in $O'$ there are two arcs to H-vertices. The frequency of the F-vertex to H-vertex arc in $O$ is $+$, that is, at least one arc is needed. This is true in $O'$. As another example, consider all H-vertices in $O'$. For each H-vertex, there is exactly one arc to a K-vertex. This is exactly what is required for the frequency of 1 for the H-vertex to K-vertex arc in $O$. After examining all frequencies in the schema tree $O$, we may conclude that $O' \triangleright O$.

Let $T'_1$ be any almost copy of $T$ in an XML data tree $T' \triangleright T$. It is possible that $T'_1$ does not contain a copy of some $r_T$-walk which contain an $?$-arc or $*$-arc. Note that this flexibility is one of the desirable features of XML. We say that $T'_1$ is missing a copy of an $r_T$-walk $C$ in $T$ if $T'_1$ does not contain a copy of $C$, otherwise $T'_1$ is said to be not missing a copy of $C$. Similarly the data tree $T'$ is said to be missing a copy of $C$ if it does not contain a copy of $C$, and not missing a copy of $C$ otherwise. In other words, $T'$ is missing a copy of $C$ if every almost copy of $T$ in $T'$ is missing a copy of $C$, and not missing a copy of $C$ if there is some almost copy of $T$ in $T'$ which is not missing a copy of $C$. As an example, $O'_1$ is missing a copy of the $r_O$-walk to the leaf with name $E$ in $O$, while $O'_2$ and $O'_3$ are not missing a copy of every $r_O$-walk of $O$. Altogether, the data tree $O'$ is not missing a copy of every $r_O$-walk of $O$.

Let $T'_1$ be any almost copy of $T$ in an XML data tree $T' \triangleright T$. It is possible that $T'_1$ does not contain a copy of some $r_T$-walk which contain an $?$-arc or $*$-arc. Note that this flexibility is one of the desirable features of XML. We say that $T'_1$ is missing a copy of an $r_T$-walk $C$ in $T$ if $T'_1$ does not contain a copy of $C$, otherwise $T'_1$ is said to be not missing a copy of $C$. Similarly the data tree $T'$ is said to be missing a copy of $C$ if it does not contain a copy of $C$, and not missing a copy of $C$ otherwise. In other words, $T'$ is missing a copy of $C$ if every almost copy of $T$ in $T'$ is missing a copy of $C$, and not missing a copy of $C$ if there is some almost copy of $T$ in $T'$ which is not missing a copy of $C$. As an example, $O'_1$ is missing a copy of the $r_O$-walk to the leaf with name $E$ in $O$, while $O'_2$ and $O'_3$ are not missing a copy of every $r_O$-walk of $O$. Altogether, the data tree $O'$ is not missing a copy of every $r_O$-walk of $O$.

![Figure 7: Two further subgraphs of $O$.](image-url)
2.1.5 Operators on Subgraphs

Examples illustrating the operators defined in this subsection will also consider the two subgraphs shown in Figure 7.

**Definition 2.9.** Let $G$ be an XML graph and let $X$ and $Y$ be two subgraphs in $G$. The **union** of $X$ and $Y$, denoted by $X \cup Y$, is the restriction of the graph union of $X$ and $Y$ to its maximal $r_G$-subgraph of $G$.

![Figure 8: An example illustrating the union and graph union of two subgraphs.](image)

**Definition 2.10.** Let $G$ be an XML graph and let $X$ and $Y$ be two subgraphs in $G$. The **intersection** of $X$ and $Y$, denoted by $X \cap Y$, is the union of all $r_G$-walks that belong to $X$ and to $Y$. The **difference** between $X$ and $Y$, denoted by $X - Y$, is the union of all $r_G$-walks belonging to $X$ but not to $Y$. In particular, $X \cap Y$ and $X - Y$ are $r_G$-subgraphs in $G$.

![Figure 9: The result of $X \cap Y$](image)  
![Figure 10: The result of $X - Y$](image)
Remark. The intersection operator is associative but the union and difference operators are not associative. The union and intersection operators are commutative but the difference operator is not.

In the absence of parenthesis, we suppose the union and intersection operator bind tighter than the difference operator. For example, by $X \cup Y - Z$ we mean $(X \cup Y) - Z$.

**Definition 2.11.** Let $G'$ and $G$ be two XML graphs, and $\phi : V_{G'} \rightarrow V_G$ be a homomorphism between them. Given an $r_G$-subgraph $H$ in $G$, the projection of $G'$ to the subgraph $H$ in $G$, denoted by $G'|_H$, is the union of all the subcopies of $H$ in $G'$. The projection $G'|_H$ is an $r_G$-subgraph of $G'$.

---

Finally the following notations will be used for convenience. We may sometimes omit the union symbol altogether, for example, we may write $XY$ instead of $X \cup Y$. Within each XML schema graph in the remainder of the thesis, leaves names are unique. Therefore, we may refer to an $r_G$-walk to some leaf carrying the name "B" simply as $\ll B \gg$. Further, we may refer to a non-empty $r_G$-subgraph $X$ by listing the names of all leaves in $X$ separated by white space. As an example, we may refer to the $r_O$-subgraph $X \cap Y$ [Figure 9] as $\ll \ll C \gg$ and the $r_O$-subgraph $X$ [Figure 7] as $\ll \ll A \ C \gg$. For two $r_G$-subgraphs $X$ and $Y$ of some graph $G$, we may use $X \subseteq Y$ to denote that $X$ is an $r_G$-subgraph of $Y$ in $G$, and more specifically $X \in Y$ to denote that $X$ is an $r_G$-walk of $Y$ in $G$.

### 2.2 Running Example

The main running example in this thesis describes information stored by a Human Resource department about employees, their bank accounts, and also details of salaries/wages.
payments made to each employee. We will segregate this information into two parts called Bank and Payment.

Both parts will include details about employees such as their name, employee ID and IRD number. A person who is liable to pay tax on his/her earnings may apply to the Inland Revenue Department for a unique IRD number which identifies them as an income tax payer of New Zealand.

In Bank, we will also include details about bank accounts to which salaries/wages payments are made. Each employee provides information on one bank account, including the bank name, account name, bank account number, and possibly information about the branch where the account is held. A bank account number consists of four components: bank number, branch number, account number and suffix number. Suppose we also need to store information about the person to contact about maintaining employees bank information. An XML schema tree for Bank, called BANK, can be found in Figure 12.

With the Payment part, we will additionally record information about salaries/wages payments made to each employee. Suppose this information includes the time of payment, cumulative number of payments up to that time, and amount paid together with details on deductions and tax. An XML schema tree for Payment will be given later in Section 4 (when we introduce identifiers).

It should be noted that we prefer using attributes wherever possible rather than text elements in the examples purely to end up with more compact XML graphs. Of course, each attribute in an XML graph $G$ with name $n$ may alternatively be modelled by a vertex $v$ of kind $E$ with name $n$ followed by a vertex $w \in Succ_G(v)$ of kind $S$ and name $n$. As an illustration of this, compare the XML graph in Figure 1 with the corresponding
2.3 Functional Dependencies in XML

We are ready to present a definition of functional dependencies for XML. We utilise the definition introduced in the first part of [15].

2.3.1 Defining XFDs

Definition 2.12. Two XML data trees $T'$ and $T$ are said to be equivalent, denoted by $T' = T$, if the isomorphism $\phi : V_{T'} \rightarrow V_T$ between $T'$ and $T$ is evaluation-preserving, that is, $val(\phi(v')) = val(v')$ holds for every $v' \in L_{T'}$.

Definition 2.13. Given an XML schema graph $T$, a functional dependency (or XFD for short) on $T$ is an expression $X \rightarrow Y$ where $X$ and $Y$ are non-empty $\tau_T$-subgraphs in $T$. Let $T'$ be an XML data tree which is compatible with $T$ and let $\phi : V_{T'} \rightarrow V_T$ be the unique homomorphism between $T'$ and $T$. Then $T'$ satisfies the XFD $X \rightarrow Y$, written as $\models_{T'} X \rightarrow Y$, if and only if for any two almost copies $T'_1$ and $T'_2$ of $T$ in $T'$ the projections $T'_1|_Y$ and $T'_2|_Y$ are equivalent whenever the projections $T'_1|_X$ and $T'_2|_X$ are equivalent and copies of $X$, i.e. $T'_1|_Y = T'_2|_Y$ whenever $T'_1|_X = T'_2|_X \equiv X$.

Example 2.3. From the information provided in Section 2.2 about the Bank part, we can specify the following XFDs:

\[
\begin{align*}
(B_{XFD1}) \quad &<\text{empID}> \rightarrow <\text{IRD#}> \\
(B_{XFD2}) \quad &<\text{empID}> \rightarrow <\text{name}> \\
(B_{XFD3}) \quad &<\text{empID}> \rightarrow <\text{bankName}\ \text{brName}\ \text{brLocation}\ \text{acctName}> \\
(B_{XFD4}) \quad &<\text{empID}> \rightarrow <\text{bankNo}\ \text{branchNo}\ \text{acctNo}\ \text{suffixNo}> \\
(B_{XFD5}) \quad &<\text{IRD#}> \rightarrow <\text{empID}>
\end{align*}
\]

The following XFDs are also required to model the banking environment we consider:

\[
\begin{align*}
(B_{XFD6}) \quad &<\text{bankName}> \rightarrow <\text{bankNo}> \\
(B_{XFD7}) \quad &<\text{bankNo}> \rightarrow <\text{bankName}> \\
(B_{XFD8}) \quad &<\text{bankName}\ \text{branchNo}> \rightarrow <\text{brName}> \\
(B_{XFD9}) \quad &<\text{bankName}\ \text{branchNo}> \rightarrow <\text{brLocation}> \\
(B_{XFD10}) \quad &<\text{bankName}\ \text{brName}> \rightarrow <\text{branchNo}> \\
(B_{XFD11}) \quad &<\text{bankName}\ \text{brLocation}> \rightarrow <\text{brName}>
\end{align*}
\]
2.3 Functional Dependencies in XML

(B_XFD12) \( \langle \text{bankName acctNo} \rangle \rightarrow \langle \text{brName acctName} \rangle \)

(B_XFD13) \( \langle \text{bankName acctName} \rangle \rightarrow \langle \text{acctNo} \rangle \)

\( B_{XF D6} \) and \( B_{XF D7} \) reflects that every bank is associated with a unique name and bank number. With \( B_{XF D8} \) to \( B_{XF D11} \), we capture the fact that for each bank, every branch is identifiable by a branch name, a branch location description and a branch number. That is, no two branches of the same bank share their location description, branch name or branch number.

It also happens that the branch at which a customer opens his/her first banking account with a bank is used for all other types of banking accounts he/she may open in future. This is represented by \( B_{XF D12} \). For each bank, each banking account belonging to a customer can be identified by an account number together with a suffix number. However, \( B_{XF D12} \) and \( B_{XF D13} \) further represent that for each bank, every customer can be identified by their account number or account name, regardless of whether the customer has several accounts of various types. A banking account may be shared by various people.

Figure 13: An XML data tree BANK' compatible with BANK.

The XML data tree BANK' in Figure 13 contains exactly two almost copies of BANK, namely \( B_1' \) and \( B_2' \) shown in Figure 14. Both almost copies contain the values “National Bank” and “0746” for \( \langle \text{bankName} \rangle \) and \( \langle \text{branchNo} \rangle \) respectively; in other words, they contain equivalent copies of \( \langle \text{bankName} \ branchNo \rangle \). However \( B_1' \) | \( \langle \text{brName} \rangle \) has
the value “PN1”, while \( B'_{2} \upharpoonright \langle \text{bankName} \rangle \) has the value “Massey University”. Also \( B'_{1} \) is not missing a copy of \( \langle \text{brLocation} \rangle \), whereas \( B'_{2} \) contains no information about the branch location. Hence, \( \text{BANK}' \) does not satisfy \( B \_xFD8 \) nor \( B \_xFD9 \).

On the other hand, \( B \_xFD6 \) is satisfied. Both \( B'_{1} \) and \( B'_{2} \) consist of the value “National Bank” for \( \langle \text{bankName} \rangle \) and both carry the value “06” for \( \langle \text{bankNo} \rangle \). That is, \( B'_{1} \upharpoonright \langle \text{bankName} \rangle = B'_{2} \upharpoonright \langle \text{bankName} \rangle \approx \langle \text{bankName} \rangle \) implies \( B'_{1} \upharpoonright \langle \text{bankNo} \rangle = B'_{2} \upharpoonright \langle \text{bankNo} \rangle \) and so \( \text{BANK}' \) satisfies \( B \_xFD6 \). Since \( B'_{2} \upharpoonright \langle \text{bankName} \rangle \upharpoonright \langle \text{brLocation} \rangle \) is missing a copy of \( \langle \text{brLocation} \rangle \), it is the case that \( B \_xFD11 \) is trivially satisfied.

One by one, we can verify that all other XFDs are satisfied by \( \text{BANK}' \). 

2.3.2 Implication and Derivation of XFDs

Analogous to the RDM, we say \( T' \) satisfies a given set \( \Sigma \) of XFDs, denoted by \( \models_{T'} \Sigma \), if \( T' \) satisfies each XFD in \( \Sigma \). As was found in the RDM, satisfaction of a given set of
2.3 Functional Dependencies in XML

XFDs by an XML data tree usually implies the satisfaction of other XFDs. The notions of implication and derivability (with respect to some rule system $\mathcal{R}$) are defined analogously to similar notions in the RDM.

Let $\Sigma$ be a set of XFDs and $X \rightarrow Y$ a single XFD. If $X \rightarrow Y$ is satisfied in every XML data tree which satisfies $\Sigma$, then $\Sigma$ implies $X \rightarrow Y$, written as $\Sigma \models X \rightarrow Y$. The semantic closure of $\Sigma$, denoted by $\Sigma^+$, is the set of all XFDs which are implied by $\Sigma$, that is, $\Sigma^+ = \{X \rightarrow Y \mid \Sigma \models X \rightarrow Y\}$.

Given a rule system $\mathcal{R}$, we say an XFD $X \rightarrow Y$ is derivable from $\Sigma$ by $\mathcal{R}$, denoted by $\Sigma \vdash_{\mathcal{R}} X \rightarrow Y$, if there is a finite sequence of XFDs, whose last element is $X \rightarrow Y$, such that each XFD in the sequence is in $\Sigma$ or can be obtained from $\Sigma$ by applying one of the inference rules in $\mathcal{R}$ to a finite number of previous XFDs in the sequence. The syntactic closure of $\Sigma$ with respect to the rule system $\mathcal{R}$, denoted $\Sigma^+_\mathcal{R}$, is the set of all XFDs which are derivable from $\Sigma$ by means of inference rules in $\mathcal{R}$, that is, $\Sigma^+_\mathcal{R} = \{X \rightarrow Y \mid \Sigma \vdash_{\mathcal{R}} X \rightarrow Y\}$. Whenever the rule system is clearly understood, we may omit $\mathcal{R}$.

An inference rule is called sound if for any given set $\Sigma$ of XFDs, every XFD which may be derived from $\Sigma$ due to that rule is also implied by $\Sigma$. A rule system $\mathcal{R}$ is sound if all inference rules in $\mathcal{R}$ are sound. In other words, $\mathcal{R}$ is sound if every XFD which is derivable from $\Sigma$ by $\mathcal{R}$ is also implied by $\Sigma$ (i.e. $\Sigma^+_\mathcal{R} \subseteq \Sigma^*$). A rule system is said to be complete if it is possible to derive every XFD which is implied by $\Sigma$ (i.e. $\Sigma^* \subseteq \Sigma^+_\mathcal{R}$).
3 XFDs in the Presence of Frequencies

In this section, we reason about XFDs in the presence of frequencies. Our main result is a sound and complete rule system (called the $\mathcal{F}$-rule system) for the derivation of XFDs in the presence of frequencies.

We begin by introducing some basic sound inference rules which we then show to be complete as well. From the basic inference rules, additional inference rules can be derived. Like in the RDM, there are various sets of inference rules which can be shown to be equivalent, that is, all the XFDs which can be derived from one set of rules can be derived using the other set of rules and vice versa. We will consider a few equivalent sets of inference rules. Lastly, we will generalise the notion of Armstrong relations to XML data trees and investigate whether XFDs in the presence of frequencies enjoy data trees which are Armstrong.

3.1 Sound Inference Rules

The first four inference rules have been taken directly from [15]. Although quite obvious and simple, for the sake of completeness we include soundness proofs for these rules.

Lemma 3.1. Let $T$ be an XML schema graph and let $X, Y, W, Z$ be $r_T$-subgraphs in $T$. The following inference rules for XFDs are sound:

1. (union rule). $X \rightarrow Y, X \rightarrow Z \quad \frac{X \rightarrow Y, X \rightarrow Z}{X \rightarrow Y \cup Z}$

2. (reflexivity axiom). $\frac{X \rightarrow Y}{Y \text{ is an } r_T\text{-subgraph of } X}$

3. (subtree rule). $\frac{X \rightarrow Y}{Z \text{ is an } r_T\text{-subgraph of } Y}$

4. (supertree rule). $\frac{W \rightarrow Y}{X \rightarrow Y} \quad W \text{ is an } r_T\text{-subgraph of } X$

Proof.

1. Assume that the union rule is not sound, that is, there is an XML data tree $T' \triangleright T$ with $\not\models_{T'} X \rightarrow Y \cup Z$ and $\models_{T'} \{X \rightarrow Y, X \rightarrow Z\}$. To violate $X \rightarrow Y \cup Z$, $T'$ must includes two almost copies $T_1', T_2'$ of $T$ such that $T_1'|_X = T_2'|_X \cong X$ and $T_1'|_{Y \cup Z} \neq T_2'|_{Y \cup Z}$. This means that there is some $r_T$-walk $C$ with $C \in Y$ or $C \in Z$ such that $T_1'|_C \neq T_2'|_C$. If $C \in Y$, then $T_1'|_Y \neq T_2'|_Y$ hence $\not\models_{T'} X \rightarrow Y$ which contradicts our assumption. Similarly if $C \in Z$ then $\not\models_{T'} X \rightarrow Z$ which also violates our assumption. Therefore by contradiction $\models_{T'} X \rightarrow Y \cup Z$. 

2. Assume that we have an XML data tree \( T' \succ T \) in which \( X \rightarrow Y \) is not satisfied and \( Y \subseteq X \). This means there must be two almost copies \( T'_1, T'_2 \) of \( T \) such that \( T'_1 |_X = T'_2 |_X \nless X \) and \( T'_1 |_Y \nless T'_2 |_Y \). It can be easily seen from Definition 2.12 [equivalence] that \( T'_1 |_X = T'_2 |_X \) if and only if \( T'_1 |_C = T'_2 |_C \) for each \( r_T \)-walk \( C \) in \( X \). Since \( Y \subseteq X \) then using the union rule and the previous observation we get \( T'_1 |_Y = T'_2 |_Y \nless Y \). This is a contradiction.

3. Assume that there is an XML data tree \( T' \succ T \) which satisfies \( X \rightarrow Y \) but violates \( X \rightarrow Z \) where \( Z \subseteq Y \). This means there is some \( r_T \)-walk \( C \in Z \) such that \( T'_1 |_C \neq T'_2 |_C \). Since \( Z \subseteq Y \) it is the case that \( C \in Y \). This means \( X \rightarrow Y \) is not satisfied which contradicts our assumption.

4. Assume \( T' \succ T \) is an XML data tree in which \( W \rightarrow Y \) is satisfied but \( X \rightarrow Y \) is not where \( W \subseteq X \). There are two almost copies \( T'_1, T'_2 \) of \( T \) such that \( T'_1 |_X = T'_2 |_X \nless X \), otherwise \( X \rightarrow Y \) cannot be violated. From \( W \subseteq X \) we get \( T'_1 |_W = T'_2 |_W \nless W \). It follows that \( T'_1 |_Y = T'_2 |_Y \), otherwise \( W \rightarrow Y \) will be violated. But this means that \( X \rightarrow Y \) is satisfied which contradicts our assumption.

We next define a root axiom which is a simplified version of the root axiom introduced in [15]. An explanation for the simplicity of our root axiom is that we do not allow element vertices in any non-empty XML graph to be leaves.

**Lemma 3.2.** Let \( T \) be an XML schema graph and \( X \) be an \( r_T \)-subgraph of \( T \). The following root axiom is sound for the inference of XFDs

\[
X \rightarrow R \quad \text{where } R \text{ is the union over all } r_T \text{-walks in } T_{\leq 1}.
\]

**Proof.** By definition, a data tree \( T' \) is compatible with an XML schema graph \( T \) if the number of arcs mapped in the homomorphism conforms to the frequencies specified in \( T \). Since \( R = \bigcup \{ C \mid C \text{ is an } r_T \text{-walk of } T_{\leq 1} \} \), there is at most one copy in \( T' \) of each \( r_T \)-walk of \( R \). Thus, any almost copy of \( T \) in \( T' \) will contain the same almost copy of \( R \). It follows that for any two almost copies \( T'_1 \) and \( T'_2 \) of \( T \) we have \( T'_1 |_R = T'_2 |_R \). Therefore \( \models_{T'} X \rightarrow R \) for any \( r_T \)-subgraph \( X \) in \( T \).

It has been observed in [15] that the transitivity rule does not hold for XML in the presence of frequencies. Consider the XFDs \( X \rightarrow Y \) and \( Y \rightarrow Z \) defined on some XML schema graph \( T \). For an XML data tree \( T' \succ T \), if any two almost copies of \( T \) are missing a copy of some \( r_T \)-walk of \( Y \), then \( T' \) trivially satisfies \( Y \rightarrow Z \). Therefore it would be possible
for two almost copies to consist of non-equivalent values for $Z$ while being equivalent and not missing a copy of every $r_T$-walk of $X$, that is, $X \rightarrow Z$ can be violated.

However we can define a restricted form of the transitivity rule which is sound for the derivation of XFDs. The main idea behind such an inference rule is to use frequencies to ensure that two almost copies are not missing a copy of every $r_T$-walk of the middle term $Y$ whenever they are not missing a copy of every $r_T$-walk of $X$ or $Z$. The notion of $Y$ being $X,Z$-compliant in the following definition accomplishes this. It should be noted that Definition 3.1 is a re-write of the same concept in [15].

**Definition 3.1.** Let $X, Y$ and $Z$ be $r_T$-subgraphs in an XML schema graph $T$. We say $Y$ is $X, Z$-compliant if and only if $Y \subseteq (X \cup C) \cup T_{\geq 1}$ for every $r_T$-walk $C$ in $Z$.

**Example 3.1.** According to the schema tree $\text{BANK}$ in Figure 12, it is the case that $\langle \text{phone name} \rangle \subseteq (\langle \text{contactPerson} \rangle \cup \langle \text{empID} \rangle) \cup \text{BANK}_{\geq 1}$. Therefore we say $\langle \text{phone name} \rangle$ is $\langle \text{contactPerson} \rangle$, $\langle \text{empID} \rangle$-compliant. It can also be verified that $\langle \text{IRD#} \rangle$ is not $\langle \text{contactPerson} \rangle$, $\langle \text{empID} \rangle$-compliant.

**Lemma 3.3.** Let $T$ be an XML schema graph and $X, Y, Z$ be $r_T$-subgraphs in $T$. The restricted-transitivity rule defined as follows is sound:

$$
\frac{X \rightarrow Y \quad Y \rightarrow Z}{X \rightarrow Z} \quad Y \text{ is } X, Z\text{-compliant.}
$$

**Proof.** Assume that there is a data tree $T' \triangleright T$ such that $\models_{T'} \{X \rightarrow Y, Y \rightarrow Z\}$ with $Y$ being $X, Z$-compliant but $\not\models_{T'} X \rightarrow Z$. Suppose the violation of $X \rightarrow C$ causes $X \rightarrow Z$ to be violated, where $C$ is an $r_T$-walk of $Z$. This means $T'$ must have two almost copies $T'_1, T'_2$ of $T$ such that $T'_1|_X = T'_2|_X \equiv X$ and $T'_1|_C \neq T'_2|_C$. By assumption we have $Y \subseteq (X \cup C) \cup T_{\geq 1}$. From $\models_{T'} X \rightarrow Y$, we know $T'_1|_Y = T'_2|_Y$. If $T'_1|_Y = T'_2|_Y \equiv Y$ then $T'_1|_C = T'_2|_C$ since $\models_{T'} Y \rightarrow Z$. Hence, $T'_1|_Y = T'_2|_Y \neq Y$. That is, $T'_1$ and $T'_2$ are missing a copy of some $r_T$-walk $B \in Y$. However $T'_1|_C \neq T'_2|_C$ tells us that $T'_1$ or $T'_2$ is not missing a copy of $C$. It follows that $T'_1$ or $T'_2$ contains every $r_T$-walk of $(X \cup C) \cup T_{\geq 1}$. Hence $B \not\subseteq (X \cup C) \cup T_{\geq 1}$ contradicting $B \in Y \subseteq (X \cup C) \cup T_{\geq 1}$.

**Example 3.2.** Recall the XML schema tree $\text{BANK}$ and all XFDs specified in Example 2.3.

There are two $r_{\text{BANK}}$-walks in $\text{BANK}_{\leq 1}$, yielding $R = \langle \text{contactPerson phone} \rangle$. Therefore, with the root axiom we may derive XFDs like $\langle \text{name bankNo branchNo acctNo suffixNo} \rangle \rightarrow \langle \text{contactPerson phone} \rangle$ and $\langle \text{bankName} \rangle \rightarrow \langle \text{contactPerson phone} \rangle$. 
The supertree rule enables us to derive from $B_{XFD9}$ the XFD $\langle\text{bankName branchNo empID}\rangle \rightarrow \langle\text{brLocation}\rangle$. Applying the subtree rule to $B_{XFD12}$ results in the two XFDs $\langle\text{bankName acctNo}\rangle \rightarrow \langle\text{brName}\rangle$ and $\langle\text{bankName acctNo}\rangle \rightarrow \langle\text{acctName}\rangle$.

By means of the reflexivity axiom, we can derive $\langle\text{bankName brName}\rangle \rightarrow \langle\text{bankName}\rangle$. Then from this new XFD and $B_{XFD10}$ and an application of the union rule we obtain $\langle\text{bankName brName}\rangle \rightarrow \langle\text{bankName branchNo}\rangle$. It is easy to see that:

$$\langle\text{bankName branchNo}\rangle \subseteq (\langle\text{bankName brName}\rangle \cup \langle\text{brLocation}\rangle) \cup \text{BANK}_{\geq 1}$$

which means $\langle\text{bankName branchNo}\rangle$ is $\langle\text{bankName brName}\rangle$, $\langle\text{brLocation}\rangle$-compliant. Therefore an application of the restricted-transitivity rule to $\langle\text{bankName brName}\rangle \rightarrow \langle\text{bankName branchNo}\rangle$ and $B_{XFD9}$ yields the XFD $\langle\text{bankName brName}\rangle \rightarrow \langle\text{brLocation}\rangle$.

We next define the notion of a unit of some $r_T$-walk which is used in the last basic inference rule presented in this section.

![Diagram](image)

Figure 15: The unit of: $\langle\text{name}\rangle$, $\langle\text{bankName}\rangle$, $\langle\text{bankNo}\rangle$, and every other $r_{\text{BANK}}$-walk in the given $r_{\text{BANK}}$-subgraph. Note that the unit of $\langle\text{contactPerson}\rangle$ and $\langle\text{phone}\rangle$ ($r_{\text{BANK}}$-walks not in the given $r_{\text{BANK}}$-subgraph) is the empty rooted graph.

**Definition 3.2.** Let $B$ be an $r_T$-walk of some XML schema graph $T$. The unit of $B$, denoted by $U_B$, is the union of all $r_T$-walks sharing some */+-arc with $B$. 

\[\square\]
There are a few observations we can make in relation to the unit of some \( r_r \)-walk which are useful for later proofs. For one, it is the case that \( U_C = U_B \) for any \( r_r \)-walk \( C \in U_B \). Furthermore, in any data tree \( T' \triangleright T \), every almost copy of \( T = U_B \) together with any almost copy of \( U_B \) form an almost copy of \( T \) in \( T' \). In particular, for any two almost copies \( T'_1, T'_2 \) of \( T \) in \( T' \), it is the case that \( T'_1 \big|_{T-U_B} \cup T'_2 \big|_{U_B} \) and \( T'_2 \big|_{T-U_B} \cup T'_1 \big|_{U_B} \) are also almost copies of \( T \) in \( T' \). The mix-and-match approach is only possible because \( T'_2 \big|_{T-U_B} \) shares with \( T'_1 \big|_{T-U_B} \) exactly those arcs (and vertices) which \( T'_2 \big|_{U_B} \) shares with \( T'_2 \big|_{T-U_B} \), and likewise \( T'_1 \big|_{U_B} \) shares with \( T'_1 \big|_{T-U_B} \) exactly those arcs which \( T'_1 \big|_{U_B} \) shares with \( T'_1 \big|_{T-U_B} \).

We are now ready to define the last inference rule required in the presence of frequencies. The rule bears a slight resemblance to the notion of “flimsy” XFDs introduced in \([22]\).

**Lemma 3.4.** Let \( T \) be an XML schema graph, \( X \) be an \( r_r \)-subgraph and \( B \) an \( r_r \)-walk of \( T \). The following noname rule is sound for the implication of XFDs:

\[
\frac{(X \cup B) \cup T_{\geq 1} - U_B) \cup X \rightarrow B}{X \rightarrow B}
\]

**Proof.** Assume there is a data tree \( T' \triangleright T \) such that \( \models_{T'} ((X \cup B) \cup T_{\geq 1} - U_B) \cup X \rightarrow B \) but \( \not\models_{T'} X \rightarrow B \). In particular, \( T' \) has two almost copies \( T'_1, T'_2 \) of \( T \) such that \( T'_1 \big|_X = T'_2 \big|_X \cong X \) and \( T'_1 \big|_B \not\cong T'_2 \big|_B \). We have \((X \cup B) \cup T_{\geq 1} - U_B) \not\subseteq X \), since otherwise \((X \cup B) \cup T_{\geq 1} - U_B) \cup X = X \) and it would follow immediately from the assumption that \( \models_{T'} X \rightarrow B \). This means there is some non-empty \( r_r \)-subgraph \( W \subseteq (X \cup B) \cup T_{\geq 1} - U_B \) such that \( W \cap X = \emptyset \). For convenience, we can now rewrite the noname rule as follows:

\[
\frac{(X \cup B) \cup T_{\geq 1} - U_B) \cup X \rightarrow B}{X \rightarrow B} = XW \rightarrow B
\]

\( T'_1 \) or \( T'_2 \) is not missing a copy of \( B \) and therefore must not be missing a copy of every \( r_r \)-walk of \((X \cup B) \cup T_{\geq 1} \). Without loss of generality assume \( T'_1 \big|_B \cong B \) and therefore \( T'_1 \big|_W \cong W \) from \( W \subseteq (X \cup B) \cup T_{\geq 1} \). There are now two cases to consider: \( T'_1 \big|_W = T'_2 \big|_W \cong W \) or \( T'_1 \big|_W \not\cong T'_2 \big|_W \).

Firstly, suppose \( T'_1 \big|_W = T'_2 \big|_W \cong W \). Recall that by assumption \( T'_1 \big|_X = T'_2 \big|_X \cong X \), therefore we have \( T'_1 \big|_{XW} = T'_2 \big|_{XW} \cong XW \). Since \( \models_{T'} XW \rightarrow B \) it follows that \( T'_1 \big|_B = T'_2 \big|_B \) which would contradict our assumption that \( \not\models_{T'} X \rightarrow B \).

So instead, let us consider the case where \( T'_1 \big|_W \not\cong T'_2 \big|_W \). Since \( W \subseteq (X \cup B) \cup T_{\geq 1} - U_B \subseteq T - U_B \), it follows that no \( r_r \)-walk of \( W \) is in \( U_B \). On the other hand, we have \( B \in U_B \) otherwise, \( B \in R \) and \( \models_{T'} X \rightarrow B \) by soundness of the root axiom which would contradict
our assumption. From $T'_1$ and $T'_2$ we can form two other almost copies of $T$, namely:

$$T'_3 = T'_1 |_{T-U_B} \cup T'_2 |_{U_B}$$

and

$$T'_4 = T'_2 |_{T-U_B} \cup T'_1 |_{U_B}.$$ 

Consider the pair of almost copies $T'_1, T'_2$ of $T$. By construction of $T'_3$, we have $T'_1 |_W = T'_3 |_W$. This means we have established $T'_1 |_{XW} = T'_3 |_{XW} \equiv XW$. Then from $\models_{T'} XW \rightarrow B$, it follows that $T'_1 |_B = T'_3 |_B$. Since $T'_3 |_B$ is just $T'_2 |_B$ then in fact $T'_1 |_B = T'_2 |_B$ which contradicts our assumption. This concludes the proof. \hfill \Box

**Example 3.3.** The only interesting XFDs on BANK which we may derive using the noname rule must consist of an $r_{\text{BANK}}$-subgraph of $<<\text{contactPerson} \ \text{phone}>>$ on the left-hand-side and the right-hand-side must be an $r_{\text{BANK}}$-walk (let us call this RHS) other than $<<\text{contactPerson}>>$ and $<<\text{phone}>>$. Altogether, this would mean that in order to apply the noname rule, the XFD $<<\text{contactPerson} \ \text{phone}>> \rightarrow \text{RHS}$ must be derivable. It is easy to see that there are no XFDs in Example 2.3 of this form, nor any which can be derived. Hence, the noname rule is not applicable for deriving any XFDs on BANK which the other inference rules cannot. \hfill \Box

**Example 3.4.** To illustrate how the noname rule may be applied, let us look at a simple scenario:

There is a small product development company specialising in manufacturing plastic prototypes. The company operates various departments and has multiple branches. It happens that each department is located at exactly one branch.

![Figure 16: An XML schema tree PD for the product development scenario.](image)

We may model this with the XML schema tree PD given in Figure 16 and the set of XFDs \{ $<<\text{brName}>> \rightarrow <<\text{brLocation}>>$, $<<\text{brLocation}>> \rightarrow <<\text{brName}>>$, $<<\text{deptName}>> \rightarrow <<\text{brName}>>$ \}. Using the noname rule we may derive the XFD $<<\text{empName}>> \rightarrow <<\text{brName}>>$. Let us verify this.
We have \(<<\text{empID empName deptName brName}}>>\) for the \(r_{PD}\)-subgraph corresponding to \((<<\text{empName}}>> \cup <<\text{brName}}>>\) \(\cup PD_{\geq 1}\), while \(U_{<<\text{brName}}>>\) is the \(r_{PD}\)-subgraph \(<<\text{brName brLocation}}>>\). This amounts to the premise of the noname rule being: \(<<\text{empName empName deptName}}>> \rightarrow <<\text{brName}}>>\). This XFD is derivable from \(<<\text{deptName}}>> \rightarrow <<\text{brName}}>>\) by means of the supertree rule. Hence we may use the noname rule to derive \(<<\text{empName}}>> \rightarrow <<\text{brName}}>>\). \(\Box\)

### 3.2 A Sound & Complete Rule System

In this section, we prove that the inference rules from Section 3.1 form a complete rule system for XFDs in the presence of frequencies. Let the \(\mathcal{F}\)-rule system consist of the following inference rules: reflexivity axiom, root axiom, subtree rule, supertree rule, union rule, restricted-transitivity rule and noname rule.

We take the usual approach to proving completeness. Consider an XML schema graph \(T\), and a given set \(\Sigma\) of XFDs on \(T\). If \(X \rightarrow Y\) cannot be derived from \(\Sigma\) by means of the inference rules, then we show that there is an XML data tree \(T'\) \(\succ T\) such that \(\models_{T'} \Sigma\) but \(\not\models_{T'} X \rightarrow Y\). Because of the union rule, this means there is some \(r_T\)-walk \(B \in Y\) such that \(X \rightarrow B\) is not derivable from \(\Sigma\) and \(T'\) does not satisfy \(X \rightarrow B\). Therefore \(T'\) must contain two almost copies \(T'_1, T'_2\) of \(T\) such that \(T'_1 |_X = T'_2 |_{X'} \equiv X\) and \(T'_1 |_B \neq T'_2 |_{B'}\). We need a general construction for such a counterexample data tree \(T'\).

Without frequencies, we can construct a counterexample data tree from the disjoint union of exactly two copies \(T'_a, T'_b\) of \(X \cup B\) in which \(T'_a |_C = T'_b |_C\) if and only if \(C \in X\). Particularly, \(T'_a, T'_b\) are each missing a copy of every \(r_T\)-walks not in \(X \cup B\). However, in the presence of frequencies, we face the additional complication that at least one almost copy of \(T\) must contain every \(r_T\)-walk of \((X \cup B) \cup T_{\geq 1}\). This means, in addition to \(X \cup B\), we also need to determine whether or not \(T'_1\) and \(T'_2\) should be equivalent for each of the remaining \(r_T\)-walks in \((X \cup B) \cup T_{\geq 1}\), keeping in mind that \(T'\) must still satisfy \(\Sigma\).

We first define the analogous of the closure of a set of attributes in the RDM.

**Definition 3.3.** Let \(T\) be an XML schema graph, \(X\) an \(r_T\)-subgraph and \(\Sigma\) a set of XFDs on \(T\). Further let \(\mathcal{R}\) be a rule system. The pre-closure \(X^+_\mathcal{R}\) of \(X\) with respect to \(\Sigma\) and the rule system \(\mathcal{R}\) is the \(r_T\)-subgraph defined as follows:

\[
X^+_\mathcal{R} = \bigcup \{Y \mid X \rightarrow Y \in \Sigma^+_\mathcal{R}\}
\]

\(\Box\)
Since $T_1|_X = T_2|_X \cong X$, to ensure $\models_T \Sigma$ we must ensure that $T_1|_{X^+_r} = T_2|_{X^+_r}$. This means that the two almost copies of $T$ must not be missing equivalent copies of every $r_T$-walk of $X^+_r \cap ((X \cup B) \cup T_{21})$. A peculiar situation is encountered: there may be XFDs not implied (hence not derivable by the $\mathcal{F}$-rule system), which need to be non-trivially satisfied in this case because $T_1$ or $T_2$ is not missing a copy of every $r_T$-walk of $(X \cup B) \cup T_{21}$. The restricted-transitivity rule means $(X^+_r)^+_r \supseteq X^+_r$, and in particular $X^+_r$ is not a closure like its counterpart attribute closure in the RDM.

![Figure 17: XML schema tree and data tree illustrating that there can be an XFD which is not derivable but which is satisfied when there are copies of certain rT-walk(s).](image)

This is illustrated by the simple XML schema tree $S$ and set $\Sigma$ of XFDs on $S$ in Figure 17(a). In the schema tree $S$, $\langle X \rangle \not\subseteq (\langle X \rangle \cup \langle D \rangle ) \cup S_{21}$, that is $\langle U \rangle$ is not $\langle X \rangle$, $\langle D \rangle$-compliant, therefore we cannot use restricted-transitivity to derive $\langle X \rangle \rightarrow \langle D \rangle$. Moreover, no other rule in the system allows us to derive $\langle X \rangle \rightarrow \langle D \rangle$. In order for a data tree to violate $\langle X \rangle \rightarrow \langle D \rangle$ it must simply be missing a copy of $\langle U \rangle$, see Figure 17(b).

However, whenever a data tree compatible with $S$ is not missing a copy of $\langle B \rangle$, it will not be missing a copy of $\langle U \rangle$. Consider the data tree $S''$ shown in Figure 17(c). $S''$ contains exactly two almost copies of $S$, let us call these $S_1''$ and $S_2''$. Recall $\models_{S''} \Sigma$ means that $\models_{S''} \langle X \rangle \rightarrow \langle U \rangle$ and $\models_{S''} \langle U \rangle \rightarrow \langle D \rangle$. It follows from $\models_{S''} \langle X \rangle \rightarrow \langle U \rangle$ and $S_1'|_{\langle X \rangle} = S_2'|_{\langle X \rangle}$ that $S_1'|_{\langle U \rangle} = S_2'|_{\langle U \rangle}$. Since $\langle U \rangle \in (\langle X \rangle \cup \langle B \rangle ) \cup S_{21}'$ it is the case that $S_1'$ and $S_2'$ are actually not missing a copy of $\langle U \rangle$. This means we have $S_1'|_{\langle D \rangle} = S_2'|_{\langle D \rangle}$ because $\models_{S''} \langle U \rangle \rightarrow \langle D \rangle$. 
Returning to our discussion, this implies that it is insufficient to stop after having considered only $X^+_T$. Because $T'_1$ and $T'_2$ are equivalent and not missing a copy of every $r_T$-walk of $X^+_T \cap ((X \cup B) \cup T_{\geq 1})$, it follows from $\models_{T'} \Sigma$ that $T'_1$ and $T'_2$ must be equivalent and not missing a copy of every $r_T$-walk of $(X^+_T \cap ((X \cup B) \cup T_{\geq 1}))^+_T \cap ((X \cup B) \cup T_{\geq 1})$. This then means $T'_1$ and $T'_2$ must be equivalent and not missing a copy of every $r_T$-walk of $((X^+_T \cap ((X \cup B) \cup T_{\geq 1}))^+_T \cap ((X \cup B) \cup T_{\geq 1}))$. Eventually there is some fix-point $X_n$ because there are only finitely many $r_T$-walks in $(X \cup B) \cup T_{\geq 1}$ in a finite schema graph. In summary, $T'_1$ and $T'_2$ must be equivalent and not missing precisely a copy of those $r_T$-walks in $X_n$ in order for $\models_{T'} \Sigma$.

This covers our general approach for constructing a counterexample, although there are a couple of small differences for the approach actually used in the proof of completeness. Recall that $T'_1 |_{T-U_B} \cup T'_2 |_{U_B}$ and $T'_2 |_{T-U_B} \cup T'_1 |_{U_B}$ are also possible almost copies of $T$ in $T'$. In particular, if $T'_1 |_{T-U_B} \not\equiv T'_2 |_{T-U_B}$ and $T'_1 |_{U_B} \not\equiv T'_2 |_{U_B}$ then there are at least four almost copies of $T$ in $T'$. In order to ensure the constructed data tree will have exactly two almost copies of $T$, we will force $T'$ to contain only one copy of $T |_{T-U_B} \cap ((X \cup B) \cup T_{\geq 1})$. Actually $T |_{T-U_B} \cap ((X \cup B) \cup T_{\geq 1})$ equals $(X \cup B) \cup T_{\geq 1} - U_B$. Therefore, we want to have $T'_1 |_{(X \cup B) \cup T_{\geq 1} - U_B} = T'_2 |_{(X \cup B) \cup T_{\geq 1} - U_B}$.

In this modified approach, there may be some $r_T$-walk $C$ in $(X \cup B) \cup T_{\geq 1} - U_B$ which is not in the $X_n$ described previously. This is rectified by actually computing the sequence of restricted pre-closures with $X_0 = ((X \cup B) \cup T_{\geq 1} - U_B) \cup X$ rather than just $X$. The noname rule means that each restricted pre-closure in the sequence is unaffected except for the additional $r_T$-subgraph $X_0 - X$.

**Example 3.5.** We demonstrate the approach described thus far with an example. Consider the XML schema tree $Q$ shown in Figure 18 together with the set $\Sigma = \{ \langle X F \rangle \rightarrow \langle C \rangle \}$ of XFDs on $Q$. Obviously we have $\langle X F \rangle \rightarrow \langle W \rangle \notin \Sigma^+_T$.

Suppose we want to construct a counterexample data tree $Q' > Q$ such that $\models_{Q'} \Sigma$ but $\not\models_{Q'} \langle X F \rangle \rightarrow \langle W \rangle$. $(\langle X F \rangle \cup \langle W \rangle) \cup Q_{\geq 1}$ is just the schema tree $Q$ without the $r_Q$-walk $\langle E \rangle$. Therefore each restricted pre-closure must not contain $\langle E \rangle$.

The sequence of restricted pre-closures is as follows:

$$\langle X F \rangle_0 = (\langle X F \rangle \cup \langle W \rangle) \cup Q_{\geq 1} - U_{\langle W \rangle} \cup \langle X F \rangle$$

$$= (\langle X F \rangle \cup \langle A B C D W \rangle - \langle A B C F W \rangle) \cup \langle X F \rangle = \langle X D \rangle \cup \langle X F \rangle = \langle X F D \rangle$$
Therefore, $Q'$ must contain two almost copies $Q_1'$ and $Q_2'$ of $Q$ which are equivalent and not missing precisely a copy of the $r_Q$-subgraph $\langle X F D B C \rangle$. Two such almost copies of $Q$ are depicted in Figure 19.

In accordance with the discussion above, we will construct $T'$ by taking the union of two copies of $(X \cup B) \cup T_2$, which are equivalent only on $X_n$. Recall that $T'$ must conform to the frequencies specified in $T$ in order for it to be compatible with $T$. Consequently, in
3 XFDs in the Presence of Frequencies

T' the two copies may need to share certain arcs and/or even copies of entire \( r_T \)-walk(s) of \( T \).

In the next definition, we provide a term to describe that two almost copies of some schema graph \( T \) in a compatible data tree \( T' \) share some \( r_T \)-walk(s). This means that two almost copies share the same copy of some \( r_T \)-walk(s) of \( T \). This concept will also be used in Section 5 to define a new notion of redundancy.

Definition 3.4. Let \( T \) be an XML schema graph. Two almost copies \( T_1', T_2' \) of \( T \) in an XML data tree \( T' \succ T \) are said to coincide on an \( r_T \)-walk \( B \) of \( T \) if and only if \( T_1' \mid_B \) and \( T_2' \mid_B \) are graph unions of exactly the same set of arcs in \( T' \). Two almost copies of \( T \) coincide on an \( r_T \)-subgraph \( Y \) of \( T \) if and only if they coincide on every \( r_T \)-walk of \( Y \). □

Example 3.6. Recall the XML data tree \( \text{BANK}' \) from Figure 13 and the extracted almost copies \( B_1', B_2' \) shown in Figure 14. \( B_1' \) and \( B_2' \) coincide on the \( r_{\text{BANK}} \)-subgraph \( \langle \text{contact\_Person\_phone} \rangle \) but do not coincide on any other \( r_{\text{BANK}} \)-walk of \( \text{BANK} \). □

With the following amalgamation operator we are able to specify how two almost copies of some schema graph should be combined to construct an XML data tree.

Definition 3.5. Let \( T \) be an XML schema graph, \( T_a, T_b \) be two almost copies of \( T \) and \( X \) be an \( r_T \)-subgraph of \( T \). The amalgamation of \( T_a \) and \( T_b \) on \( X \), denoted \( T_a \ll X \rr T_b \), is the XML data tree obtained by taking the graph union of \( T_a \) and \( T_b \) in such a way that \( T_a \) and \( T_b \) coincide on \( X \), and \( T_a \) and \( T_b \) only share all arcs in their projections to \( X \cup T_{\leq 1} \).

Recall that \( T_{a1} \mid_{(X \cup W) \rr T_{21} - W} \cup T_{b1} \mid_{W} \) and \( T_{b1} \mid_{(X \cup W) \rr T_{21} - W} \cup T_{a1} \mid_{W} \) are also almost copies of \( T \) in an XML data tree containing \( T_a \) and \( T_b \). Further, from \( X_0 = ((X \cup W) \cup T_{21} - W) \cup X \subseteq X_n \) we know that \( T_{a1} \mid_{(X \cup W) \rr T_{21} - W} = T_{b1} \mid_{(X \cup W) \rr T_{21} - W} \). In order for the constructed data tree to contain exactly two almost copies of \( T \), we require that \( T_a' \) and \( T_b' \) are amalgamated on \( (X \cup W) \cup T_{\geq 1} - W \).

Example 3.7. Let us continue with constructing the counterexample from Example 3.5. We need to construct \( Q' \) from two copies \( Q'_a \) and \( Q'_b \) of \( \langle \langle X F \rangle \cup \langle W \rangle \rangle \cup Q_{\geq 1} = \langle \langle X F A B C D W \rangle \rangle \) which are equivalent on the \( r_Q \)-subgraph \( \langle \langle X F D B C \rangle \rangle \). Incidentally, these can simply be the two almost copies of \( Q \) from Figure 19, that is, \( Q'_a = Q'_1 \) and \( Q'_b = Q'_2 \).

From Example 3.5, we have that \( \langle \langle X F \rangle \cup \langle W \rangle \rangle \cup Q_{\geq 1} - U_{\langle W \rangle} = \langle \langle X D \rangle \rangle \). Therefore we amalgamate \( Q'_a \) and \( Q'_b \) on \( \langle \langle X D \rangle \rangle \).

\( }
3.2 A Sound & Complete Rule System

Figure 20: The XML data tree $Q' = Q'_a \Pi_{[X \cup D]} Q'_b$ where $Q' \succ Q$. Here $Q'_a$ and $Q'_b$ correspond to the almost copies $Q'_1$ and $Q'_2$ from Figure 19.

The result of $Q'_a \Pi_{[X \cup D]} Q'_b$ is the XML data tree $Q'$ in Figure 20. Note that, $Q'$ precisely contains the two almost copies $Q'_1$ and $Q'_2$. Though we have left out some vertices' names for convenience, the homomorphism between $Q'$ and $Q$ is the name-preserving mapping which maps every vertex from $Q'$ to the vertex carrying the same name in $Q$. By also examining the frequencies, it can easily be verified that $Q' \succ Q$. □

Theorem 3.5. The $F$-rule system is sound and complete for the derivation of XFDs in the presence of frequencies.

Proof. Soundness of the inference rules has already been proven in Lemma 3.1, Lemma 3.2, Lemma 3.3 and Lemma 3.4. It remains to show that the inference rules form a complete rule system. Let $T$ be an XML schema graph and $\Sigma$ a set of XFDs on $T$. Let $X \rightarrow Y \notin \Sigma^+$. That is, there must be an $\tau_T$-walk $B \in Y$ such that $X \rightarrow B$ cannot be derived, otherwise by means of the union rule $X \rightarrow Y$ would be derivable. We construct a counterexample data tree $T' \succ T$ such that $\models_{\tau_T} \Sigma$ and $\not\models_{\tau_T} X \rightarrow B$.

Consider a sequence of restricted pre-closures $X_0, X_1, X_2, \ldots, X_{n-1}, X_n, X_{n+1}, X_{n+2}, \ldots$ where $X_n = X_{n+1} = X_{n+2} \ldots$ for $n \geq 0$, defined as follows:

\[
X_0 = ((X \cup B) \cup T_{\geq 1} - U_B) \cup X
\]
\[
X_1 = (X_0)^+ \cap ((X \cup B) \cup T_{\geq 1})
\]
\[
X_2 = (X_1)^+ \cap ((X \cup B) \cup T_{\geq 1})
\]
\[
\vdots
\]
\[ \begin{align*}
X_{n-1} &= (X_{n-2})_F^+ \cap ((X \cup B) \cup T_{\geq 1}) \\
X_n &= (X_{n-1})_F^+ \cap ((X \cup B) \cup T_{\geq 1}) \\
\vdots
\end{align*} \]

Let \( X_F^B = X_n \). Consider the XML data tree \( T' = T_a' \cup_{(X \cup B) \cup T_{\geq 1} - u_B} T_b' \) where \( T_a', T_b' \) are two copies of \( (X \cup B) \cup T_{\geq 1} \) with

\[ T_a'|_W = T_b'|_W \text{ if and only if } W \subseteq X_F^B \]

This is always possible since \( T_a'|_W \cap (X \cup B) \cup T_{\geq 1} - u_B = T_b'|_W \cap (X \cup B) \cup T_{\geq 1} - u_B \). Further, \( U_B \) must contain at least the \( r_T \)-walk \( B \), otherwise there is no \(+/-\)-arc in \( B \) which means \( B \in R \) and \( X \rightarrow B \) is derivable by means of the root axiom which would contradict our assumption. Moreover the resulting data tree \( T' \) contains exactly two almost copies of \( T \): \( T_1' = T_a' \) and \( T_2' = T_b' \).

Firstly, we need to show that \( T' \) satisfies every XFD in \( \Sigma \). Assume to the contrary that some \( U \rightarrow V \in \Sigma \) is not satisfied by \( T' \). There must be some \( r_T \)-walk \( C \in V \) such that \( U \rightarrow C \) is not satisfied by \( T' \). From the construction, we have \( U \subseteq X_F^B = X_n \), otherwise \( U \rightarrow C \) cannot be violated. From \( U \rightarrow C \in \Sigma \) we get \( C \in U_F^+ \subseteq (X_n)^+_F \). Furthermore \( C \in ((X \cup B) \cup T_{\geq 1}) \), otherwise \( T' \) would be missing a copy of \( C \) and \( U \rightarrow C \) would not be violated. Altogether \( C \in (X_n)^+_F \cap ((X \cup B) \cup T_{\geq 1}) = X_{n+1} = X_n = X_F^B \). It follows that \( T_1'|_C = T_2'|_C \) which contradicts our assumption that \( U \rightarrow C \) is not satisfied by \( T' \). Hence by contradiction \( \models_{T'} U \rightarrow V \).

Lastly, we need to show that \( X \rightarrow Y \) is violated by \( T' \). If \( B \in X_F^B = X_n \), then \( X_{n-1} \rightarrow B \in \Sigma_F^+ \) from the definition of \( X_n \). Also, we have \( X_{n-1} \subseteq (X_{n-2})_F^+ \) by definition and it follows that \( X_{n-2} \rightarrow X_{n-1} \). Further \( X_{n-1} \subseteq (X_{n-2} \cup B) \cup T_{\geq 1} \) since \( X_{n-1} \subseteq (X \cup B) \cup T_{\geq 1} \) and \( X \subseteq X_{n-2} \). This means \( X_{n-1} = (X_{n-2})_B \) is \( B \)-compliant. Thus application of the restricted-transitivity rule yields \( X_{n-3} \rightarrow B \in \Sigma_F^+ \). Following the same reasoning, we can obtain \( X_{n-3} \rightarrow B \in \Sigma_F^+ \), then \( X_{n-4} \rightarrow B \in \Sigma_F^+ \), and so on until eventually we end up with \( X_0 \rightarrow B \in \Sigma_F^+ \). Recall \( X_0 = ((X \cup B) \cup T_{\geq 1} - u_B) \cup X \) and so we can use the noname rule to obtain \( X \rightarrow B \in \Sigma_F^+ \). This would contradict our assumption, hence \( B \not\in X_F^B \). According to the construction, \( T' \) contains two almost copies of \( T \) which are non-equivalent on \( B \) but equivalent and not missing a copy of every \( r_T \)-walk of \( X \). This means \( \not\models_{T'} X \rightarrow B \) hence \( \not\models_{T'} X \rightarrow Y \). \( \square \)
3.3 Additional Inference Rules for XFDs

In this section we identify some additional inference rules derivable from the basic rules given in Section 3.1.

Lemma 3.6. Let $T$ be an XML schema graph and $X, Y, W, Z$ be $r_T$-subgraphs in $T$. The additional inference rules for XFDs are sound:

1. (extension rule). \[
\frac{X \rightarrow Y}{X \rightarrow X \cup Y}
\]
2. (augmentation rule). \[
\frac{X \rightarrow Y}{X \cup W \rightarrow Y \cup W}
\]
3. (intersection rule). \[
\frac{X \rightarrow Y, X \rightarrow Z}{X \rightarrow Y \cap Z}
\]
4. (restricted-pseudo-transitivity). \[
\frac{X \rightarrow Y, Y \cup W \rightarrow Z}{X \cup W \rightarrow Z} \quad Y \text{ is } (X \cup W), Z\text{-compliant.}
\]

Proof.

1. From the reflexivity axiom and $X \subseteq X$ we obtain $X \rightarrow X$. Then by means of the union rule and $X \rightarrow Y$, we get $X \rightarrow X \cup Y$.

2. By means of the supertree rule and $X \rightarrow Y$, we get $X \cup W \rightarrow Y$. From the reflexivity axiom, $X \cup W \rightarrow W$ since $W \subseteq X \cup W$. Finally using the union rule we obtain $X \cup W \rightarrow Y \cup W$.

3. Using the union rule, we get $X \rightarrow Y \cup Z$. Since $Y \cap Z \subseteq Y \cup Z$, by means of the subtree rule it is the case that $X \rightarrow Y \cap Z$.

4. By means of the augmentation rule, $X \rightarrow Y$ implies $X \cup W \rightarrow Y \cup W$. $W$ is always $(X \cup W), Z\text{-compliant}$ since $W \subseteq X \cup W$. Moreover, it follows from $Y$ being $(X \cup W), Z\text{-compliant}$ that $Y \cup W$ is $(X \cup W), Z\text{-compliant}$. Thus by restricted-transitivity rule we can infer $X \cup W \rightarrow Z$.

We now identify sets of inference rules which are equivalent to each other in the derivation of XFDs. As a consequence of Theorem 3.5, these results immediately allow us to identify alternative sound and complete rule systems for the derivation of XFDs in the presence of frequencies.

Proposition 3.1. Let $S$ denote the set of inference rules for XFDs consisting of the reflexivity axiom, union rule and subtree rule.
1. Every XFD derivable from $SU\{\text{augmentation rule}\}$ is derivable from $SU\{\text{supertree rule}\}$ and vice versa.

2. Every XFD derivable from $SU\{\text{augmentation rule, restricted-pseudo-transitivity rule}\}$ is derivable from $SU\{\text{augmentation rule, restricted-transitivity}\}$ and vice versa.

3. Every XFD derivable from $SU\{\text{supertree rule, restricted-pseudo-transitivity rule}\}$ is derivable from $SU\{\text{supertree rule, restricted-transitivity}\}$ and vice versa.

Proof.

1. Lemma 3.6 has shown that every XFD derivable by augmentation rule is derivable by means of the supertree, reflexivity and union inference rules which are all in $SU\{\text{supertree rule}\}$.

   It remains to show that every XFD derivable using the supertree rule is also derivable from $SU\{\text{augmentation rule}\}$. By application of the augmentation rule to $X \rightarrow Y$ we obtain $X \cup W \rightarrow Y \cup W$. Then by means of the subtree rule we obtain $X \cup W \rightarrow Y$. The augmentation rule and subtree rule are both in $SU\{\text{augmentation rule}\}$.

2. Lemma 3.6 also shows that the restricted-pseudo-transitivity rule is derivable by means of the restricted-transitivity rule and augmentation rule.

   Conversely, the restricted-transitivity rule is derivable from $SU\{\text{augmentation rule, restricted-pseudo-transitivity rule}\}$. Suppose we have $X \rightarrow Y, Y \rightarrow Z$ and $Y$ is $X, Z$-compliant. Let $W = \emptyset$. Using the sequence of derivation from the above proof of 1, $Y \cup W \rightarrow Z$ is derivable by means of the augmentation rule and subtree rule. Since $Y$ is $X, Z$-compliant, it is $(X \cup W), Z$-compliant. Therefore using the restricted-pseudo-transitivity rule we obtain $X \cup W \rightarrow Z$. This means $X \rightarrow Z$ since $X \cup W = X$, which is the conclusion we need for the restricted-transitivity rule.

3. This is immediate from the proof of 1 and 2 above.

Corollary 3.1. The sets of inference rules consisting of:

- reflexivity axiom, subtree rule, union rule, root axiom, noname rule, and
- augmentation rule or supertree rule, and
- restricted-pseudo-transitivity rule or restricted-transitivity rule

are sound and complete.
3.4 Armstrong XML Data Trees

For the relational data model, it is possible to construct Armstrong relations for certain classes of integrity constraints. A relation \( r \) over a relational schema \( R \) is said to be Armstrong with respect to a set of functional dependencies \( \Sigma \) over \( R \) if \( r \) satisfies precisely those functional dependencies implied by \( \Sigma \) and violates all other functional dependencies. We can define a similar notion for XML data trees.

**Definition 3.6.** Let \( T \) be an XML schema graph and \( \Sigma \) a set of XFDs on \( T \). An XML data tree \( T' \succ T \) is said to be Armstrong with respect to \( \Sigma \) if and only if for every XFD \( X \rightarrow Y \) over \( T \), \( \models_{T'} X \rightarrow Y \) if and only if \( X \rightarrow Y \in \Sigma^+ \).

The immediate consequence of Definition 3.6 and the sound and complete \( F \)-axiom system is that, in the presence of frequencies, \( T' \) is Armstrong with respect to \( \Sigma \) if and only if for every XFD \( X \rightarrow Y \) over \( T \), \( \models_{T'} X \rightarrow Y \) if and only if \( X \rightarrow Y \in \Sigma^+ \).

XFDs are said to enjoy Armstrong XML data trees if for any XML schema graph \( T \) and any set \( \Sigma \) of XFDs on \( T \), it is possible to construct an XML data tree \( T' \succ T \) such that \( T' \) satisfies precisely \( \Sigma \) and violates all XFDs not implied by \( \Sigma \). It is straightforward to show that XFDs do not enjoy Armstrong XML data trees in the presence of frequencies.

**Theorem 3.7.** XFDs in the presence of frequencies do not enjoy Armstrong XML data trees.

**Proof.** It is sufficient to give an example XML schema graph \( T \) and a set of XFDs on \( T \) for which no Armstrong data tree exists. Recall the schema graph from Figure 17(a) and the corresponding set of XFDs. It is easy to see that \( \langle X \rangle \rightarrow \langle D \rangle \text{, } \langle X \rangle \rightarrow \langle B \rangle \notin \Sigma^+ \). We proceed to show that it is not possible to construct a data tree \( T' \succ T \) which satisfies \( \Sigma \) but violates both \( \langle X \rangle \rightarrow \langle D \rangle \) and \( \langle X \rangle \rightarrow \langle B \rangle \).

Assume there is an XML data tree \( T' \succ S \) which violates \( \langle X \rangle \rightarrow \langle D \rangle \) and \( \langle X \rangle \rightarrow \langle B \rangle \). Since \( \nexists_{T'} \langle X \rangle \rightarrow \langle D \rangle \), there are two almost copies \( T'_1, T'_2 \) of \( S \) such that \( T'_1 \mid_{\langle X \rangle} = T'_2 \mid_{\langle X \rangle} \cong \langle X \rangle \) and \( T'_1 \mid_{\langle D \rangle} \neq T'_2 \mid_{\langle D \rangle} \). From \( \models_{T'} \langle X \rangle \rightarrow \langle U \rangle \) it follows that \( T'_1 \mid_{\langle U \rangle} = T'_2 \mid_{\langle U \rangle} \). If the two almost copies are not missing a copy of \( \langle U \rangle \) then \( T'_1 \mid_{\langle D \rangle} = T'_2 \mid_{\langle D \rangle} \) because \( \models_{T'} \langle U \rangle \rightarrow \langle D \rangle \). Hence \( T'_1 \) and \( T'_2 \) must be missing a copy of \( \langle U \rangle \). However, \( T'_1 \) and \( T'_2 \) can only be missing a copy of \( \langle U \rangle \) if they are missing a copy of \( \langle B \rangle \). In this case we have \( T'_1 \mid_{\langle B \rangle} = T'_2 \mid_{\langle B \rangle} \) which then yields \( \models_{T'} \langle X \rangle \rightarrow \langle B \rangle \). We have obtained a contradiction. This completes our proof. \( \square \)
4 XFDs in the Presence of Frequencies and Identifiers

In addition to frequencies, we now consider the situation where certain attributes are only assigned values which are unique in an XML data tree. We refer to such attributes as *identifier-attributes*. In particular, an attribute of type ID in a DTD is an identifier-attribute in the corresponding XML schema graph. If no DTD is available then it is again up to the designer to add suitable identifiers to the generated XML graph. We first revise some definitions from Section 2.1 to account for the presence of identifier-attributes.

4.1 Revised XML Graph Model

We will use "I" to differentiate an identifier-attribute from an ordinary attribute. The kind assignment in Definition 2.2 [XML graph] is thus extended to: kind : V_G → {E, A, I, S}. The possible frequencies for an arc a = (v, w) where kind(w) = I is the same as for kind(w) = A, that is, freq(a) = ? or 1. We add this to Definition 2.6 [XML schema graph].

We call an r_T-walk to some identifier-attribute an *identifier*.

Let the set Σ(BANKID) of XFDs on BANKID include XFD5 to XFD13 from Example 2.3 and the following:

\[(B_{XFD14}) \xrightarrow{\langle \text{empID} \rangle} \xrightarrow{\langle \text{E.id} \rangle} \]

Figure 21: An XML schema tree BANKID which extends BANK by an identifier.

Let V_G^I consists of all vertices in V_G of kind I. Leaves are now vertices of kind A, I or S, that is L_G = V_G^A ∪ V_G^S ∪ V_G^I. It is not necessary to modify Definition 2.7 [XML data tree] and Definition 2.12 [equivalent].
Let \( \Sigma(\text{PAYMENTID}) \) be the set of XFDs on \( \text{PAYMENTID} \) consisting of:

- \((P.XFD1) \quad \langle \text{empID}\rangle \rightarrow \langle E._id\rangle\)
- \((P.XFD2) \quad \langle \text{IRD#}\rangle \rightarrow \langle \text{empID}\rangle\)
- \((P.XFD3) \quad \langle \text{E._id} \ 	ext{year}\rangle \rightarrow \langle \text{AP._id}\rangle\)
- \((P.XFD4) \quad \langle \text{E._id} \ 	ext{pmtNo}\rangle \rightarrow \langle \text{PD._id}\rangle\)
- \((P.XFD5) \quad \langle \text{E._id} \ 	ext{date}\rangle \rightarrow \langle \text{PD._id}\rangle\)

Values assigned to identifier-attributes need to be unique in an XML data tree \( T' \), that is, for every string value \( s \in \text{STRING} \) if there exists a vertex \( v \in V_T \) such that \( \text{val}(v) = s \) then for every other leaf \( u \) we have \( \text{val}(u) \neq s \). We refer to this as the unique identifier value constraint. The revision of Definition 2.8 [compatible] simply requires that \( T' \) also satisfies the unique identifier value constraint.

**Example 4.1.** In the remainder of the section, we mainly consider the second part of the running example, that is the payments records. An XML schema tree \( \text{PAYMENTID} \) modeling the Payment part is shown in Figure 22. Consider the XML data tree \( \text{PAYMENTID}' \) depicted in Figure 23.

The name-preserving mapping which maps every vertex from \( \text{PAYMENTID}' \) to the vertex carrying the same name in \( \text{PAYMENTID} \) is a homomorphism between \( \text{PAYMENTID}' \) and \( \text{PAYMENTID} \). It is easy to verify that this homomorphism complies with the frequencies specified in \( \text{PAYMENTID} \).

Now look at all vertices of kind \( I \) in \( \text{PAYMENTID}' \). The value of each vertex of kind \( I \) does not occur anywhere else in \( \text{PAYMENTID}' \). This means \( \text{PAYMENTID}' \) satisfies the unique identifier value constraint. Therefore \( \text{PAYMENTID}' \) is compatible with \( \text{PAYMENTID} \).
Some examples in which the unique identifier value constraint is violated are:

- if the value “e_1” was changed to “2003”, or
- if the values “e_1” and “ap_1” were changed to “id_1”, or
- if the value “ap_3” was changed to “ap_1”.

\[ \text{Figure 23: An XML data tree PAYMENTID' compatible with PAYMENTID.} \]

4.2 Sound Inference Rules

It is easy to see that all inference rules which are sound in the presence of frequencies are also sound in the presence of frequencies and identifiers. However, a few other inference rules are required to obtain a sound and complete rule system in the presence of frequencies and identifiers.

The first rule stems from the uniqueness of values taken by identifier-attribute. For an \( r_T \)-subgraph \( X \), let \( X_{ID} \) be the union of all identifiers in \( X \), that is, \( X_{ID} = \bigcup \{ I \mid I \in X \text{ and } I \text{ is an identifier in } T \} \).
Lemma 4.1. Let $T$ be an XML schema graph and $X$ an $r_T$-subgraph of $T$ with $X_{ID}$ being non-empty. The noname2 axiom, as defined below, is sound:

$$X_{ID} \rightarrow X_{ID} \cup T_{\leq 1}$$

Proof. Suppose there is a data tree $T' > T$ such that there are two almost copies of $T$ with $T'_1|_{X_{ID}} = T'_2|_{X_{ID}} \cong X_{ID}$. Since $X_{ID}$ consists only of identifiers, $T'_1$ and $T'_2$ must coincide on $X_{ID}$ due to the unique identifier value constraint. Further, there is only one almost copy $S'$ of $X_{ID} \cup T_{\leq 1}$ in $T'$ such that $S'|_{X_{ID}} = T'_1|_{X_{ID}} = T'_2|_{X_{ID}}$. Therefore $T'_1$ and $T'_2$ must in fact coincide on $X_{ID} \cup T_{\leq 1}$. This implies that $T'_1|_{X_{ID} \cup T_{\leq 1}} = T'_2|_{X_{ID} \cup T_{\leq 1}}$. □

Example 4.2. In PAYMENT_ID there are three identifiers: $<<E\_id>>$, $<<AP\_id>>$ and $<<PD\_id>>$. The noname2 axiom allows us to derive the following XFDs:

- $<<E\_id>> \rightarrow <<E\_id\ name\ empID\ IRD\#>>$
- $<<AP\_id>> \rightarrow <<AP\_id\ year\ E\_ID\ name\ empID\ IRD\#>>$
- $<<PD\_id>> \rightarrow PAYMENT\_ID$

Remark. If we allow an XFD to be an expression $X \rightarrow Y$ where $X$ is a possibly empty $r_T$-subgraph, then we can rewrite the root axiom from Lemma 3.2 such that the noname2 axiom is a generalisation of the rewritten root axiom.

We next extend the notion of a unit of some $r_T$-walk to account for the presence of identifiers. This then allows us to derive a simple generalisation of the noname rule given in Lemma 3.4.

Definition 4.1. Let $X$ be an $r_T$-subgraph and $B$ be an $r_T$-walk of some XML schema graph $T$. The unit of $B$ relative to $X$, denoted by $U^X_B$, is the union of all $r_T$-walks sharing some */+ - arc $A$ with $B$ where $A$ is not in $X_{ID}$.

Example 4.3. Consider the $r_{PAYMENT\_ID}$-subgraph $<<E\_id\ name\ AP\_id>>$ in PAYMENT_ID. For convenience, let us denote this simply by $X$ [Figure 24(a)]. Then we have $X_{ID} = <<E\_id\ AP\_id>>$ [Figure 24(b)]. The arc from the vertex with name “annualPayments” to the vertex carrying the name “paymentDetails” is the only */+ - arc which is in $<<pmtNo>>$ but not in $X_{ID}$. Therefore $U^X_{<<pmtNo>>}$ is the $r_{PAYMENT\_ID}$-subgraph $<<PD\_id\ pmtNo\ date\ grossAmt\ taxAmt\ deductions>>$ [Figure 24(c)]. □
Figure 24: XML trees relating to the computation of the unit of \( \langle \langle \text{pmtNo}\rangle \rangle \) relative to \( \langle \langle \text{E.id name AP.id}\rangle \rangle \).

Analogous to \( U_B \), for any \( r_T \)-walk \( C \in U_B^X \), it is the case that \( U_C^X = U_B^X \). It remains to check whether for any two almost copies \( T_1, T_2 \) of \( T \) in some data tree \( T' \triangleright T \), it is still true that \( T_1 |_{T - \overline{U_B^X}} \cup T_2 |_{U_B^X} \) and \( T_2 |_{T - \overline{U_B^X}} \cup T_1 |_{U_B^X} \) are almost copies of \( T \) in \( T' \).

If \( X_{ID} \) is empty, that is, there is no identifier in \( X \), then \( U_B^X = U_B \). Obviously in this case, \( T_1 |_{T - \overline{U_B^X}} \cup T_2 |_{U_B^X} \) and \( T_2 |_{T - \overline{U_B^X}} \cup T_1 |_{U_B^X} \) are almost copies of \( T \) from the observation we made before. Suppose instead that \( X_{ID} \) is non-empty. The above observation is not true unless an additional condition is satisfied. Let \( I \in X_{ID} \) be an identifier which shares with each \( r_T \)-walk of \( U_B - U_B^X \) the last */+arc which that \( r_T \)-walk shares with \( U_B^X \). For any two almost copies of \( T \) such that \( T_1 |_{I} = T_2 |_{I} = I \), we can observe that \( T_1 |_{T - \overline{U_B^X}} \cup T_2 |_{U_B^X} \) and \( T_2 |_{T - \overline{U_B^X}} \cup T_1 |_{U_B^X} \) are also almost copies of \( T \). Similar to previously, this mix-and-match is possible because the unique identifier value constraint guarantees that \( T_2 |_{U_B^X} \)
shares with $T_1 \mid_{T-U_B^X}$ exactly those arcs (and vertices) which $T_2 \mid_{U_B^X}$ shares with $T_2 \mid_{T-U_B^X}$ and, $T_1 \mid_{U_B^X}$ shares with $T_2 \mid_{T-U_B^X}$ exactly those arcs which $T_1 \mid_{U_B^X}$ shares with $T_1 \mid_{T-U_B^X}$

Example 4.4. Let us reconsider $U^X_{\langle \text{pmtNo} \rangle}$ from Figure 24(c). It is the case that $U_{\langle \text{pmtNo} \rangle} = \text{PAYMENTID}$, and hence $U_{\langle \text{pmtNo} \rangle} - U^X_{\langle \text{pmtNo} \rangle}$ is $\langle E\.id \ name \ empID \ IRD\# \ AP\_id \ year \rangle$. For convenience, let us call this subgraph $Y$. The only identifier in $X_{ID}$ which shares with each $r_{\text{PAYMENTID}-walk}$ in $Y$ the last $*/+$-arc which that $r_{\text{PAYMENTID}-walk}$ shares with $U^X_{\langle \text{pmtNo} \rangle}$ is $\langle \text{AP\_id} \rangle$. Therefore, for any two almost copies of $\text{PAYMENTID}$ which are equivalent and not missing a copy of $\langle \text{AP\_id} \rangle$, it is possible to form two almost copies by exchanging their almost copies of $U^X_{\langle \text{pmtNo} \rangle}$ and $\text{PAYMENTID} - U^X_{\langle \text{pmtNo} \rangle} = Y$.

![Diagram](image)

Figure 25: A modified XML schema tree PAYMENTID2

Suppose we modify $\text{PAYMENTID}$ into $\text{PAYMENTID2}$ shown in Figure 25. Instead of $\langle \text{name} \rangle$, we model that a name consist of a first name together with potentially many middle names and a surname. Under $\text{PAYMENTID2}$, everything in the preceding discussion still holds. In particular, $U^X_{\langle \text{pmtNo} \rangle}$ is the same as shown in Figure 24(c). Again $\langle \text{AP\_id} \rangle$ is still the only identifier in $X_{ID}$ which shares with each $r_{\text{PAYMENTID2}-walk}$ in $U_{\langle \text{pmtNo} \rangle} - U^X_{\langle \text{pmtNo} \rangle}$ the last $*/+$-arc which that $r_{\text{PAYMENTID2}-walk}$ shares with $U^X_{\langle \text{pmtNo} \rangle}$. Therefore, for any two almost copies of $\text{PAYMENTID2}$ which are equivalent and not missing a copy of $\langle \text{AP\_id} \rangle$, it is possible to form two almost copies by exchanging their almost copies of $U^X_{\langle \text{pmtNo} \rangle}$ and $\text{PAYMENTID2} - U^X_{\langle \text{pmtNo} \rangle}$.

\[\square\]
Lemma 4.2. Let T be an XML schema graph, X an $r_T$-subgraph of T and B an $r_T$-walk of T. The generalised noname rule defined as follows is sound for the derivation of XFDs:

$$\frac{(X \cup B) \cup T_{\geq 1} - U_B^X \cup X \rightarrow B}{X \rightarrow B}$$

Proof. The proof is analogous to that of Lemma 3.4. Suppose there is some data tree $T' \triangleright T$ with $\models_{T'} ((X \cup B) \cup T_{\geq 1} - U_B^X) \cup X \rightarrow B$ but $\not\models_{T'} X \rightarrow B$. That is, $T'$ has two almost copies $T'_1$, $T'_2$ of $T$ such that $T'_1 |_X = T'_2 |_X \equiv X$ and $T'_1 |_B \neq T'_2 |_B$. We have $((X \cup B) \cup T_{\geq 1} - U_B^X) \subseteq X$, otherwise $((X \cup B) \cup T_{\geq 1} - U_B^X) \cup X = X$ which would immediately mean $\models_{T'} X \rightarrow B$ by assumption. Therefore there is some non-empty $r_T$-subgraph $W \subseteq ((X \cup B) \cup T_{\geq 1} - U_B^X)$ such that $W \cap X = \emptyset$. We can then rewrite the generalised noname rule as follows:

$$\frac{(X \cup B) \cup T_{\geq 1} - U_B^X \cup X \rightarrow B}{X \rightarrow B} = \frac{XW \rightarrow B}{X \rightarrow B}$$

One of $T'_1$ and $T'_2$ must not be missing a copy of $B$ and thus not missing a copy of every $r_T$-walk of $(X \cup B) \cup T_{\geq 1}$. Without loss of generality, assume $T'_1 |_B \equiv B$ and so $T'_1 |_W \equiv W$ since $W \subseteq (X \cup B) \cup T_{\geq 1}$. There are now two cases to consider: $T'_1 |_W = T'_2 |_W \equiv W$ and $T'_1 |_W \neq T'_2 |_W$.

Firstly, suppose $T'_1 |_W = T'_2 |_W \equiv W$. Recall that by assumption $T'_1 |_X = T'_2 |_X \equiv X$, therefore we have $T'_1 |_X \cap W = T'_2 |_X \cap W \equiv XW$. Since $\models_{T'} XW \rightarrow B$ it follows that $T'_1 |_B = T'_2 |_B$ which contradicts our assumption that $\not\models_{T'} X \rightarrow B$.

So, let us consider instead that $T'_1 |_W \neq T'_2 |_W$. Since $W \subseteq ((X \cup B) \cup T_{\geq 1} - U_B^X) \subseteq T - U_B^X$, it follows that no $r_T$-walk of $W$ is in $U_B^X$. If $B \notin U_B^X$ then there is no */+-arc which is in $B$ but not in an $r_T$-walk of $X_{ID}$. That is $B \in R$ if $X_{ID}$ is empty, or $B \in X_{ID} \cup T_{\leq 1}$ and application of the noname2 axiom followed by application of the subtree rule states that $\models_{T'} X_{ID} \rightarrow B$. In either case, $T'_1 |_B = T'_2 |_B$ which would contradict our assumption. Hence $B \in U_B^X$. From $X_{ID} \subseteq X$ we obtain $T'_1 |_{X_{ID}} = T'_2 |_{X_{ID}} \equiv X_{ID}$.

Therefore we can form two other almost copies of $T$ as follows:

- $T'_3 = T'_1 |_{T - U_B^X} \cup T'_2 |_{U_B^X}$
- $T'_4 = T'_2 |_{T - U_B^X} \cup T'_1 |_{U_B^X}$

Consider the pair of almost copies $T'_1$ and $T'_3$. We have $T'_1 |_W = T'_3 |_W$ and altogether $T'_1 |_XW = T'_3 |_XW \equiv XW$. From $\models_{T'} XW \rightarrow B$, it follows that $T'_1 |_B = T'_3 |_B$. Since $T'_3 |_B$ is just $T'_2 |_B$ then in fact $T'_1 |_B = T'_2 |_B$ which contradicts our assumption. \(\square\)
Note that if $X_{ID}$ is an empty $r_T$-subgraph then the generalised noname rule reduces to the noname rule of Lemma 3.4.

### 4.3 A Sound & Complete Rule System

Let the $I$-rule system for XFDs in the presence of frequencies and identifiers be the set containing the following inference rules: reflexivity axiom, root axiom, subtree rule, supertree rule, union rule, restricted-transitivity rule, noname2 axiom and generalised noname rule.

Similar to Section 3.2, consider a sequence of restricted pre-closures $X_0, X_1, X_2, \ldots, X_{n-1}, X_n, X_{n+1}, X_{n+2}, \ldots$ where $X_n = X_{n+1} = X_{n+2} \ldots$ for $n \geq 0$, now computed using the $I$-rule system:

\[
\begin{align*}
X_0 &= ((X \cup B) \cup T_{\geq 1} - U_B^X) \cup X \\
X_1 &= (X_0)^+ \cap ((X \cup B) \cup T_{\geq 1}) \\
X_2 &= (X_1)^+ \cap ((X \cup B) \cup T_{\geq 1}) \\
& \vdots \\
X_{n-1} &= (X_{n-2})^+ \cap ((X \cup B) \cup T_{\geq 1}) \\
X_n &= (X_{n-1})^+ \cap ((X \cup B) \cup T_{\geq 1}) \\
& \vdots
\end{align*}
\]

Let $X^B_I = ((X_n \cup B) \cup T_{\geq 1} - U_B^{X_n}) \cup X_n$. Due to the soundness of the generalised noname axiom, if $X_n \rightarrow A \not\in \Sigma^+_I$ then $X^B_I \rightarrow A \not\in \Sigma^+_I$ or $A \subseteq X^B_I$. In particular, this means that $X^B_I = (X^B_I)^+ \cap ((X \cup B) \cup T_{\geq 1})$ and so it is sufficient for us to consider $X^B_I$.

There may be $r_T$-walks in $X^B_I$ which are not functionally determined by $X$. Analogous to Section 3.2, we nevertheless construct a counterexample data tree from two almost copies of $T$ which are equivalent on $X^B_I$ in order to ensure that the resulting data tree consists of exactly two almost copies of $T$. An abstract illustration of the structure of an XML schema graph and a constructed XML data tree compatible with the schema graph is shown in Figure 26 and Figure 27.

**Theorem 4.3.** The $I$-rule system consisting of the reflexivity axiom, root axiom, subtree rule, supertree rule, union rule, restricted-transitivity rule, noname2 axiom and generalised noname rule is sound and complete for the derivation of XFDs in the presence of frequencies and identifiers.
Consider $X^B_T$ as outlined above. Consider the data tree $T' = T'_a \Pi (X \cup B) \cup T_{\geq 1} \cup T'_b$ with $T'_a, T'_b$ being two copies of $(X \cup B) \cup T_{\geq 1}$ such that

$$T'_a |_W = T'_b |_W$$

if and only if $W \subseteq X^B_T$

This is always possible and the resulting data tree $T'$ will contain exactly two almost copies of $T$: $T'_1 = T'_a$ and $T'_2 = T'_b$.

Firstly, we need to show that $T'$ satisfies every XFD in $\Sigma$. Assume that some $U \rightarrow V \in \Sigma$ is not satisfied by $T'$. Then there must be some $\tau_T$-walk $C \in V$ such that $\not\models_{T'} U \rightarrow C$. We have $U \subseteq X^B_T$ and $C \not\in X^B_T$ with $C \in ((X \cup B) \cup T_{\geq 1})$, otherwise $U \rightarrow C$ cannot be violated. By application of the supertree rule to $U \rightarrow C \in \Sigma$ we obtain $X^B_T \rightarrow C \in \Sigma_T$. Since $C \notin X^B_T = (X \cup B) \cup T_{\geq 1} - U^X_B$ we have $C \in U^X_B$. This gives $U^X_C = U^X_B$ which implies $((X \cup C) \cup T_{\geq 1} - U^X_C) \cup X_n = X^B_T$. Therefore it follows from the generalised noname rule that $X_n \rightarrow C \in \Sigma_T$, that is, $C \in (X_n)^T$. Altogether $C \in (X_n)^T \cap ((X \cup B) \cup T_{\geq 1}) = X_{n+1} = X_n$, that is, $C \in X^B_T$. This is a contradiction hence we may conclude that $\models_{T'} U \rightarrow V$. 

Proof. Soundness of the inference rules has already been proven in Lemma 3.1, Lemma 3.2, Lemma 3.3, Lemma 4.1 and Lemma 4.2. It remains to show that the $T$-rule system is complete in the presence of frequencies and identifiers. Let $T$ be an XML schema graph and $\Sigma$ a set of XFDs on $T$. Suppose $X \rightarrow Y \notin \Sigma_T$. That is, there is some $\tau_T$-walk $B \in Y$ such that $X \rightarrow B$ cannot be derived. We construct a counterexample data tree $T' \triangleright T$ such that $\models_{T'} \Sigma$ and $\not\models_{T'} X \rightarrow B$.

Figure 26: A diagram illustrating the structure of an XML schema graph $T$ and the various subgraphs of $(X \cup B) \cup T_{\geq 1}$ identifiable when computing $X^B_T$.

Figure 27: A diagram illustrating the structure of a constructed XML data tree $T' \triangleright T$. We use diagonal stripes versus horizontal stripes on the bottom-right to identify two isomorphic but non-equivalent $\tau_T$-subgraphs.
Secondly, we show that the XFD $X \rightarrow Y \notin \Sigma_T^+$ is not satisfied by $T'$. Suppose $B \in X_T^B$. Then $X_T^B \rightarrow B$ and by means of the \textit{generalised noname rule} $X_n \rightarrow B$. Clearly $B \in (X \cup B) \cup T$ and so $B \in (X_n)^+ \cap ((X \cup B) \cup T) = X_{n+1} = X_n$. It follows that $X_{n-1} \rightarrow B \in \Sigma_T^+$ from the definition of $X_n$. Further $X_{n-1} \subseteq (X_{n-2})^+$, therefore it follows that $X_{n-2} \rightarrow X_{n-1}$. Also $X_{n-1} \subseteq (X_{n-2} \cup B) \cup T$ since $X \subseteq X_{n-2}$ and $X_{n-1} \subseteq (X \cup B) \cup T$. This means $X_{n-1}$ is $X_{n-2}, B$-compliant. Therefore $X_{n-2} \rightarrow B \in \Sigma_T^+$ is derived by means of the \textit{restricted-transitivity rule}. Following the same reasoning, we get $X_{n-3} \rightarrow B \in \Sigma_T^+$, then $X_{n-4} \rightarrow B \in \Sigma_T^+$, and so on until eventually we obtain $X_0 \rightarrow B \in \Sigma_T^+$. $X_0 = ((X \cup B) \cup T \cup U_B^1) \cup X$ and so another application of the \textit{generalised noname rule} yields $X \rightarrow B \in \Sigma_T^+$ which contradicts our assumption. Hence $B \notin X_T^B$. Then by construction $\not \models_{T'} X \rightarrow B$ and thus $\not \models_{T'} X \rightarrow Y$. \hfill $\square$
In addition to the axiomatisation of functional dependencies, another important objective of design theory is the design of “good” database schemas. For various data models, a primary justification for a schema being “good” (i.e. a desirable property), apart from the absence of update anomalies and simplified integrity checking, is the absence of redundancy. Normal forms have been proposed as syntactic characterisations with which to determine whether a schema has certain desirable properties. In this section, we derive a new XML normal form for XFDs in the presence of frequencies and identifiers which is both necessary and sufficient for the absence of redundancy. We will define a notion of redundancy in Section 5.2, however we begin with a discussion of trivial XFDs.

5.1 Trivial XFDs

An XFD on an XML schema graph $T$ is called trivial if and only if they are satisfied by every XML data tree $T' \succ T$.

**Proposition 5.1.** Let $T$ be an XML schema tree and $X, Y$ be two non-empty $r_T$-subgraphs in $T$. An XFD $X \rightarrow Y$ on $T$ is trivial if and only if one of the following conditions holds:

1) $Y \subseteq X$

2) $Y \subseteq X_{ID} \cup T_{\leq 1}$

**Proof.** (If) For each of the cases above, we show that every data tree $T' \succ T$ satisfies the XFD $X \rightarrow Y$ and is therefore trivial. Firstly, if $Y \subseteq X$, the reflexivity axiom states that every data tree $T' \succ T$ satisfies the XFD $X \rightarrow Y$.

For the second case where $Y \subseteq X_{ID} \cup T_{\leq 1}$. If $X_{ID}$ is empty then $Y \subseteq R$. The root axiom states that every data tree satisfies the XFD $X \rightarrow R$. Since $Y \subseteq R$, the subtree rule further states that every data tree $T' \succ T$ also satisfies the XFD $X \rightarrow Y$. Suppose instead that $X_{ID}$ is non-empty, then the noname2 axiom states that every data tree satisfies the XFD $X_{ID} \rightarrow X_{ID} \cup T_{\leq 1}$. Since $X_{ID} \subseteq X$, by supertree rule, we have that every data tree also satisfies $X \rightarrow X_{ID} \cup T_{\leq 1}$. Finally since $Y \subseteq X_{ID} \cup T_{\leq 1}$, the subtree rule again states that every data tree also satisfies $X \rightarrow Y$.

Under each condition, we have shown that $X \rightarrow Y$ is a trivial dependency.

(Only If) It remains to show that all trivial XFDs must satisfy at least one of the specified conditions. Assume that $X \rightarrow Y$ is a trivial XFD on $T$ and none of the two conditions hold, that is, $Y \not\subset X$ and $Y \not\subseteq X_{ID} \cup T_{\leq 1}$. 
5.2 Redundancy with respect to XFDs

We need to construct an XML data tree \( T' \supseteq T \) in which \( X \rightarrow Y \) is violated. Consider the data tree \( T' = T'_a \Pi_{(X_{ID} \cup T_{\leq 1})} T'_b \) with \( T'_a, T'_b \) being copies of \( T \) such that

\[
T'_a|_W = T'_b|_W \text{ if and only if } W \subseteq X \text{ or } W \subseteq X_{ID} \cup T_{\leq 1}
\]

Observe that the amalgamation is always possible because every \( r_T \)-walk not in \( X_{ID} \cup T_{\leq 1} \) must contain at least one *+/--arc and \( T'_a, T'_b \) may only be non-equivalent on those \( r_T \)-walks.

Since \( Y \not\subseteq X \) and \( Y \not\subseteq X_{ID} \cup T_{\leq 1} \) hold, it is clear that \( \not\models_{T'} X \rightarrow Y \). Therefore by contradiction we may conclude that trivial XFDs must satisfy one of the two conditions. 

5.2 Redundancy with respect to XFDs

In the RDM, redundancy with respect to functional dependencies considers each functional dependency to be describing a basic unit of information when retrieving or updating data. A relation which satisfies a given set of functional dependencies, and contains two tuples identical on such a unit of information is said to be redundant. If we simply rewrite this notion for the XML graph model, we obtain the following definition for redundancy:

Let \( T \) be an XML schema graph and \( \Sigma \) a set of XFDs on \( T \). We say \( T \) is redundant with respect to \( \Sigma \) if and only if there is some XML data tree \( T' \supseteq T \) such that \( \models_{T'} \Sigma \) and for some non-trivial XFD \( X \rightarrow Y \in \Sigma \) with \( r_T \)-walk \( B \in Y \), there exists two almost copies \( T'_1, T'_2 \) of \( T \) in \( T' \) with \( T'_1|_X_B = T'_2|_X_B \cong X_B \).

Example 5.1. All XFDs in \( \Sigma(PAYMENTID) \) on \( PAYMENTID \) [Figure 22] are non-trivial. Consider the XFD:

\[
(P\_XFD1) \quad \langle \text{empID} \rangle \rightarrow \langle E\_id \rangle
\]

The two almost copies of \( PAYMENTID \) in \( PAYMENTID' \) shown in Figure 28 are equivalent and not missing a copy of both \( r_{PAYMENTID} \)-walk of \( \langle \text{empID} \ E\_id \rangle \). This means \( P\_XFD1 \) causes \( PAYMENT \) to be redundant with respect to \( \Sigma(PAYMENTID) \) according the above definition. However the two almost copies actually share the same copy of \( \langle \text{empID} \ E\_id \rangle \) in \( PAYMENTID' \).

Example 5.1 illustrates that the above definition is not quite adequate in the framework of XML. The unit of information is not redundant since we cannot delete it from either
almost copies without losing information. Similar to nested relations, the hierarchical structure in XML enables us to avoid some redundancy which would be unavoidable in the RDM. In order to adapt a notion of redundancy, we need the additional requirement that the two almost copies must not share the same almost copy of the right-hand-side of the XFD, that is, they do not coincide [Definition 3.4] on the right-hand-side.

**Definition 5.1.** Let \( T \) be an XML schema graph and \( \Sigma \) a set of XFDs on \( T \). We say \( T \) is redundant with respect to \( \Sigma \) if and only if there is some XML data tree \( T' \succ T \) such that \( \models_{T'} \Sigma \) and for some non-trivial XFD \( X \rightarrow Y \in \Sigma \) with \( r_T \text{-walk} \ B \in Y - X \) there exists two almost copies \( T'_1, T'_2 \) of \( T \) in \( T' \) with \( T'_1 |_{XB} = T'_2 |_{XB} \cong XB \) but \( T'_1 \) and \( T'_2 \) do not coincide on \( B \).

**Example 5.2.** According to Definition 5.1 the XFD

\[(P \_XFD1) \quad \ll < empID > \rightarrow < E\_id > \]

is no longer seen to cause PAYMENTID to be redundant with respect to \( \Sigma(PAYMENTID) \).

If the right-hand-side of an XFD contains only identifiers then the XFD cannot cause an XML schema tree to be redundant due to the unique identifier value constraint. So the only XFD in \( \Sigma(PAYMENTID) \) that may cause some concern is

\[(P \_XFD2) \quad \ll IRD\# \rightarrow < empID > \]

Since \( \ll empID > \), \( \ll E\_id > \) -compliant, by means of the restricted-transitivity rule we can derive \( \ll IRD\# > \rightarrow < E\_id > \) where \( < E\_id > \) is an identifier. It is easy to see that for any data tree compatible with PAYMENTID, for any
two almost copies of PAYMENTID which are equivalent and not missing a copy of \(<IRD\#\ empID>\), they must be equivalent to and not missing a copy of \(<E_id>\). In fact, because \(<E_id>\) is an identifier, any two almost copies of PAYMENTID coincide on \(<E_id>\). Since \(<empID>\in <E_id>\cup PAYMENTID_{\leq 1}\), the two almost copies must also coincide on \(<empID>\). This means PAYMENTID is non-redundant with respect to \(\Sigma(PAYMENTID)\).

Example 5.3. Now consider the XML schema tree BANKID from Figure 21. Suppose we have the XML data tree modified from the one in Figure 13 such that \(\Sigma(BANKID)\) and the unique identifier value constraint are satisfied. The resulting data tree would contain information about two employees who have supplied the same bank account details. One explanation for this would be that a married couple working in the company have both given their joint-account details. Therefore, \(BXF D6\) to \(BXF D13\) cause BANKID to be redundant with respect to \(\Sigma(BANKID)\).

Similar to the RDM, we can prove that a schema graph \(T\) is redundant with respect to \(\Sigma\) precisely if \(T\) is redundant with respect to \(\Sigma^*\). In other words, a schema graph being redundant is invariant under the replacement of a set of XFDs by an equivalent set. It should be noted that according to Theorem 4.3, \(\Sigma^* = \Sigma_T^+\) in the presence of frequencies and identifiers.

Theorem 5.1. Let \(T\) be an XML schema graph and \(\Sigma\) a set of XFDs on \(T\). Then \(T\) is redundant with respect to \(\Sigma\) if and only if \(T\) is redundant with respect to \(\Sigma^*\).

Proof: (Only If) The redundancy of \(T\) with respect to \(\Sigma^*\) whenever \(T\) is redundant with respect to \(\Sigma\) is obvious since \(\Sigma \subseteq \Sigma^*\), and \(\models_T \Sigma\) implies \(\models_T \Sigma^*\) by definition of \(\Sigma^*\).

(If) It remains to show that redundancy of \(T\) with respect to \(\Sigma^*\) also implies that \(T\) is redundant with respect to \(\Sigma\). Consider the chain

\[\Sigma = \Sigma_0 \subseteq \Sigma_1 \subseteq \ldots \subseteq \Sigma_k = \Sigma_T^+ = \Sigma^*\]

where \(\Sigma_{i+1}\) results from \(\Sigma_i\) for \(i \geq 0\), by a single application of one of the inference rules from the \(I\)-rule system. We show that there is already some XFD in \(\Sigma_i\) which causes \(T\) to be redundant with respect to \(\Sigma_i\) whenever \(T\) is redundant with respect to \(\Sigma_{i+1}\) for any \(i \geq 0\).

Assume that \(T\) is redundant with respect to \(\Sigma_{i+1}\). This means that some non-trivial XFD \(X \rightarrow Y \in \Sigma_{i+1}\) which causes \(T\) to be redundant with respect to \(\Sigma_{i+1}\). Further, for some \(T\)-walk \(B \in Y - X\), there is an XML data tree \(T' \triangleright T\) such that \(\models_{T'} \Sigma_{i+1}\) which contains two almost copies \(T'_1, T'_2\) of \(T\) such that \(T'_1|_{XB} = T'_2|_{XB} \cong XB\) but \(T'_1\) and \(T'_2\) do...
not coincide on $B$. If $X \rightarrow Y \in \Sigma_i$, then there is nothing to show. It remains to look at $X \rightarrow Y \in \Sigma_{i+1} - \Sigma_i$.

Clearly $\models_{r^r} \Sigma_{i+1}$ implies $\models_{r^r} \Sigma_i$ since $\Sigma_i \subseteq \Sigma_{i+1}$. Since $X \rightarrow Y$ is non-trivial, Proposition 5.1 implies that it has not been derived by means of the reflexivity axiom, root axiom or noname2 axiom. We proceed by considering the cases where $X \rightarrow Y$ has been derived by means of any of the remaining axioms in the $r$-rule system.

Assume that $X \rightarrow Y$ has been derived using the union rule, i.e. $Y = W \cup Z$ and $X \rightarrow W, X \rightarrow Z \in \Sigma_i$. It must be that $B \in W - X$ or $B \in Z - X$. If $B \in W - X$ then $X \rightarrow W$ causes $T$ to be redundant with respect to $\Sigma_i$. Similarly if $B \in Z - X$ then $X \rightarrow Z$ causes $T$ to be redundant with respect to $\Sigma_i$. In either case, $T$ is redundant with respect to $\Sigma_i$.

Next assume that $X \rightarrow Y$ has been derived by means of the subtree rule, i.e. $Y \sim W$ with $X \rightarrow W \in \Sigma_i$. From $B \in Y - X$ and $Y \subseteq W$ we infer $B \in W - X$. It immediately follows that $T$ is redundant with respect to $\Sigma_i$ due to $X \rightarrow W$.

Thirdly, suppose that $X \rightarrow Y$ has been derived using the supertree rule, i.e. $W \sim X$ with $W \rightarrow Y \in \Sigma_i$. Since $W \subseteq X$ and $T_1|_{X^1} = T_2|_{X^1} \subseteq X$, it is the case that $T_1|_{W^1} = T_2|_{W^1} \subseteq W$.

From $B \in Y - X$ and $W \subseteq X$ we infer $B \in Y - W$. Therefore $T$ is redundant with respect to $\Sigma_i$ because of $W \rightarrow Y$.

Suppose $X \rightarrow Y$ has been derived by means of the restricted-transitivity rule, i.e. $W$ is $X, Y$-compliant and $X \rightarrow W, W \rightarrow Y \in \Sigma_i$. Recall that $W$ is $X, Y$-compliant if and only if $W \subseteq (X \cup C) \cup T_{\geq 1}$ for each $r_T$-walk $C \in Y$. In particular, we have $W \subseteq (X \cup B) \cup T_{\geq 1}$.

From this and the fact that $\models_{r^r} X \rightarrow W$ we get $T_1|_{W^1} = T_2|_{W^1} \subseteq W$. Either $B \not\in W$ or $B \in W$. If $B \not\in W$ then $B \in Y - W$ and it immediately follows that $W \rightarrow Y$ causes $T$ to be redundant with respect to $\Sigma_i$. Suppose instead that $B \in W$. From assumption $B \not\in X$, therefore $B \in W - X$, in which case $X \rightarrow W$ causes $T$ to be redundant with respect to $\Sigma_i$.

Finally, assume that $X \rightarrow Y$ has been derived using the generalised noname rule, i.e. $X' = ((X \cup Y) \cup T_{\geq 1} - U^X) \cup X$ with $Y = B$ being a single $r_T$-walk and $X' \rightarrow Y \in \Sigma_i$.

Rewriting our initial assumption gives $T_1|_{X^Y} = T_2|_{X^Y} \cong XY$ but $T_1$ and $T_2$ do not coincide on $Y$, and $Y \not\in X$. If $Y \in X'$ then there is no *+/arc which is in $Y$ but not in $X_{ID}$. That is $Y \in X_{ID} \cup T_{\geq 1}$ meaning that $X \rightarrow Y$ is trivial by Proposition 5.1. It therefore remains to consider the case $Y \not\in X'$.

$T_1$ and $T_2$ are not missing a copy of every $r_T$-walk of $X'$ since $X' \subseteq (X \cup Y) \cup T_{\geq 1}$ and neither a copy of $X$ nor a copy of $Y$ are missing from either almost copies. It
is the case that either $T'_1 |_{X'} = T'_2 |_{X'}$ or $T'_1 |_{X'} \neq T'_2 |_{X'}$. In the first case, we know that $X' \rightarrow Y$ causes $T$ to be redundant with respect to $\Sigma_i$. So consider the latter case where $T'_1 |_{X'} \neq T'_2 |_{X'}$. Since $X_{ID} \subseteq X$ we have $T'_1 |_{X_{ID}} = T'_2 |_{X_{ID}} \cong X_{ID}$. This allows us to apply the observation from Section 4.2, that is, from $T'_1$ and $T'_2$ we obtain another almost copy of $T$, namely $T'_3 = T'_1 |_{T - U'_X} \cup T'_2 |_{U'_Y}$. It is easy to see that $T'_1 |_{X'} = T'_3 |_{X'} \cong X'$ since $X' \subseteq (T - U'_X) \cup X$. From $Y \not\subseteq X'$ we infer $Y \in U'_X$. This means $T'_3 |_{Y}$ is just $T'_2 |_{Y}$, so it follows that $T'_1$ and $T'_3$ do not coincide on $Y$. But this means that $X' \rightarrow Y$ causes $T$ to be redundant with respect to $\Sigma_i$. □

5.3 $X^I\text{NF}$: An XML Normal Form Utilising Identifiers

In the RDM, a syntactic characterisation of a relation schema being non-redundant with respect to a set of FDs is the Boyce-Codd Normal Form (BCNF). The definition of BCNF is not easily adaptable to the XML framework due to the difficulty of adapting the notion of keys from the RDM to XML. As far as we are aware, the notion of keys in XML (e.g. [1, 7, 8, 12]) currently only provide a means for identifying and referencing specific vertices.

Our proposed normal form for XML definition avoids referring to any notion of keys in XML. Instead, we propose to make use of the uniqueness of identifier values in order to guarantee non-redundancy. Consider a non-trivial XFD of the form $X \rightarrow Y$. Our proposed normal form requires that $Y \in I \cup T_{\leq 1}$ for some identifier $I$, where for any two almost copies $T'_1, T'_2$ of the schema tree such that $T'_1 |_{X} = T'_2 |_{X} \cong X$ it is the case that $T'_1, T'_2$ are equivalent and not missing a copy of $I$. Due to the uniqueness of identifier value, $T'_1$ and $T'_2$ would then necessarily coincide on the identifier and thus also coincide on $Y$. Clearly the identifier $I$ can be in $X^+_T$, but $I$ can also be in $X^+_T$ defined as follows.

Let $X_T^B = ((X \cup B) \cup T_{\geq 1} - U_B^X) \cup X_n$ where the sequence $X_0, X_1, X_2, ..., X_{n-1}, X_n, X_{n+1}, ...$ of restricted pre-closures with $X_n = X_{n+1} = X_{n+2} = ...$ is computed as follows:

- $X_0 = ((X \cup B) \cup T_{\geq 1} - U_B^X) \cup X$
- $X_1 = (X_0)^+_T \cap ((X \cup B) \cup T_{\geq 1})$
- $X_2 = (X_1)^+_T \cap ((X \cup B) \cup T_{\geq 1})$
- ...
- $X_{n-1} = (X_{n-2})^+_T \cap ((X \cup B) \cup T_{\geq 1})$
- $X_n = (X_{n-1})^+_T \cap ((X \cup B) \cup T_{\geq 1})$
- ...

where the pre-closures
Definition 5.2. Let $T$ be an XML schema graph, $X$ an $r_T$-subgraph and $B$ an $r_T$-walk of $T$. $B$ is said to be relatively identified by $X$ if and only if there exists some identifier $I$ in $T$ such that $I \in X_B^T$ and $B \in I \cup T_{\leq 1}$.

Remark. For an XFD $X \rightarrow B$, if $B$ is an identifier then $B$ is relatively identified by $X$.

Definition 5.3. Let $T$ be an XML schema graph and $\Sigma$ a set of XFDs on $T$. We say that $T$ is in XML with Identifiers Normal Form (X$^I$NF) with respect to $\Sigma$ if and only if for every non-trivial XFD $X \rightarrow B \in \Sigma^*$ where $B$ is a single $r_T$-walk of $T$, it is the case that $B$ is relatively identified by $X$.

Remark. If there are no identifiers in $T$ then $T$ is in X$^I$NF with respect to $\Sigma$ if and only if every XFD $X \rightarrow B \in \Sigma^*$ is trivial.

With the following Lemma and Theorem we show that X$^I$NF is a necessary and sufficient condition for non-redundancy.

Lemma 5.2. Let $T$ be an XML schema graph and $\Sigma$ a set of XFDs on $T$. Consider a data tree $T' \triangleright T$ such that $\models_{T'} \Sigma$ and the sequence of restricted pre-closures used to compute $X_B^T$ (see above). For every $r_T$-walk $A \in X_n - X_0$, any two almost copies $T_1, T_2$ of $T$ with $T_1|_X = T_2|_X \cong X$ and $T_i|_B \cong B$ for $i = 1$ or $2$, it is the case that $T_1|_A = T_2|_A \cong A$.

Proof. Let $A \in X_n - X_0$. From $A \not\in X_0 = (X \cup B) \cup T_{\geq 1} - U_B^X$ we infer that $A \in U_B^X$. Without loss of generality assume that $T_1|_B \cong B$. This means $T_1|_{X_0} \cong X_0$ since $T_1$ is not missing a copy of every $r_T$-walk of $X$ and $B$. If $T_1|_{X_0} = T_2|_{X_0} \cong X_0$ then $T_1|_{X_n} = T_2|_{X_n} \cong X_n$ and of course $T_1|_A = T_2|_A \cong A$. Therefore suppose $T_1|_{X_0} \neq T_2|_{X_0}$. Since $T_1|_{X_{ID}} = T_2|_{X_{ID}} \cong X_{ID}$ we can consider a third almost copy of $T$, namely $T_3 = T_1|_{T - U_B^X} \cup T_2|_{U_B^X}$. We now have $T_1|_{X_0} = T_3|_{X_0} \cong X_0$ and thus $T_1|_A = T_3|_A \cong A$. In particular, this means $T_1|_A = T_3|_A \cong A$. But $T_3|_A$ is just $T_2|_A$ so in fact $T_1|_A = T_2|_A \cong A$.

Theorem 5.3. Let $T$ be an XML schema graph and $\Sigma$ a set of XFDs on $T$. Then $T$ is in X$^I$NF with respect to $\Sigma$ if and only if $T$ is non-redundant with respect to $\Sigma$.

Proof. (Only If) Let $T$ be in X$^I$NF and assume that $T$ is redundant with respect to $\Sigma$. A direct implication of Theorem 5.1 is that $T$ is redundant with respect to $\Sigma^*$. Therefore there is some XML data tree $T' \triangleright T$ such that $\models_{T'} \Sigma$ and for some non-trivial XFD $X \rightarrow B \in \Sigma^*$ with $r_T$-walk $B \not\subset X$, there exists two almost copies $T_1, T_2$ of $T$ in $T'$ with $T_1|_{XB} = T_2|_{XB} \cong XB$ but $T_1$ and $T_2$ do not coincide on $B$. We can assume that $B$ is a single $r_T$-walk without loss of generality. Since $T$ is in X$^I$NF and $X \rightarrow B$ is non-trivial,
we have $B$ is relatively identified by $X$. That is, there is some identifier $I$ in $T$ such that $I \in X^B_\geq$ and $B \in I \cup T_{\leq 1}$.

If $T_1|_I = T_2|_I \cong I$ then $T'_1$ and $T'_2$ must coincide on $I$ because of the unique identifier value constraint. Then $B \in I \cup T_{\leq 1}$ would further imply that $T'_1$ and $T'_2$ coincide on $B$. This would contradict our assumption, therefore assume $T'_1|_I \neq T'_2|_I$. As a direct result of Lemma 5.2, $I \not\in X_n - X_0$. Moreover $I \not\subset X$ since $T'_1|_X = T'_2|_X \cong X$ by assumption. This leaves the cases where either (1) $I \in X_0 - X$, or (2) $I \in X^B_\geq - X_n$.

Firstly suppose $I \in X_0 - X$, that is $I \in ((X \cup B) \cup T_{\geq 1} - U^X_B) - X$. In particular $I \not\in U^X_B$ and therefore $B \not\in U^X_B$ since $B \in I \cup T_{\leq 1}$. This means that there is no */+-arc which is in $B$ but not in $X_{ID}$. If $X_{ID}$ is empty then there is no */+-arc in $B$ and $B \in R$. But then $X \to B$ would be trivial and also $T'_1, T'_2$ would coincide on $B$ thus contradicting our assumptions. Hence there is some identifier $J \in X_{ID} \subseteq X$ such that $B \in J \cup T_{\leq 1}$. Clearly $T_1|_J = T_2|_J \cong J$. Then $T'_1$ and $T'_2$ coincide on $J$ and therefore also coincide on $B$ because $B \in J \cup T_{\leq 1}$. This is a contradiction to our assumption that there are two almost copies $T'_1, T'_2$ of $T$ in $T'$ with $T'_1|_B = T'_2|_B \cong XB$ but $T'_1$ and $T'_2$ not coinciding on $B$.

Now consider the case where $I \in X^B_\geq - X_n$, that is $I \in ((X_n \cup B) \cup T_{\geq 1} - U^X_{B^n}) - X_n$. Similar to before, $I \not\in U^X_{B^n}$ so $B \not\in U^X_{B^n}$ and there is no */+-arc in $B$ but not in $(X_n)_{ID}$. Like above, $(X_n)_{ID}$ must not be empty and there is some identifier $J \in (X_n)_{ID}$ with $B \in J \cup T_{\leq 1}$. Either $J \in X_n - X_0$ or $J \in X_0 - X$ or $J \in X$.

For $J \in X$, it is obvious that $T'_1|_J = T'_2|_J \cong J$. If $J \in X_n - X_0$ then $T'_1|_J = T'_2|_J \cong J$ by Lemma 5.2. By the same argument as above, both cases result in $T'_1$ and $T'_2$ coinciding on $J$ and thus coinciding on $B$. Finally consider the case where $J \in X_0 - X$. This is just the first case discussed above. Following the same argument as previously, we conclude that $T'_1$ and $T'_2$ coincide on $B$.

In each case we obtain a contradiction, therefore it must be that $T$ is non-redundant with respect to $\Sigma$.

(If) On the other hand, we need to show that if $T$ is not in X'NF with respect to $\Sigma$ then $T$ is redundant with respect to $\Sigma$. Assume that $T$ is not in X'NF with respect to $\Sigma$. Let $X \to B \in \Sigma^*$ be a non-trivial XFD where $B$ is not relatively identified by $X$. We show that it is possible to construct an XML data tree $T' \triangleright T$ witnessing that $T$ is redundant with respect to $\Sigma^*$. More specifically, it will be the case that $|=T' \Sigma$ and $T'$ contains two almost copies $T'_1, T'_2$ such that $T'_1|_B = T'_2|_B \cong XB$ but $T'_1, T'_2$ do not coincide on $B$.

Recall the XML data tree construction from Theorem 4.3: namely $T' = T'_a \Pi_{(X_n \cup B) \cup T_{\geq 1} - U^X_B} T'_b$ with $T'_a, T'_b$ being two copies of $(X \cup B) \cup T_{\geq 1}$ such
that

\[ T_a' |_W = T_b' |_W \text{ if and only if } W \subseteq X_T^B \]

The resulting data tree \( T' \) contains exactly two almost copies of \( T \): \( T_1' = T_a' \) and \( T_2' = T_b' \).

Analogous to the proof of Theorem 4.3, we can show that \( \models T' \). Obviously \( X \subseteq X_T^B \) and so \( T_1' |_X = T_2' |_X \cong X \). It follows from \( X \rightarrow B \in \Sigma^* \) that \( B \in X_T^B \) and therefore \( T_1' |_B = T_2' |_B \cong B \). Suppose \( B \in (X_n \cup B) \cup T_{\geq 1} - U_B^{X_n} \). Then \( B \not\in U_B^{X_n} \) and it follows that there is no */+-arc in \( B \) but not in \((X_n)_{ID}\). In other words \( B \in (X_n)_{ID} \cup T_{\leq 1} \). Since \((X_n)_{ID} \subseteq X_T^B \), if \((X_n)_{ID} \) is non-empty then there is some identifier \( I \in (X_n)_{ID} \subseteq X_T^B \) such that \( B \in I \cup T_{\leq 1} \). This means \( B \) would be relatively identified by \( X \) which would contradict our assumption. On the other hand, if \((X_n)_{ID} \) is empty then there is actually no */+-arc in \( B \) and \( B \in R \subseteq (X_n)_{ID} \cup T_{\leq 1} \). This would contradict that \( X \rightarrow B \) is non-trivial. Hence \( B \not\in (X_n \cup B) \cup T_{\geq 1} - U_B^{X_n} \). In particular \( B \in U_B^{X_n} \) and therefore by construction \( T_1' \) and \( T_2' \) do not coincide on \( B \).

### 5.4 Elegantly Checking X\( iNF \)

According to Definition 5.3, in order to check whether an XML schema graph \( T \) is in \( X'iNF \) we need to examine all XFDs in \( \Sigma^* \) with a single \( r_T \)-walk on the right-hand-side. This is rather impractical because we must first compute \( \Sigma^* \), therefore we investigate a more elegant approach to check for \( X'iNF \).

Let \( \Sigma \) be a set of XFDs and let \( X^{\Sigma} = \bigcup \{ Y \mid X \rightarrow Y \in \Sigma \} \) denote the union of \( r_T \)-subgraphs specified in \( \Sigma \) to be functionally determined by \( X \). This allows us to restate the definition of \( X'iNF \) as follows: for every \( r_T \)-subgraph \( X \) such that there is an XFD \( X \rightarrow Y \in \Sigma^* \) and for every \( r_T \)-walk \( B \in X^{\Sigma^*} \) if \( X \rightarrow B \) is non-trivial then \( B \) is relatively identified by \( X \). In the next theorem, we show that in order to determine whether or not \( T \) is in \( X'iNF \), it is sufficient to examine all XFDs in \( \Sigma \). That is, we would need to check that for every \( r_T \)-subgraph \( X \) such that there is an XFD \( X \rightarrow Y \in \Sigma \), and for every \( r_T \)-walk \( B \in X^{\Sigma} \) if \( X \rightarrow B \) is non-trivial then \( B \) is relatively identified by \( X \).

We say an XFD \( X \rightarrow Y \in \Sigma \) causes \( T \) to violate \( X'iNF \) if there is an \( r_T \)-walk \( B \in Y \) such that \( X \rightarrow B \in \Sigma^* \) is non-trivial and \( B \) is not relatively identified by \( X \). Naturally, there is no XFD \( X \rightarrow Y \in \Sigma^* \) which causes \( T \) to violate \( X'iNF \) if and only if \( T \) is in \( X'iNF \) with respect to \( \Sigma \). Similarly, there is no XFD \( X \rightarrow Y \in \Sigma \) which causes \( T \) to violate \( X'iNF \) if and only if for every \( r_T \)-subgraph \( X \) such that there is an XFD \( X \rightarrow Y \in \Sigma \), and for every \( r_T \)-walk \( B \in X^{\Sigma} \) if \( X \rightarrow B \) is non-trivial then \( B \) is relatively identified by
X. This alternative characterisation of X"NF enables us to provide a simple proof for the next theorem.

**Theorem 5.4.** Let $T$ be an XML schema graph and $\Sigma$ a set of XFDs on $T$. $T$ is in $X"NF$ with respect to $\Sigma$ if and only if for every $r_T$-subgraph $X$ such that there is an XFD $X \rightarrow Y \in \Sigma$, and for every $r_T$-walk $B \in X^{\Sigma}$ if $X \rightarrow B$ is non-trivial then $B$ is relatively identified by $X$.

**Proof.** (Only If) Since $\Sigma \subseteq \Sigma^*$, it is easy to see that if no XFD in $\Sigma^*$ causes $T$ to violate X"NF, it must be the case that no XFD in $\Sigma$ causes $T$ to violate X"NF.

(If) We need to show that if no XFD in $\Sigma$ causes $T$ to violate X"NF then no XFD in $\Sigma^*$ causes $T$ to violate X"NF. Let there be a chain

$$\Sigma = \Sigma_0 \subset \Sigma_1 \subset \ldots \subset \Sigma_k = \Sigma^+_T = \Sigma^*$$

where $\Sigma_{i+1}$ results from $\Sigma_i$, $i \geq 0$ by a single application of one of the inference rules in the $T$-rule system. We will show that if there is an XFD $X \rightarrow Y \in \Sigma_{i+1}$ which causes $T$ to violate X"NF, then there is already some XFD in $\Sigma_i$ which causes $T$ to violate X"NF.

Assume that no XFD in $\Sigma_i$ causes $T$ to violate X"NF while some XFD in $\Sigma_{i+1}$ causes $T$ to violate X"NF. This means the single XFD $X \rightarrow Y \in \Sigma_{i+1} - \Sigma_i$ with $i \geq 0$ causes $T$ to violate X"NF. That is, there is an $r_T$-walk $B \in Y$ such that $X \rightarrow B$ is non-trivial and $B$ is not relatively identified by $X$. Since $X \rightarrow B$ is non-trivial $X \rightarrow Y$ must be non-trivial. Therefore $X \rightarrow Y$ has not been derived by means of the reflexivity axiom, root axiom or noname2 axiom in accordance with Proposition 5.1. We now consider the cases where $X \rightarrow Y$ has been derived by any of the remaining inference rules in the $T$-rule system.

Assume that $X \rightarrow Y$ has been derived by means of the union rule, i.e. $Y = W \cup Z$ and $X \rightarrow W, X \rightarrow Z \in \Sigma_i$. We have $B \in W$ or $B \in Z$. Due to the initial assumptions, if $B \in W$ then $X \rightarrow W \in \Sigma_i$ causes $T$ to violate X"NF. Similarly, if $B \in Z$ then $X \rightarrow Z \in \Sigma_i$ causes $T$ to violate X"NF.

Secondly assume that $X \rightarrow Y$ has been derived using the subtree rule, i.e. $Y \subseteq Y'$ and $X \rightarrow Y' \in \Sigma_i$. Since $Y \subseteq Y'$ and $B \in Y$, it follows that $B \in Y'$. Again the initial assumptions immediately mean $X \rightarrow Y' \in \Sigma_i$ causes $T$ to violate X"NF.

The remainder of the proof will utilise the following observation. Let $V$ and $W$ be two $r_T$-subgraphs in $T$. If $V \subseteq W$ then it follows from $V_{ID} \subseteq W_{ID}$ that $U_B^W \subseteq U_B^V$. Further, we have $(V \cup B) \cup T_{\geq 1} \subseteq (W \cup B) \cup T_{\geq 1}$ and thus $V_0 = ((V \cup B) \cup T_{\geq 1} - U_B^V) \cup V \subseteq ((W \cup B) \cup T_{\geq 1} - U_B^W) \cup W = W_0$. It immediately follows that $V^F_B \subseteq W^F_B$. 


Suppose $X \rightarrow Y$ has been derived using the supertree rule, i.e. $X' \subseteq X$ and $X' \rightarrow Y \in \Sigma_i$. Suppose $B$ is relatively identified by $X'$, that is, there is some identifier $I$ such that $I \in (X')^P_F$ and $B \in I \cup T_{\leq 1}$. The above observation yields $(X')^P_F \subseteq X^P_F$ from $X' \subseteq X$. Hence $I \in X^P_F$. This would mean $B$ is relatively identified by $X$, contradicting our assumption. Hence $B$ is not relatively identified by $X'$. But this means that $X' \rightarrow Y \in \Sigma_i$ causes $T$ to violate $X'\text{NF}$.

Next assume $X \rightarrow Y$ has been derived by means of the restricted-transitivity rule, i.e. $W$ is $X,Y$-compliant and $X \rightarrow W, W \rightarrow Y \in \Sigma_i$. Recall that $W$ being $X,Y$-compliant implies $W \subseteq (X \cup B) \cup T_{\geq 1}$. Together with $X \rightarrow W \in \Sigma_i$ we get $W \subseteq X_n$ where $X_n$ occurs in the sequence of restricted pre-closures used to compute $X^P_F$. The observation above gives $W^P_F \subseteq (X_n)^P_F = X^P_F$. Suppose $B$ is relatively identified by $W$. Then there is some identifier $I \in W^P_F$ such that $B \in I \cup T_{\leq 1}$. It follows that $I \in X^P_F$ and $B$ is relatively identified by $X$ which would be a contradiction. Hence $B$ is not relatively identified by $W$, in which case $W \rightarrow Y \in \Sigma_i$ causes $T$ to violate $X'\text{NF}$.

Finally, suppose that $X \rightarrow Y$ has been derived using the generalised noname rule, i.e. $X' = ((X \cup Y) \cup T_{\geq 1} - U^F_Y) \cup X$ with $Y = B$ being a single $r_r$-walk of $T$ and $X' \rightarrow Y \in \Sigma_i$. We have $X' = ((X \cup Y) \cup T_{\geq 1} - U^F_Y) \cup X = X_0$. In particular, $X' \subseteq X_0$ and therefore $(X')^P_F \subseteq (X_0)^P_F = X^P_F$. Suppose $B$ is relatively identified by $X'$, that is, there is some identifier $I \in (X')^P_F$ with $B \in I \cup T_{\leq 1}$. Consequently $I \in X^P_F$ and $B$ is relatively identified by $X$, a contradiction. Therefore $B$ is not relatively identified by $X'$. Then $X' \rightarrow Y \in \Sigma_i$ causes $T$ to violate $X'\text{NF}$.

Example 5.4. Recall that in Example 5.2 we observed that all XFDs in $\Sigma(PAYMENTID)$ apart from $P_XFD2$ contain only identifiers on the right-hand-side. Further, we saw that $\langle \text{IRD#} \rangle \rightarrow \langle \text{E.id} \rangle$ is derivable from $\Sigma(PAYMENTID)$. It is the case that $(\langle \text{IRD#} \rangle \cup \langle \text{empID} \rangle \cup PAYMENTID_{\leq 1})$ includes $\langle \text{E.id} \rangle$. Particularly, this means $\langle \text{E.id} \rangle$ will be in $(\langle \text{IRD#} \rangle)_{X,\text{empID}}$.

In fact, every non-trivial XFD in $\Sigma(PAYMENTID)$ each $r_{PAYMENTID}$-walk on the right-hand-side is relatively identified by the left-hand-side. Therefore we conclude that PAYMENTID is in $X'\text{NF}$ with respect to $\Sigma(PAYMENTID)$. This confirms the observation in Example 5.2 that PAYMENTID is non-redundant with respect to $\Sigma(PAYMENTID)$.

Example 5.5. We can also verify that BANKID is not in $X'\text{NF}$ with respect to $\Sigma(BANKID)$, i.e. supporting that BANKID is indeed redundant with respect to $\Sigma(BANKID)$ by Theorem 5.3.
5.5 “Redundancy” as a Design Quality

For a simple example, consider the non-trivial XFD

\[(B_{XFD6}) \quad \langle \text{bankName} \rangle \rightarrow \langle \text{bankNo} \rangle\]

From the sequence of restricted pre-closures, we obtain

\[\langle \text{bankName} \rangle_1 \langle \text{bankNo} \rangle = \langle \text{bankName} \; \text{bankNo} \rangle\]

There is no identifier at all, hence \(\langle \text{bankNo} \rangle\) is not relatively identified by \(\langle \text{bankName} \rangle\). So \(B_{XFD6}\) is witness that BANKID is not in \(X^\circ NF\) with respect to \(\Sigma(\text{BANKID})\).

As another example, consider the XFD

\[(B_{XFD12}) \quad \langle \text{bankName} \; \text{acctNo} \rangle \rightarrow \langle \text{brName} \; \text{acctName} \rangle\]

For convenience, we simply use \(X\) to refer to \(\langle \text{bankName} \; \text{acctNo} \rangle\). It is easy to verify that \(X \rightarrow \langle \text{brName} \rangle\) is non-trivial. The sequence of restricted pre-closures for \(X\) relative to \(\langle \text{brName} \rangle\) is as follows:

\[
\begin{align*}
X_0 &= X \\
X_1 &= X \cup \langle \text{brName} \; \text{acctName} \rangle \\
X_2 &= X \cup \langle \text{brName} \; \text{acctName} \; \text{branchNo} \rangle = X_3 = X_4 = \ldots & \text{by } B_{XFD10}
\end{align*}
\]

Again there is no identifier in \(X_n\) (where \(n = 2\)) therefore \(\langle \text{brName} \rangle\) is not relatively identified by \(\langle \text{bankName} \; \text{acctNo} \rangle\) and \(B_{XFD12}\) shows that BANKID is not in \(X^\circ NF\) with respect to \(\Sigma(\text{BANKID})\).

\[\square\]

5.5 “Redundancy” as a Design Quality

In our definition of redundancy, we have considered XFDs as representing a unit of information. In accordance with the same notion in the RDM, we have considered a piece of information to be redundant if it is inferable from other information stored in an XML data tree which satisfies the XFD representing the unit of information. However, this means we are only required to ensure that data corresponding to the right-hand-side of each dependency is not stored redundantly. The replication of data corresponding to the left-hand-side is ignored.
Example 5.6. Let us consider a simplified zip code system. Suppose we need to store data about the zip code of each location in New Zealand where the location details include the name of the city, suburb, and street. It happens that the street together with the zip code determines the city in which the street is located and the street together with the suburb determines the zip code. We can model this in various ways. Consider the two approaches presented in Figure 29 and Figure 30.

We can verify that ZIPA is in XMLNF with respect to $\Sigma(ZIPA)$ and ZIPB is in XMLNF with respect to $\Sigma(ZIPB)$. According to Theorem 5.3, this means that both schema trees are considered to be non-redundant with respect to their corresponding set of XFDs.

Observe that in each of the given XML data tree, there are three almost copies of the compatible schema tree with valuation of “Kent St” and “1001” for $\langle\text{street zip}\rangle$. In each case, the three almost copies coincide on $\langle\text{city}\rangle$ but do not coincide on $\langle\text{street zip}\rangle$. □
5.5 "Redundancy" as a Design Quality

\[ \Sigma(\text{ZipB}) \text{ consists of:} \]

- \((ZB.XFD1) \langle \text{street} \, \text{zip} \rangle \rightarrow \langle \text{city} \rangle\)
- \((ZB.XFD2) \langle \text{street} \, \text{suburb} \rangle \rightarrow \langle \text{zip} \rangle\)
- \((ZB.XFD3) \langle \text{city} \rangle \rightarrow \langle \text{CZC} \, \text{id} \rangle\)
- \((ZB.XFD4) \langle \text{street} \, \text{suburb} \, \text{zip} \rangle \rightarrow \langle \text{ZP} \, \text{id} \rangle\)

Figure 30: Another XML schema tree \(\text{ZIPB}\) for the zip code example, together with a set \(\Sigma(\text{ZIPB})\) of XFDs on \(\text{ZIPB}\) and a compatible XML data tree.

The above example suggests that the generalisation of non-redundancy in Definition 5.1 may be too weak. We can alternatively consider the following definition of redundancy:

Let \(T\) be an XML schema graph and \(\Sigma\) a set of XFDs on \(T\). We say that \(T\) is redundant with respect to \(\Sigma\) if and only if there is some XML data tree \(T' \triangleright T\) such that \(\models_{T'} \Sigma\) and for some non-trivial XFD \(X \rightarrow Y \in \Sigma\) with \(r_T\)-walk \(B \in Y - X\) there exist two almost copies \(T'_1, T'_2\) of \(T\) in \(T'\) with \(T'_1 \mid_{XB} = T'_2 \mid_{XB} \cong XB\) but \(T'_1\) and \(T'_2\) do not coincide on any \(r_T\)-walk of \(XB\).

However, there is one simple argument against using such a definition: if the information about the left-hand-side of an XFD is lost or missing, there is no way to derive this information from the rest/remaining information.

The main question that needs to be asked as a result of this discussion is how redundancy should be defined in the context of XML and whether non-redundancy should be an important quality aspect for the design of XML schemas.
6 Related Work

6.1 Relational Databases with Null Values

We refer the reader to [19] for a general introduction to relations with null values.

Work on functional dependencies in relational databases with null values dates back to as early as 1979, carried out by Lien [20]. This work was continued in [21]. Lien provides an axiomatisation for functional dependencies and an axiomatisation for multivalued dependencies in relational databases with null values. It is one of the earliest papers to remark that the transitivity rule is not sound in the presence of missing information.

The axiomatisation of Lien can also be found in [6] where it is generalised by Athena and Morfuni for functional dependencies in the presence of null values (NFDs) together with existence constraints (ECs) over flat relations. An existence constraint is an expression of the form \( e : X \vdash Y \) which is satisfied by a relation if each tuple \( t \) which is \( X \)-total (i.e. \( t[X] \) does not contain any null values) is also \( Y \)-total. Like frequencies, ECs offer a means to control the presence of missing values. In particular, ECs are required for defining a restricted form of the transitivity rule which is sound in the presence of null values. ECs may express some, but not all, frequencies and conversely frequencies may express some, but not all, ECs.

Consequently the discussion of NFDs with ECs in [6] has some similarities with the discussion in Section 3. The restricted-transitivity rule and restricted-pseudo-transitivity rule resembles the transitivity rule with ECs [6, pg.15] and the \( J_3 \) rule [6, pg.19] respectively. The sound and complete Athena-Morfuni rule system for NFDs and ECs (see Theorem 11 in [6, pg.20]) has some similarity with the \( \mathcal{F} \)-rule system.

However the Athena-Morfuni rule system also contains additional inference rules for the derivation of ECs which are not required for frequencies. More importantly, the \( \mathcal{F} \)-rule system contains two additional inference rules to the Athena-Morfuni rule system: the root axiom, and the noname rule. The root axiom exists due to the cardinality constraint of “at most once” specified by frequencies, while the noname rule arises from the nesting structure of data. There is no comparable feature in flat relations with nulls; this may explain the non-availability of rules similar to the root axiom and noname rule in the Athena-Morfuni rule system.
6.2 XML and Semistructured Databases

In this section, we identify more specifically related work focusing on functional dependencies in the context of XML or semistructured databases.

One of the first papers to address the issue of designing “good” XML schemas is [10] by Embley and Mok. The main purpose of the paper is the translation of arbitrary conceptual-model hypergraphs, used to express sets of integrity constraints, into scheme-tree forests.\(^2\) No notion of functional dependency is defined; instead the concept of functional constraints expressible by conceptual-model hypergraphs is considered. The paper includes a definition of a normal form called XNF. A scheme-tree forest is said to be in XNF if it does not contain “potential redundancy” and is as compact as possible in terms of the number of scheme trees. The notion of potential redundancy with respect to a functional constraint \(X \rightarrow Y\) checks whether each value assigned to an attribute in \(Y\) occurs exactly once in each scheme-tree instance, particularly we note that the definition disregards the values for \(X\). One significant limitation of this work by Embley and Mok is that it is difficult to verify syntactically whether a given XML schema can be considered as a “good” design.

In [12], a notion of path constraints was briefly mentioned. However, to the best of our knowledge, the first work to define a notion of functional dependencies for XML is Lee et al [16]. In this paper, functional dependencies for XML (called FD\(_{XML}\)) are defined over paths rooted at any element in an XML document. This is facilitated by including a “header path” within each FD\(_{XML}\) expression. The remaining part of an FD\(_{XML}\) is a functional constraint of the form \(P_{x_1}, \ldots, P_{x_n} \rightarrow P_y\) where each \(P_i\) must be a path to an element. Attributes can only be optionally included if they are key for the element to which they are attached. Lee et al also attempt to characterise “well-structured FD\(_{XML}\)”. One condition for an FD\(_{XML}\) being well-structured is that the header path, followed by each path in the left-hand-side of the FD\(_{XML}\) followed by the single path on the right-hand-side must form a path. This condition is based on earlier works on functional dependencies in semistructured databases including [17, 38]. A limitation of FD\(_{XML}\) being well-structured is that we are not able to express functional dependencies between subelements of different elements or functional dependencies where subelements determine an element in which they are nested. An example provided in [16] shows that for “flat XML data”, it is not meaningful to have well-structured FD\(_{XML}\). In particular, well-structured FD\(_{XML}\) is not a generalisation of the notion of functional dependencies in the RDM. Also well-structured FD\(_{XML}\) does not recognise some functional dependencies expressible over nested relations.

\(^2\)Embley and Mok later discuss how DTDs can be generated from scheme-tree forests in [11]
Overall, the discussions in [16] are quite informal.

One of the best-known research works on functional dependencies for XML is [2], a short version of the journal paper [4], by Arenas and Libkin. The focus of the paper is on how to design DTDs in order to avoid two “commonly present” problems in poor XML schema design, namely redundancy and update anomalies. Arenas and Libkin define the notions of functional dependencies in XML (which we will refer to as XML FDs) and their satisfaction using the concept of “tree tuple”, which is similar to the total unnesting of a nested relation. A normal form for XML (called XNF) is also introduced which is later shown to guarantee the absence of redundancy using an information theoretic approach [3]. In [2, 4] it is illustrated and formally shown that XNF is a generalisation of BCNF and the nested normal form NNF introduced by Mok et al in [26].

Among all the literature, XML FDs based on “tree tuples” are the most similar to subgraph-based XFDs from [14, 15]. In particular, the concept of “tree tuple” closely corresponds to the concept of almost copies of an XML schema graph, and both generalise a “no information” interpretation of null values from the RDM [5, Chapt. 6] for defining satisfaction of functional dependencies in XML. We refer the reader to [5] for definitions of strong and weak satisfaction of functional dependencies in relations with null values and various different interpretations of null values. The “no information” interpretation of null values is common for functional dependencies on relations with null values, for example in [6, 18, 20, 21].

One difference between the “tree tuple” approach and the subgraph-based approach is that the former requires the existence of DTDs while the latter does not. With DTDs, disjunction is permitted, which is not considered in the XML graph model. It should be noted that, in contrast to XFDs, XML FDs may include paths from the unique root vertex to any vertices, including internal vertices. One motivation for not considering such paths to internal vertices is that internal vertices do not have counterparts in the RDM. Instead identifier-attributes may be used to refer to particular vertices. This is more in line with original intentions of XML and provides more flexibility: identifier-attributes are specified if desired, but not compulsory. Overall, we expect that X'NF proposed in this thesis implies Arenas and Libkin’s XNF if identifier-attributes are compulsory.

No axiomatisation of XML FDs was given by Arenas and Libkin. However, some complexity results were given in [2, 4] about the implication problem for XML functional dependencies over various classes of DTDs. One important result is that XML functional dependencies cannot be finitely axiomatised. The finite axiomatisation of XFDs is one of the major results of this thesis. The provided proof in [4] suggests that arbitrary disjunction contributes to the XML functional dependencies not being finitely axiomatisable.
Recall that we do not consider disjunction. Our resolution of disjunction considers XML schemas which are similar to “simple” DTDs whereby every disjunctive expression can be rewritten as a simple regular expression containing no disjunction. The implication problem for functional dependencies over simple DTDs is shown to be solvable in quadratic time.

The normalisation strategy of Arenas and Libkin assumes a certain degree of non-missing information in order to ensure losslessness; any path which participates in an XML FD is assumed to be non-missing in the corresponding XML data tree. In [4], it is suggested that we can relax this assumption by converting a schema permitting missing information into a collection of subschemas identifying every possible data structure which may occur due to missing information. The XML FD then only applies to the subschema which is the same as the original schema. We remark that this approach may lead to exponential growth in the size of an XML schema which is hardly desirable. Another problem with the normalisation approach of Arenas and Libkin is that it is unlikely to result in an ideal data structure as the normalisation process usually generates very flat structures.

In the last two years, Vincent et al is another group in the research community who have investigated how to adapt functional dependencies for XML. Recent works include: [22, 28, 31, 33, 34, 35, 36]. The main focus of research has been directed towards the study of functional dependencies in XML which are strongly satisfied (called strong XFDs). A normal form is given which guarantees the absence of redundancy and also an axiomatisation of strong XFDs. The normal form with respect to strong XFDs (called XNF) proposed in these papers is a slight modification of the one introduced in [2, 4]. This alteration is required because of the mixed-content elements permitted by Vincent et al but ignored by Arenas and Libkin.

Similar to [2, 4], functional dependencies are defined in terms of paths to arbitrary vertices including internal vertices. But unlike Arenas and Libkin, no notion of frequencies is considered. A major distinguishing feature of works by Vincent et al is the concept of strong satisfaction. Similar to relations with null values, Vincent et al propose that we think of an XML tree with missing information as representing a collection of “complete” XML trees with non-missing information. An XML tree $T$ then strongly satisfies an XFD $\varphi$ if every complete XML trees represented by $T$ satisfy $\varphi$. Expressed in the framework of this thesis, an XML data tree containing at least one almost copy which is not a copy of the given XML schema graph is said to contain missing information. In particular, this implies that the “unknown” interpretation (values exist but not currently known) is used for information deemed to be missing. We remark that the “no information” interpretation is more general than the “unknown” interpretation as it also includes the
“does not exist” interpretation (values do not exist). Due to the flexibility of XML data structure, we argue that it is more natural to use the “no information” or “does not exist” interpretation of missing information.

Although the inference rules investigated by Vincent et al are shown to be sound for strong XFDs, they are only proven to be complete for strong XFDs with a single path on the left-hand-side (called unary XFDs). In contrast to the inference rules in Section 3 and Section 4, the inference rules proposed by Vincent et al are not easily compared to inference rules for functional dependencies in the RDM. We also highlight that the transitivity rule is sound for strong XFDs but not sound for XFDs discussed in this thesis.

In [22], Vincent et al have also studied primary XFDs (only paths to leaves) which is similar to subgraph-based XFDs without identifiers and frequencies. In [22], the focus is placed on the issue of designing XML documents. An analogy of transitive dependencies and partial dependencies is generalised from the RDM for primary XFDs. It is suggested that the presence of transitive and partial dependencies leads to redundancy and therefore should be eliminated/avoided. The paper illustrated this with an example but provides no formal justification. Vincent et al have also introduced a new notion of functional dependencies called “local XFDs” [23], and give a possible generalisation of the notion of multivalued dependencies and defined a normal form with respect to these multivalued dependencies in [29, 30, 32].

Finally there is the subgraph-based approach to functional dependencies for XML [14, 15] on which we have based the work of this thesis. [15] includes a sound and complete rule system for XFDs on XML schema graphs with no frequencies and no identifiers and also suggests what inference rules should constitute an axiomatisation of XFDs with frequencies and XFDs with identifiers. In contrast to this thesis, leaves in [14, 15] may be of kind $E$. An important contribution of [14, 15] is to provide a framework in which various notions of functional dependencies in XML can be defined and studied.
7 Conclusion

In this thesis, we have studied a subgraph-based approach toward functional dependencies for XML, which we have referred to as XFDs. We have utilised the definition of XFDs for the XML graph model introduced in [14, 15].

The first main result of the research is an axiomatisation for XFDs in the presence of frequencies and also an axiomatisation for XFDs in the presence of frequencies and identifiers. In the presence of frequencies, we have presented a sound and complete rule system, denoted the $\mathcal{F}$-rule system, which includes the reflexivity axiom, subtree rule, supertree rule, union rule, restricted-transitivity rule and noname rule. In the presence of identifiers, we have generalised the noname rule and added a new noname2 axiom to obtain a sound and complete rule system denoted as the $\mathcal{I}$-rule system.

In discussing a completeness proof for the $\mathcal{F}$-rule system, we have observed that there may exist XFDs which are not implied in general but may be satisfied due to the non-trivial interaction between the XML schema and the XFDs. This has necessitated the consideration of a sequence of pre-closures in addition to a simple analogy of an attribute closure in the RDM.

We have also discussed alternative sound and complete rule systems for implication of XFDs in the presence of frequencies by showing that certain sets of inference rules are equivalent. The notion of Armstrong relation has also been generalised for XML data trees and with a simple proof we have shown that XFDs in the presence of frequencies do not enjoy Armstrong XML data trees.

For the second part of our investigation, we have defined a notion of redundancy in the context of XML, and have devised a normal form called $X^\lceil\text{NF}$ which guarantees non-redundancy. In the definition of redundancy, we have considered an XFD to be representing a unit of information. An XML schema graph is then said to contain redundancy with respect to some XFD $X \rightarrow Y$ if it contains two distinguishable non-empty almost copies of $Y$, with the copies of $X$ attached to each almost copy of $Y$ being equivalent. $X^\lceil\text{NF}$ makes use of identifiers to guarantee that this cannot occur. We have also discussed a more elegant approach to verifying whether an XML schema graph is in $X^\lceil\text{NF}$. Similar to the RDM, it is sufficient to examine XFDs in a given set of XFDs, rather than all implications of the given set of XFDs.
7 CONCLUSION

7.1 Future Work

There are many other areas of research which still need to be investigated to proceed towards developing a theory for the design of XML schemas.

The implication problem in the context of XML relates to the ability to decide whether an XFD $X \rightarrow Y$ is implied by a given set $\Sigma$ of XFDs. In our framework, due to Theorem 3.5 and Theorem 4.3, this is equivalent to deciding whether $Y \in X^+_R$ where $\mathcal{R}$ is either the $\mathcal{F}$-rule system or the $\mathcal{I}$-rule system. Using the inference rules to compute the set of all derivable XFDs is quite impractical. Therefore, it is necessary to develop a simple algorithm for generating $X^+_R$ for an arbitrary schema graph $T$, an arbitrary set $\Sigma$ of XFDs and an arbitrary $r_T$-subgraph $X$ in $T$. The study of the related work suggests that an initial algorithm may be derivable from algorithms in [6] since many inference rules in this thesis can be easily mapped to rules in [6].

In this thesis, we have proposed a normal form in the presence of frequencies and identifiers. In particular, redundancy is prevented by the uniqueness property of identifiers. Another direction of research is to investigate a normal form for XML schemas in the absence of identifiers. This may involve generalising the notion of multivalued dependencies to the context of XML and examining existing normal forms for nested relations.

In Section 5.5 we have suggested that one important area still to be addressed is the formal characterisation of properties of “bad” XML schema design. Up to now, it has been assumed that, similar to the RDM, redundancy and update anomalies are two important quality aspects of XML schemas. However, apart from [33] there has been no formal definition of any update anomalies in the context of XML, and little to no formal definition of redundancy can be found in the literature. It is vital in the study of how to design “good” XML schema that we are able to identify “good” schemas. It is important to investigate whether redundancy and update anomalies carry the same importance for XML as they did for the RDM, and also to identify other potentially desirable properties for XML data which may not exist for the RDM.

In this thesis, we have not considered how to transform an XML schema which violates X'NF into one that does not. We have left this for future research. It is likely that the normalisation approach introduced by Arenas and Libkin [2, 4] can be translated to the framework in this thesis. Another area for future research is the study of XFDs in the presence of references. References may be used to ensure losslessness during normalisation, for minimising redundancy when designing XML schemas and for increasing the expressiveness of XFDs.
With respect to functional dependencies, it is also possible to investigate other notions of functional dependencies, such as XFDs based on the notion of pre-image and XFDs containing disjunctions. As with the RDM, different classes of dependencies interact with one another. Currently no research has been directed towards studying the interaction among different notions of dependencies. Another possible research direction is to study XFDs under different assumptions. For example, also to consider disjunction and recursion in XML schemas, permit mixed-content data and consider document order of XML elements.
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