

XML SCHEMA REFINEMENT THROUGH FORMAL CONCEPT ANALYSIS

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ABSTRACT. As XML becomes a popular data representation and exchange format over the web, XML schema design has become an important research area. Formal Concept Analysis (FCA) has been widely applied in many fields recently. In this paper, we propose the application of FCA to find functional dependencies (FDs) in XML databases. Our work is based on the definitions of the Generalized Tree Tuple, XML functional dependency and XML key notion presented by [22]. We propose a framework which parses the XML document and constructs the Formal Context corresponding to the flat representation of the XML data. The obtained Conceptual Lattice is a useful graphical representation of the analyzed XML document's elements and their hierarchy. The software also finds the keys and functional dependencies in XML data, which are attribute implications in the constructed Formal Context. The scheme of the XML document is transformed in GTT-XNF using the detected functional dependencies.

Keywords and phrases: XML design, Formal Concept Analysis, XML Functional Dependency, XML Normal Forms.

1. INTRODUCTION

In the last few years several papers discussed the relationship between Formal Concept Analysis (FCA) and relational databases [8, 10]. Our approach intends to extend these results by reformulating the XML functional dependency inference with an FCA viewpoint.

FCA is a mathematical theory of concept hierarchies which is based on Lattice Theory. It is used as a technique for data analysis, knowledge representation; it is a useful tool to represent knowledge contained in a database.

Designing XML data means to choose an appropriate XML schema, which usually come in the form of DTD (Document Type Definition) or XML Scheme. A big number of classical database subjects have been reexamined in the XML

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context [7, 1, 18, 17, 3] because XML became more and more popular. Discovering XML data redundancies from the data itself becomes necessary and it is an integral part of the schema refinement (or re-design) process.

Recently, there were several attempts to define XFDs (see [6, 16, 9, 19]) but in general, these approaches have different semantics regarding the *tree tuple* and *closest node* XFDs and do not preserve the semantics of FDs when relational data is mapped to XML via arbitrary nesting.

Functional dependencies (FDs) are a key factor in XML design. Our paper proposes a framework to mine FDs from an XML database; it is based on the notions of Generalized Tree Tuple, XML functional dependency and XML key notion presented by [22]. Our contribution is the construction of the formal context for a tuple class or the whole XML document. Non-leaf and leaf level elements (or attributes) and corresponding values are inserted in the formal context, then the concept lattice of the XML data is constructed too. The obtained Conceptual Lattice is a useful graphical representation of the analyzed XML document's elements and their hierarchy. The software also finds the keys in the XML document. The set of implications resulted from this concept lattice will be equivalent to the set of functional dependencies that hold in that database.

This paper is an extended version of the short conference paper that appears as [12]. The key additions to this journal paper are Section 2, which discusses related work, Section 3 presents the necessary definitions of Functional dependency for XML data and GTT-XNF normal form. In Section 4 it is explained in detail how these two techniques are combined to mine functional dependencies. As a novelty of this article is the transformation of a given XML Scheme to a scheme in GTT-XNF form. Finally, Section 5 summarizes the conclusions and future work.

2. RELATED WORK

The first authors who presented the problem of finding functional dependencies in many-valued context were Ganter and Wille [8]. Different authors [14, 15] use FCA concepts and methods like agree sets, maximal sets and closed sets, which are closely related to the concept of closed sets and generators, described previously, to avoiding the transformation of the original database. The authors use these concepts to find efficient algorithms to extract functional dependencies from a relational database. [4] studied the lattice characterization and its properties for Armstrong and symmetric dependencies. Hereth has already described the relationship between FCA and functional dependencies in [10], he has introduced the formal context of functional dependencies. In this context, implications hold for functional dependencies. The paper [11]

presents an FCA based approach to detect functional dependencies in a relational database table.

The first authors who formally defined XML FD and normal form (XNF) were Arenas and Libkin introducing the so-called *tree tuple* approach [1]. In [13] and [18], the authors used a *path-based* approach and built their XML FD notion in a way similar to the XML Key notion proposed in [5].

Yu and Jagadish [22] show, that these XML FD notions are insufficient and propose a Generalized Tree Tuple (GTT) based XML functional dependency and key notion, which include particular redundancies involving set elements. Based on these concepts, the GTT-XNF normal form is presented too.

In later work [2], Arenas and Libkin provided a formal justification for the use of XNF in XML database design, using the classical information theory approach. A measure of the information content of data (independent of updates and queries) is introduced, as entropy of a suitably chosen probability distribution. A formal definition of a well designed XML schema was given and the fact that XNF is both a necessary and sufficient condition for an XML schema to be well designed was proved.

Vincent et al. in [17] investigated the problem of justifying XML normal forms [18], in the terms of *closest node* XFDs using redundancy elimination. In [17], a normal form for XML documents is proposed and it has been proved to be a necessary and sufficient condition for the elimination of redundancy.

3. FUNCTIONAL DEPENDENCY FOR XML DATA

Arenas and Libkin introduced first the so-called *tree tuple* notion in [1], they have defined functional dependency in XML data and XNF normal form for XML. Redundancies in XML data have several distinct features due to the heterogeneous nature of XML data, which makes them richer in semantics as compared with redundancies in relational data. Yu and Jagadish [22] show, that the XML FD notion introduced by [1] doesn't include all possible features of an XML document and propose a Generalized Tree Tuple (GTT) based XML functional dependency and XML key notion, which include particular redundancies involving set elements. They propose the GTT-XNF normal form too based on these notions. As [22] we treat leaf level elements and attributes in the same manner. The definitions of this section are based on [22].

Definition 1. (Schema) *A schema is defined as a set $S = (E, T, r)$, where:*

- *E is a finite set of element labels;*
- *T is a finite set of element types, and each $e \in E$ is associated with a $\tau \in T$, written as $(e : \tau)$, τ has the next form:*
 $\tau ::= \text{str} \mid \text{int} \mid \text{float} \mid \text{SetOf } \tau \mid \text{Rcd}[e_1 : \tau_1, \dots, e_n : \tau_n];$

- $r \in E$ is the label of the root element, whose associated element type can not be `SetOf` τ .

This definition contains some basic constructs in XML Scheme [20]. There are a lot of other datatypes defined at [20], but it is not relevant for our problem to enumerate them. Types `str`, `int` and `float` are the system defined *simple types* and `Rcd` indicate *complex scheme elements* (elements with children elements). Keyword `SetOf` is used to indicate *set schema elements* (elements that can have multiple matching data elements sharing the same parent in the data). We will treat attributes and elements in the same way, with a reserved "@" symbol before attributes.

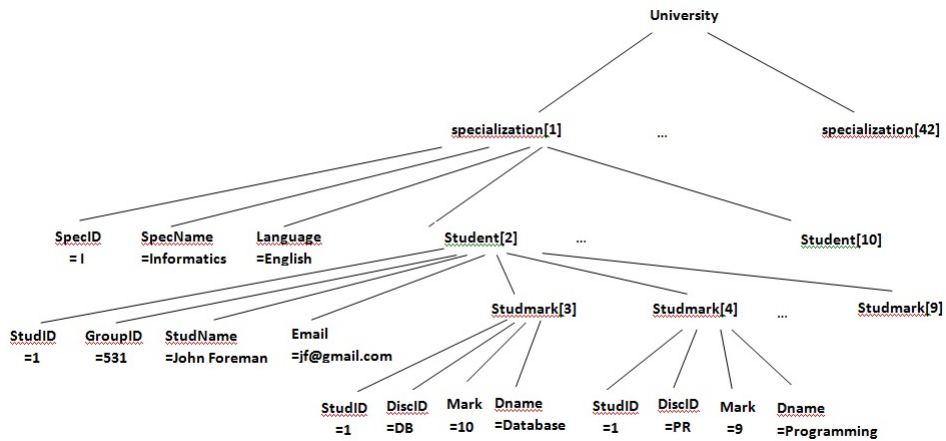


FIGURE 1. Example tree

The examples of this paper are based on XML tree of Figure 1.

Example 1. The scheme $S_{University}$ of XML document from Figure 1 is:

```

University:Rcd
  specialization:SetOf Rcd
    SpecID: str
    SpecName: str
    Language: str
    Student: SetOf Rcd
      StudID: int
      GroupID: str
      StudName: str
      Email:str

```

```

Studmark: SetOf Rcd
  StudID: int
  DiscID: str
  Mark: int
  DName: str

```

A schema element e_k can be identified through a path expression, $path(e_k) = /e_1/e_2/.../e_k$, where $e_1 = r$, and e_i is associated with type $\tau_i ::= \text{Rcd} [\dots, e_{i+1} : \tau_{i+1}, \dots]$ for all $i \in [1, k - 1]$. A path is *repeatable*, if e_k is a set element. We adopt XPath steps "." (self) and ".." (parent) to form a relative path given an anchor path.

Definition 2. (Data tree) *An XML database is defined to be a rooted labeled tree $T = \langle N, \mathcal{P}, \mathcal{V}, n_r \rangle$, where:*

- N is a set of labeled data nodes, each $n \in N$ has a label e and a node key that uniquely identifies it in T ;
- $n_r \in N$ is the root node;
- \mathcal{P} is a set of parent-child edges, there is exactly one $p = (n', n)$ in \mathcal{P} for each $n \in N$ (except n_r), where $n' \in N, n \neq n', n'$ is called the parent node, n is called the child node;
- \mathcal{V} is a set of value assignments, there is exactly one $v = (n, s)$ in \mathcal{V} for each leaf node $n \in N$, where s is a value of simple type.

We assign a node key, referred to as @key, to each data node in the data tree in a pre-order traversal. A data element n_k is a descendant of another data element n_1 if there exists a series of data elements n_i , such that $(n_i, n_{i+1}) \in \mathcal{P}$ for all $i \in [1, k - 1]$. Data element n_k can be addressed using a path expression, $path(n_k) = /e_1/.../e_k$, where e_i is the label of n_i for each $i \in [1, k]$, $n_1 = n_r$, and $(n_i, n_{i+1}) \in \mathcal{P}$ for all $i \in [1, k - 1]$.

A data element n_k is called *repeatable* if e_k corresponds to a set element in the schema. Element n_k is called a *direct descendant* of element n_a , if n_k is a descendant of n_a , $path(n_k) = \dots/e_a/e_1/.../e_{k-1}/e_k$, and e_i is not a set element for any $i \in [1, k - 1]$.

In considering data redundancy, it is important to determine the equality between the "values" associated with two data elements, instead of comparing their "identities" which is represented by @key. So, we have:

Definition 3. (Element-value equality) *Two data elements n_1 of $T_1 = \langle N_1, \mathcal{P}_1, \mathcal{V}_1, n_{r1} \rangle$ and n_2 of $T_2 = \langle N_2, \mathcal{P}_2, \mathcal{V}_2, n_{r2} \rangle$ are element-value equal (written as $n_1 =_{ev} n_2$) if and only if:*

- n_1 and n_2 both exist and have the same label;

- There exists a set M , such that for every pair $(n'_1, n'_2) \in M$, $n'_1 =_{ev} n'_2$, where n'_1, n'_2 are children elements of n_1, n_2 , respectively. Every child element of n_1 or n_2 appears in exactly one pair in M .
- $(n_1, s) \in \mathcal{V}_1$ if and only if $(n_2, s) \in \mathcal{V}_2$, where s is a simple value.

Definition 4. (Path-value equality) Two data element paths p_1 on $T_1 = \langle N_1, \mathcal{P}_1, \mathcal{V}_1, n_{r1} \rangle$ and p_2 on $T_2 = \langle N_2, \mathcal{P}_2, \mathcal{V}_2, n_{r2} \rangle$ are path-value equal (written as $T_1.p_1 =_{pv} T_2.p_2$) if and only if there is a set M' of matching pairs where

- For each pair $m' = (n_1, n_2)$ in M' , $n_1 \in N_1$, $n_2 \in N_2$, $path(n_1) = p_1$, $path(n_2) = p_2$, and $n_1 =_{ev} n_2$;
- All data elements with path p_1 in T_1 and path p_2 in T_2 participate in M' , and each such data element participates in only one such pair.

The definition of functional dependency in XML data needs the definition of so called Generalized Tree Tuple.

Definition 5. (Generalized tree tuple) A generalized tree tuple of data tree $T = \langle N, \mathcal{P}, \mathcal{V}, n_r \rangle$, with regard to a particular data element n_p (called pivot node), is a tree $t_{n_p}^T = \langle N^t, \mathcal{P}^t, \mathcal{V}^t, n_r \rangle$, where:

- $N^t \subseteq N$ is the set of nodes, $n_p \in N^t$;
- $\mathcal{P}^t \subseteq \mathcal{P}$ is the set of parent-child edges;
- $\mathcal{V}^t \subseteq \mathcal{V}$ is the set of value assignments;
- n_r is the same root node in both $t_{n_p}^T$ and T ;
- $n \in N^t$ if and only if: 1) n is a descendant or ancestor of n_p in T , or 2) n is a non-repeatable direct descendant of an ancestor of n_p in T ;
- $(n_1, n_2) \in \mathcal{P}^t$ if and only if $n_1 \in N^t$, $n_2 \in N^t$, $(n_1, n_2) \in \mathcal{P}$;
- $(n, s) \in \mathcal{V}^t$ if and only if $n \in N^t$, $(n, s) \in \mathcal{V}$.

A generalized tree tuple is a data tree projected from the original data tree. It has an extra parameter called a pivot node. In contrast with tree tuple defined in [1], which separate sibling nodes with the same path at all hierarchy levels, the generalized tree tuple separate sibling nodes with the same path above the pivot node. See an example generalized tree tuple of tree from Figure 1 in Figure 2. Based on the pivot node, generalized tree tuples can be categorized into tuple classes:

Definition 6. (Tuple class) A tuple class C_p^T of the data tree T is the set of all generalized tree tuples t_n^T , where $path(n) = p$. Path p is called the pivot path.

Definition 7. (XML FD) An XML FD is a triple $\langle C_p, LHS, RHS \rangle$, written as $LHS \rightarrow RHS$ w.r.t. C_p , where C_p denotes a tuple class, LHS is a set of paths $(P_i, i = [1, n])$ relative to p , and RHS is a single path (P_r) relative to p .

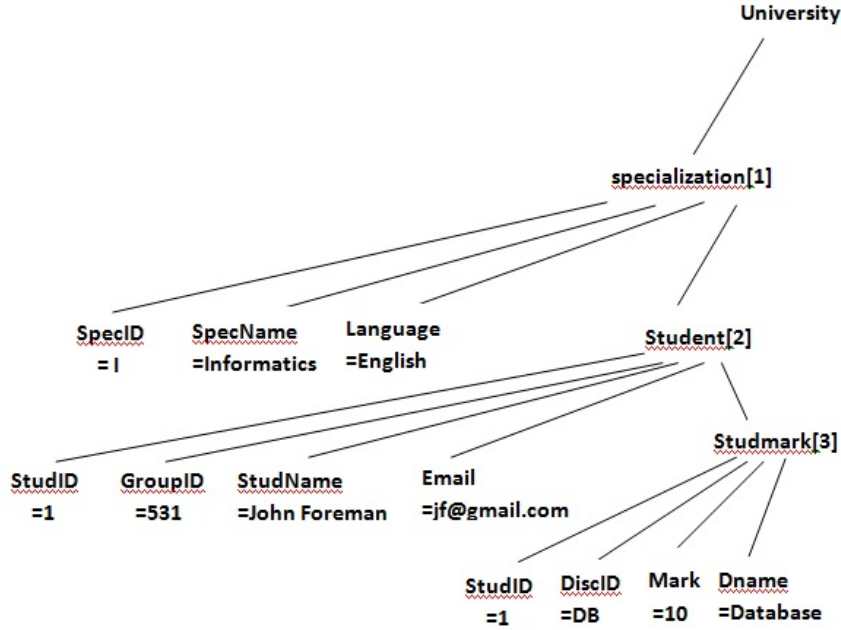


FIGURE 2. Example tree tuple

An XML FD holds on a data tree T (or T satisfies an XML FD) if and only if for any two generalized tree tuples $t_1, t_2 \in C_p$

- $\exists i \in [1, n]$, $t_1.P_i = \perp$ or $t_2.P_i = \perp$, or

- If $\forall i \in [1, n]$, $t_1.P_i =_{pv} t_2.P_i$, then $t_1.P_r \neq \perp, t_2.P_r \neq \perp, t_1.P_r =_{pv} t_2.P_r$.

A null value, \perp , results from a path that matches no node in the tuple, and $=_{pv}$ is the path-value equality defined in Definition 4.

Example 2. (XML FD) In our running example whenever two disciplines agree on *DiscID* values, they have the same *DName*. This can be formulated as follows:

$$./DiscID \rightarrow ./DName \text{ w.r.t } C_{Studmark}$$

Another example is:

$$./Student/GroupID \rightarrow ./SpecID \text{ w.r.t } C_{specialization}$$

In our approach we find the XML keys of a given XML document, so we need the next definition:

Definition 8. (XML key) An XML Key of a data tree T is a pair $\langle C_p, LHS \rangle$, where T satisfies the XML FD $\langle C_p, LHS, ./@key \rangle$.

Example 3. We have the XML FD: $\langle C_{Student}, ./StudentID, ./Student@key \rangle$, which implies that $\langle C_{Student}, ./StudentID \rangle$ is an XML key.

Tuple classes with repeatable pivot paths are called *essential tuple classes*.

Definition 9. (Interesting XML FD) *An XML FD $\langle C_p, LHS, RHS \rangle$ is interesting if it satisfies the following conditions:*

- $RHS \notin LHS$;
- C_p is an essential tuple class;
- RHS matches to descendent(s) of the pivot node.

Definition 10. (XML data redundancy) *A data tree T contains a redundancy if and only if T satisfies an interesting XML FD $\langle C_p, LHS, RHS \rangle$, but does not satisfy the XML Key $\langle C_p, LHS \rangle$.*

4. OVERVIEW OF THE APPROACH

In this section we describe the methodology of a general approach to use FCA to build tools that identify functional dependencies in XML documents. To achieve this, as a first step, we need to define the objects and attributes of interest and create models of XML in terms of FCA context. Our approach is carried out by a sequence of processing steps. The output of each step provides the input to the next step. Every step is illustrated with an example. Our method is supported by a framework named FCAMineXFD. We will now describe each processing step in detail.

4.1. Constructing the Formal Context, the Input to FCA. In this step the most important issue is how to map the XML document to metamodel entities. Our software can analyze the whole XML document or a *tuple class* C_p given by the path p . Tuple-based XML FD notion proposed in the above section suggests a natural technique for XFD discovery. XML data can be converted into a fully unnested relation, a single relational table, and apply existing FD discovery algorithms directly. Given an XML document, which contains at the beginning the schema of the data, we create generalized tree tuples from it.

Each tree tuple in a tuple class has the same structure, so it has the same number of elements. We use the flat representation which converts the generalized tree tuples into a flat table. Each row in the table corresponds to a tree tuple in the XML tree. In the flat table there are non-leaf and leaf level elements (or attributes) introduced from the tree.

For non-leaf level nodes the associated keys (see Section 3) are used as values.

Applying our experience in detecting functional dependencies in relational databases (see more details in [11]), we use the definitions introduced by

Hereth in [10]. Hereth gives the translation from the relational database into a power context family and based on it he defines the formal context of functional dependencies as follows:

Definition 11. Let $\vec{\mathbb{K}}$ be a power context family, and let $m \in M_k$ be an attribute of the k -th context. Then, the formal context of functional dependencies of m with regard to $\vec{\mathbb{K}}$ is defined as $FD(m, \vec{\mathbb{K}}) := (m^{I_k} \times m^{I_k}, \{1, 2, \dots, k\}, J)$ with $((g, h), i) \in J : \Leftrightarrow \pi_i(g) = \pi_i(h)$ with $g, h \in m^{I_k}$ and $i \in \{1, 2, \dots, k\}$.

The π is the relational algebra projection operation. In the next paragraph we will see how we construct this formal context of functional dependencies.

In this step the formal context of functional dependencies for XML data is built, mapping from metamodel entities to FCA objects and attributes.

- Choice of FCA Attributes: *PathEnd/ElementName*

Due to space considerations we will not specify the whole path to the element (or attribute) names, only the end of the path. FCA attribute names are built from the end of the path to the element: *PathEnd* and element name as follows:

- for non-leaf level nodes the name of the attribute is constructed as: `<ElementName>+”@key”` and its value will be the associated key value as specified in Section 3. More elements, which have the same path, will have the same attribute name, but the values will be different.
- the leaves (actually not the values of the leaves, but the element names of the leaves) of the tree tuple.
- Choice of Objects: the objects are considered to be the tree tuple pairs, actually the tuple pairs of the flat table. The key values associated to non-leaf elements and leaf element’s values are used in these tuple pairs.
- Choice of Properties: the mapping between objects and attributes is defined by a binary relation, this incidence relation of the context shows which attributes of this tuple pairs have the same value.

The analyzed XML document may have a large number of tree tuples. Creating the tree tuple pairs, our context table may have a very large number of rows, therefore, we need to clear the concepts of irrelevant entities. We filter the tuple pairs and we leave out those pairs in which there are no common attributes, by an operation called ”clarifying the context”, which does not alter the conceptual hierarchy.

Example 4. The beginning of the formal context of our running example for tuple class $C_{specialization}$ can be seen in Figure 3. There are only a few

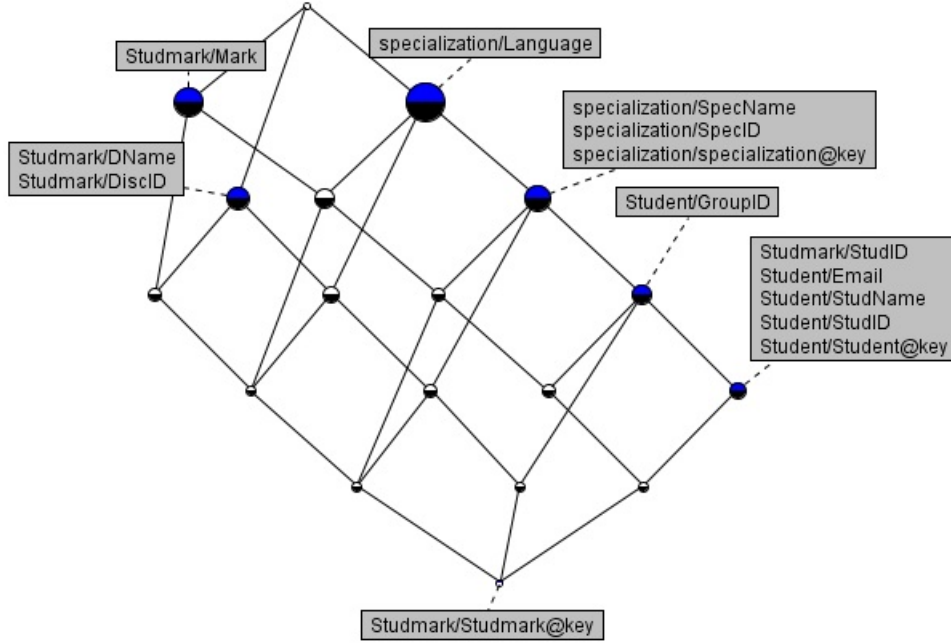


FIGURE 4. Concept Lattice of functional dependencies' Formal Context for tuple class $C_{specialization}$

$StudID$, $Student/StudName$, $Student/Student@key$, $Student/Email$ implies concept with label $Student/GroupID$.

4.4. Mining XFDs according to the concept hierarchy. In this step, we examine the candidate concepts resulting from the previous steps and use them to explore XFDs. Once the lattice is constructed, we can interpret each concept and generate the list of all functional dependencies.

The relationship between FDs in databases and implications in FCA was pointed out in [8]: a FD $X \rightarrow Y$ holds in a relation r over R iff the implication $X \rightarrow Y$ holds in the context (G, R, I) where $G = \{(t_1, t_2) | t_1, t_2 \in r, t_1 \neq t_2\}$ and $\forall A \in R, (t_1, t_2)IA \Leftrightarrow t_1[A] = t_2[A]$.

This means that objects of the context are couples of tuples and each object intent is the agree set of this couple. Thus, the implications in this lattice corresponds to functional dependencies in XML.

Example 7. Analyzing the Conceptual Lattice obtained for tuple class $C_{Student}$ (Figure 4) we can detect functional dependencies like:

$$\langle C_{Student}, ./StudID, ./GroupID \rangle$$

$$\langle C_{Student}, ./Student@key, ./GroupID \rangle$$

$$\langle C_{Student}, ./StudName, ./GroupID \rangle$$

$$\langle C_{Student}, ./Email, ./GroupID \rangle$$

In the lattice we list only the attributes, these are relevant for our analysis. Let there be a concept, labeled by A, B and a second concept labeled by C . A, B and C are FCA attributes. Let concept labeled by A, B be the subconcept of concept labeled by C . Therefore tuple pairs of concept labeled by A, B have the same values for attributes A, B , but for attribute C too. Tuple pairs of concept labeled by C do not have the same values for attribute A , nor for B , but have the same value for attribute C . Tuple pairs of every subconcept of concept labeled by A, B have the same values for attributes A, B . The labeling of the lattice is simplified by putting each attribute only once, at the highest level. We analyze attributes A and B . If we have only $A \rightarrow B$, then A would be a subconcept of B . If only $B \rightarrow A$ holds then B should be a subconcept of A . We have $A \rightarrow B$ and $B \rightarrow A$, that's why they come side by side in the lattice. So attributes from a concept imply each other.

Example 8. In concept node with label *specialization/specialization@key, specialization/SpecID, specialization/SpecName* the associated objects are tree tuple pairs, where the values for *specialization/SpecID* are the same. So we have the next XML FDs:

$$\langle C_{specialization}, ./SpecID, ./SpecName \rangle$$

$$\langle C_{specialization}, ./SpecID, ./specialization@key \rangle$$

$$\langle C_{specialization}, ./specialization@key, ./SpecID \rangle$$

$$\langle C_{specialization}, ./specialization@key, ./SpecName \rangle$$

$$\langle C_{specialization}, ./SpecName, ./specialization@key \rangle$$

$$\langle C_{specialization}, ./SpecName, ./SpecID \rangle$$

Software FCAMineXFD found many functional dependencies. A part of these XML FD-s are in Figure 5.

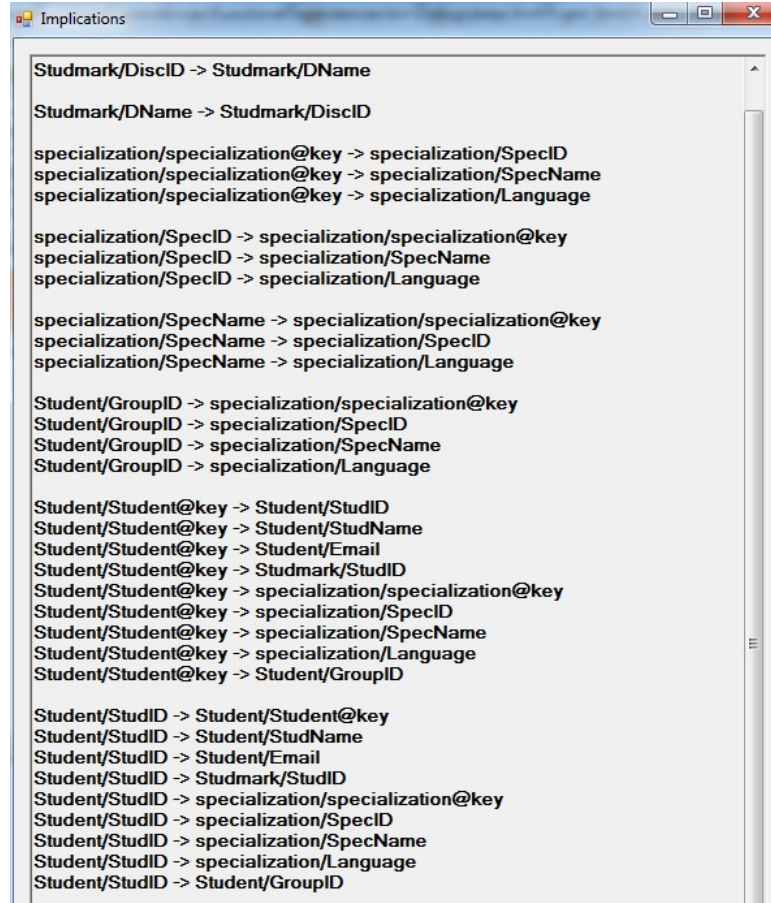


FIGURE 5. Some of the functional dependencies in tuple class $C_{specialization}$

Example 9. In the concept lattice for the XML document of Example 1 we can see the hierarchy of the analyzed data. The node labeled by *specialization/Language* is on a higher level, than node labeled by *specialization/SpecName*. The *specialization* node with three attributes is a subconcept of node labeled *specialization/Language*. The *Student* node in XML is child of *specialization* node. In the lattice, the node labeled with the key of Student, is subconcept of *specialization* node, so the hierarchy is visible. These are 1:n relationships, from *Specialization* to *Group*, from *Group* to *Students*, from *Students* to *Studmark*.

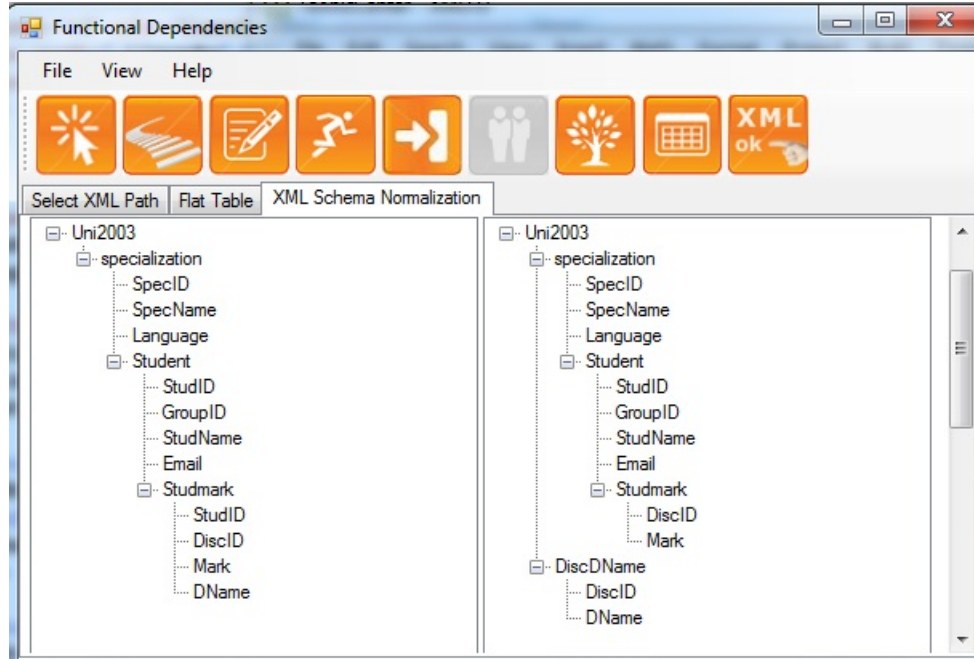


FIGURE 6. The proposed new scheme of University XML data

The information about *Disciplines* is on the other side of the lattice. *Disciplines* are in n:m relationship with *Students*, linked by *Studmark* node in this case.

Therefore, we say that FCA can serve as a guideline for dependency mining.

4.5. Finding XML keys. The implications found by FCAMineXFD contain some FDs with RHS as $./@key$ values. These can be used to detect the keys in XML.

Example 10. In tuple class $C_{Student}$ we have XML FD: $\langle C_{Student}, ./StudentID, ./Student@key \rangle$, which implies that $\langle C_{Student}, ./StudentID \rangle$ is an XML key.

Example 11. Let us look at XML FD-s of Example 8. There are two FDs with RHS as $./specialization@key$ in tuple class $C_{specialization}$, so the detected XML keys are: $\langle C_{specialization}, ./SpecID \rangle$, $\langle C_{specialization}, ./SpecName \rangle$.

4.6. Detecting XML data redundancy. Having the set of functional dependencies for XML data in a tuple class, we can detect interesting functional dependencies. In essential tuple class $C_{Studmark}$, the XML FD $\langle C_{Studmark},$

$\langle ./DiscID, ./DName \rangle$ found by the software in Figure 5 is an interesting FD, but $\langle C_{Studmark}, ./DiscID \rangle$ is not an XML key. So it is a data redundancy.

The same reason applies for XML FD $\langle C_{Studmark}, ./DName, ./DiscID \rangle$.

4.7. Normalization. Given the set of dependencies discovered by our tool, we adopt the normalization algorithm of [22] to convert one XML schema into a correct one. See the resulting scheme in Figure 6.

5. CONCLUSION AND FUTURE WORK

This paper introduces an approach for mining functional dependencies in XML documents based on FCA. We proposed a framework to analyze XML documents using Concept Analysis. Based on the flat representation of XML, we constructed the concept lattice. We analyzed the resulted concepts, which allowed us to discover a number of interesting dependencies. Our framework offers an interactive visualization for dependency exploration. Taking in consideration our preliminary results, we believe that FCA is a promising technique in XML database design too. We had also previously used FCA to explore functional dependencies in relational databases, see more details in [11]. In this paper, we complemented the information with XML design exploration.

Given the set of dependencies discovered by our tool, we propose a correct XML schema. We have started to use our approach on several case studies. We plan to develop our own FCA tool because Conexp is limited w.r.t. number of rows in the formal context.

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