Information preserving XML schema embedding

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Information Preserving XML
Schema Embedding

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A fundamental concern of data integration in an XML context is the ability to embed one or more source documents in a target document so that (a) the target document conforms to a target schema and (b) the information in the source documents is preserved. In this paper, information preservation for XML is formally studied, and the results of this study guide the definition of a novel notion of schema embedding between two XML DTD schemas represented as graphs. Schema embedding generalizes the conventional notion of graph similarity by allowing an edge in a source DTD schema to be mapped to a path in the target DTD. Instance-level embeddings can be derived from the schema embedding in a straightforward manner, such that conformance to a target schema and information preservation are guaranteed. We show that it is NP-complete to find an embedding between two DTD schemas. We also outline efficient heuristic algorithms to find candidate embeddings, which have proved effective by our experimental study. These yield the first systematic and effective approach to finding information preserving XML mappings.

Categories and Subject Descriptors: H.2.5 [Database Management]: Heterogeneous Databases—Data translation

General Terms: Algorithms, Design, Languages, Management, Performance, Theory

Additional Key Words and Phrases: Data transformation, information integration, information preservation, schema embedding, schema mapping, XML, XSLT

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1. INTRODUCTION

A central technical issue for the exchange, migration and integration of XML data is to find mappings from documents of a source XML (DTD) schema to documents of a target schema. In practice such a mapping, referred to as an XML mapping, often needs to (1) guarantee type-safety, that is, the target document produced by the mapping should conform to the target schema; and (2) preserve information, that is, the target documents should not lose original information of the source data. Criteria for information preservation include: (1) invertibility [Hull 1986]: can one recover the source document from the target? and (2) query preservation: for a certain XML query language, can all queries on source documents in that language be answered on target documents by queries in the same language? We now illustrate these concepts with an example.

Example 1.1. Consider two source DTDs $S_0, S_1$ and a target DTD $S$ represented as graphs in Figure 1 (we omit the str–PCDATA– child under cno, credit, title, year, term, instructor, gpa in Figure 1(c)). A document of $S_0$ contains information of classes taught at a school, and a document of $S_1$ contains student data of the school. The user wants to map the document of $S_0$ and the document of $S_1$ to a single instance of $S$, which is to collect data about courses and students of the school in the last five years. Here we use edges of different types to denote various constructs of a DTD, namely, solid edges for a concatenation type (a unique occurrence of each child), dashed edges for disjunction (one and only one child), and star edges (edges labeled ‘∗’) for Kleene star (zero or more child).

Here type safety requires that school documents produced by integrating instances of $S_0$ and $S_1$ are guaranteed to conform to the target DTD $S$. Invertibility asks for the ability to reconstruct the original class and student documents from an integrated school document, while query preservation requires the ability to answer XML queries expressed in a language $L$ (e.g., XPath) and posed on class and student documents by equivalent queries that are expressed in the same language $L$ but are posed on the school document.

Type safety is typically necessary since it concerns whether or not XML mappings make sense. In many applications one also wants XML mappings to be information preserving. For example, in data exchange between two schemas or in data migration from one schema to another [Lenzerini 2002], one often wants to reconstruct the source document and thus requires the XML mapping to be invertible. As observed in Fagin [2006], inverse mappings are also useful in developing new mappings via mapping composition. It is also common in practice that users care more about query answerability than the ability to restore the original documents. As an example, in a P2P system [Kementsietsidis et al. 2003; Halevy et al. 2004], for any query $Q$ posed on a local document residing in one peer, one wants to be able to find the same query answer via a query $Q'$ posed on another peer; furthermore, while $Q'$ may be different from (yet equivalent to) $Q$, $Q'$ and $Q$ should be expressible in the same query language $L$, for example, XPath. In other words, the XML mappings from data at one peer to another peer should be query preserving. Note that in query rewriting it is also required that the rewritten query should be expressible in the same language.
as that of the original query [Halevy 2000; Lenzerini 2002]. For all the reasons that this requirement is important for query rewriting, it is also needed for query preservation. In particular, the language in which the original query $Q$ is given may be only language supported by the system or is the language that the user wants to use. Furthermore, the user should not be penalized by paying the higher price for evaluating and optimizing queries in a richer language than that of the original query, for example, XQuery.

While one can certainly define XML mappings in a query language such as XQuery or XSLT, such queries may be large and complex, and as a result time-consuming to construct by hand. Worse still, type safety may be hard to
check for mappings defined in XQuery or XSLT [Alon et al. 1995]. In practice one often wants a systematic method to define XML mappings that are guaranteed to be type safe. When it comes to information preservation, a number of fundamental questions are open. Can one determine whether an XML mapping is information preserving? Is there an efficient method to find information preserving XML mappings, or better still, to define XML mappings that are guaranteed to be invertible and/or query preserving w.r.t. a popular XML query language, for example, XPath?

While type safety and information preservation are clearly desirable, an additional feature is the ability to map documents of DTDs that have different structures. A given source DTD may differ in structure from a desired target DTD. This is commonly encountered in data integration, where the target DTD needs to accommodate data from multiple sources and thus may not be similar to any of the sources in structure; in Figure 1, for example, the school DTD is quite different from the class and student DTDs.

Background. While information preservation has been studied for traditional database transformations [Abiteboul and Hull 1988; Hull 1986; Miller et al. 1993, 1994], to our knowledge, no previous work has considered it for XML mappings. In fact, a variety of tools and models have been proposed for finding XML mappings at schema- or instance-level [Doan et al. 2001; Madhavan et al. 2001; Melnik et al. 2002; Melnik et al. 2003; Miller et al. 2001; Milo and Zohar 1998]; however, none has addressed invertibility and query preservation for XML. Most tools either focus on highly similar structures, or adopt a strict graph similarity model like simulation [Abiteboul et al. 2000] to match structures, which is incapable of mapping DTDs with different structures such as those shown in Figure 1, and can ensure neither invertibility nor query preservation w.r.t. XML query languages. Another issue is that it is unclear that mappings found by some of these tools guarantee type safety when it comes to complex XML DTDs.

Contributions. In response to the practical need, we investigate fundamental questions associated with XML mappings. Furthermore, we propose a method for defining XML mappings that are guaranteed to be both type safe and information preserving. Here information preservation will be characterized by both invertibility and query preservation. More specifically, this work makes the following contributions.

First, as criteria for information preservation we revisit the notions of invertibility and query preservation Abiteboul and Hull 1988; Hull 1986; Miller et al. 1993, 1994] for XML mappings. While the two notions coincide for relational mappings w.r.t. relational calculus [Hull 1986], we show that they are in general different for XML mappings w.r.t. XML query languages. Furthermore, we show that it is undecidable to determine whether or not an XML mapping defined in a small fragment of XQuery or XSLT is information preserving.

Second, to cope with the undecidability result, we introduce an XML mapping framework based on a novel notion of schema embeddings. A schema embedding is a natural extension of graph similarity in which an edge in a source DTD schema may be mapped to a path, rather than a single edge, in a target DTD. For example, the source DTDs $S_0$ and $S_1$ of Figure 1 can both be embedded in
S, while there is no sensible mapping from them to S based on graph similarity. From a schema embedding, an instance-level XML mapping can be directly produced that has all the properties mentioned above. In particular, such mappings are invertible, query preserving w.r.t. regular XPath (an extension of XPath introduced in Marx [2004]), and ensure type safety. As with schema-mapping techniques for other data models, by automatically producing this mapping the user is saved from the burden of writing and type-checking a complex mapping query. Moreover, we show that the inverse and query translation functions for the mapping are efficient.

Third, we provide an algorithm to translate queries posed against a source schema into queries against the document as embedded in the target schema. In order to accomplish this translation in low-polynomial time, we introduce a mild augmentation of nondeterministic finite state automata to represent regular XPath queries; based on this notion we then develop a schema-directed translation algorithm producing an automaton for the target schema. While automaton may itself be translated into regular XPath, this translation subsumes the translation of finite-state automata to regular expressions, an EXPTIME-complete problem [Ehrenfeucht and Zeiger 1976].

Fourth, we provide algorithms to compute schema embeddings. We show that it is NP-complete to find an embedding between two DTDs, even when the DTDs are nonrecursive. Thus practical algorithms for finding embeddings are necessarily heuristic. We have implemented our algorithms and conducted an experimental study based on mapping schemas taken from real-life and benchmark sources to copies of these schemas with varying amounts of introduced noise. These experiments verify the accuracy and efficiency of our heuristics on schemas up to a few hundred nodes in size, supporting the practical applicability of schema embedding. We omit the details of the algorithms and experimental results due to the lack of space, but we suggest the reader consult [Bohannon et al. 2005].

Schema embeddings are a promising tool for automatically computing information preserving XML mappings, and are particularly suited for common information integration cases where the target schema is more general and thus more complex than the source. To the best of our knowledge, this work is the first to study information preservation in the generic XML context, and it yields a systematic and effective approach to defining and finding type safe and information preserving XML mappings.

Organization. The remainder of the article is organized as follows. Section 2 reviews DTDs and XPath, and revisits invertibility and query preservation for XML mappings. Section 3 investigates basic properties of invertibility and query preservation, establishing equivalence, separation and complexity results for XML mappings. Section 4 defines the notion of schema embedding and shows that schema embedding guarantees information preservation and type safety. Section 5 shows that the problem of finding schema embedding is intractable, and outlines our algorithms for computing schema-embedding candidates. Related work is discussed in Section 6, followed by topics for future work in Section 7.
2. DTDS, XPath, Information Preservation

In this section we review DTDS and (regular) XPath, and revisit the notions of information preservation [Hull 1986; Miller et al. 1994] for XML.

2.1 DTDS

To simplify the discussion, consider DTDS of the form \((E, P, r)\), where \(E\) is a finite set of element types; \(r\) is a distinguished type in \(E\), called the root type; \(P\) defines the element types: and for each \(A\) in \(E\), \(P(A)\) is a regular expression of the form:

\[
\alpha ::= \text{str} | \epsilon | B_1, \ldots, B_n | B_1 + \cdots + B_n | B^* \]

where \text{str} denotes PCDATA, \(\epsilon\) is the empty word, \(B\) is a type in \(E\) (referred to as a child of \(A\)), and ‘+’, ‘,’ and ‘*’ denote disjunction (with \(n > 1\), concatenation and the Kleene star, respectively. We refer to \(A \rightarrow P(A)\) as the production of \(A\). Note that this form of DTDS does not lose generality since any DTD \(S\) can be converted to \(S'\) of this form (in linear time) by introducing new element types, and (regular) XPath queries on \(S\) can be rewritten into equivalent (regular) XPath queries on \(S'\) in \text{PTIME} [Benedikt et al. 2005].

Schema Graphs. We represent a DTD \(S\) as a labeled graph \(G_S\), referred to as the graph of \(S\). For each element type \(A\) in \(S\), there is a unique node labeled \(A\) in \(G_S\), referred to as the A node. From the A-node there are edges to nodes representing child types in \(P(A)\), determined by the production \(A \rightarrow P(A)\) of \(A\). There are three different types of edges indicating different DTD constructs. Specifically, if \(P(A) = B_1, \ldots, B_n\) then there is a solid edge from the A node to each \(B_i\) node, referred to as an AND edge; it is labeled with a position \(k\) if \(B_i\) is the \(k\)-th occurrence of a type \(B\) in \(P(A)\) (the label can be omitted if \(B_i\)'s are distinct). If \(P(A) = B_1 + \cdots + B_n\) then there is a dashed edge from the A node to each \(B_i\) node (w.l.o.g. assume that \(B_i\)'s are distinct in disjunction), referred to as an OR edge. If \(P(A) = B^*\), then there is a solid edge with a “*” label from the A node to the \(B\) node, referred to as a star edge. When it is clear from the context, we shall use the DTD and its graph interchangeably, both referred to as \(S\); similarly for A element type and A node.

A DTD is said to be recursive if and only if its graph is cyclic.

For example, Figure 1 shows graphs representing three DTDS, where Figures 1(a) and 1(c) depict recursive DTDS.

An XML instance \(T\) of a DTD \(S\) is an ordered, node-labeled tree that conforms to \(S\). That is, (1) there is a unique node, the root, in \(T\) labeled with \(r\); (2) each node in \(T\) is labeled either with an \(E\) type \(A\), called an A element, or with \text{str}, called a text node; (3) each A element has a list of children of elements and text nodes such that their labels are a word in the regular language defined by \(P(A)\); and (4) each text node carries a string value (PCDATA) and is a leaf. We denote by \(I(S)\) the set of all instances of \(S\).

Two XML trees \(T_1\) and \(T_2\) are said to be equal, denoted by \(T_1 = T_2\), if \(T_1\) and \(T_2\) are isomorphic by an isomorphism that is the identity on string values. More specifically, for a node \(n_1\) in \(T_1\) and a node \(n_2\) in \(T_2\), we say that \(n_1\) and \(n_2\) are
equal, denoted by \( n_1 = n_2 \), if the following conditions are satisfied. (1) If both \( n_1 \) and \( n_2 \) are text nodes, then they carry the same string value. (2) If both \( n_1 \) and \( n_2 \) are elements, then they are both labeled with the same tag and moreover, their children are pairwise equal, i.e., their children are lists \([v_1, \ldots, v_k]\) and \([u_1, \ldots, u_k]\), respectively, and \( v_i = u_i \) for all \( i \in [1, k] \). We say that \( T_1 = T_2 \) if \( r_1 = r_2 \), where \( r_1 \) and \( r_2 \) are the root nodes of \( T_1 \) and \( T_2 \), respectively. Intuitively, if \( T_1 \) and \( T_2 \) are equal then they have the identical structure carrying the same string values (observable values).

Assume a countably infinite set \( U \) of node ids. For each XML node \( v \) in \( T \), we assume that \( v \) is associated with a distinct node id \( id(v) \in U \), and denote the set of all node ids in \( T \) by \( \text{dom}(T) \). Note that a text node is also associated with a node id and it carries PCDATA.

A DTD \( S \) is consistent if it has no useless element types, that is, each element type of \( S \) appears in \( I(S) \). For standard context-free grammars (CFGs) it has been well studied how to drop all useless types from a CFG [Hopcroft and Ullman 1979], in quadratic time. Along the same lines we can convert any DTD \( S \) to a consistent \( S' \) in \( O(|S|^2) \) time such that \( I(S') = I(S) \). Thus in the sequel we only consider consistent DTDs.

### 2.2 XPath and Regular XPath

We consider a class of regular XPath queries proposed and studied in Marx [2004], denoted by \( \mathcal{X}_R \) and defined as follows:

\[
\begin{align*}
p & ::= \epsilon \ | \ A \ | \ p/text() \ | \ p/p \ | \ p \cup p \ | \ p^* \ | \ p[q], \\
q & ::= p \ | \ p/text() = ‘c’ \ | \ position() = k \ | \ ¬q \ | \ q \land q \ | \ q \lor q,
\end{align*}
\]

where \( \epsilon \) is the empty path (self), \( A \) is a label (element type), \( ‘\cup’ \) is the union operator, \( ‘/’ \) is the child-axis, and \( * \) is the Kleene star; \( q \) is a qualifier, \( p \) is an \( \mathcal{X}_R \) expressions, \( k \) is a natural number, \( c \) is a string constant, and \( \neg, \land, \lor \) are the Boolean negation, conjunction and disjunction operators, respectively. We shall use a special qualifier \( \text{true} \), which always holds and is definable in \( \mathcal{X}_R \) (e.g., \( \text{[true]} \) can be defined as \( \{\epsilon\} \)).

An XPath [Clark and DeRose 1999] fragment of \( \mathcal{X}_R \), denoted by \( \mathcal{X}' \), is defined by replacing \( p^* \) with \( p/\!/p \) in the definition above, where \( /\!/ \) is the descendant-or-self-axis.

A (regular) XPath query \( p \) is evaluated at a context node \( v \) in an XML tree \( T \); its result, denoted by \( v[p/\!] \), is the set consisting of (a) node ids in \( \text{dom}(T) \) of those nodes reachable via \( p \) from \( v \), and (b) string values (PCDATA) if \( p \) contains a sub-query of the form \( p'/\!text() \), e.g., when \( p \) is \( A/C/\!text() \cup A/B \) [Clark and DeRose 1999; Marx 2004]. We use \( p(T) \) to denote \( v[p/\!] \) if \( v \) is the root node of \( T \). While node ids are non-printable, commercial systems typically provide APIs that allow one to define a function \( f \) such that (a) it maps node ids in \( \text{dom}(T) \) to observable values and (b) it behaves the same as the identity function on string values (e.g., Xerces [Xerces and Xalan], Galax [Siméon and Fernandez]).
2.3 Invertibility and Query Preservation

For XML DTDs $S_1$ and $S_2$, a (data) instance mapping $\sigma_d : I(S_1) \rightarrow I(S_2)$ is invertible if there exists an inverse $\sigma_d^{-1}$ of $\sigma_d$ such that for any XML instance $T \in I(S_1)$, $\sigma_d^{-1}(\sigma_d(T)) = T$, where $f(T)$ denotes the result of applying a function (or mapping, query) $f$ to $T$. In other words, the composition $\sigma_d^{-1} \circ \sigma_d$ is equivalent to the identity mapping $id$, which maps an XML document to itself.

For an XML query language $L$, a mapping $\sigma_d$ is query preserving w.r.t. $L$ if there exists a computable function $Tr : L \rightarrow L$ such that for any XML query $Q \in L$ and any $T \in I(S_1)$, $Q(T) = Tr(Q)(\sigma_d(T))$, i.e., $Q = Tr(Q) \circ \sigma_d$.

In a nutshell, invertibility is the ability to recover the original source XML document from the target document; query preservation w.r.t. regular XPath as follows. With an XML mapping $\sigma_d : S_1 \rightarrow S_2$ we associate a (partial) node id mapping $\text{idM()}$ that, given an XML instance $T$ of the source schema, maps $\text{dom}(\sigma_d(T))$ to $\text{dom}(T)$ and it is the identity mapping on string values (furthermore, $\text{idM()}$ also recovers the original tag of the node $v$ in $T$ if $\text{idM()}$ maps a node from $\sigma_d(T)$ to $v$; we omit this to simplify the discussion). We say that $\sigma_d$ is query preserving w.r.t. regular XPath if there exists a computable function $Tr$ such that for any regular XPath query $Q$ and any $T \in I(S_1)$, $Q(T) = \text{idM(Tr(Q)(\sigma_d(T)))}$, i.e., $\text{idM()}$ recovers the original query result $Q(T)$ from $\text{Tr}(Q)(\sigma_d(T))$. This assures that $Q(T)$ and $\text{idM(Tr(Q)(\sigma_d(T)))}$ return the same set of node ids (carrying their original tags in $T$). Assuming a countably infinite set $\mathcal{V}$ of observable values, then for any function $f$ that maps nodes ids in $\text{dom}(T)$ to $\mathcal{V}$ and maps string values to themselves, $f(Q(T)) = f(\text{Tr}(Q)(\sigma_d(T)))$; that is, they yield the same set of observable values no matter what printable values are associated with those node ids via user-defined mapping function and system-provided APIs.

Example 2.1. Figure 2 depicts a source schema $S_1$ (on the left) and a target schema $S_2$ (on the right). A mapping $\sigma_d : I(S_1) \rightarrow I(S_2)$ is indicated by the arrows, while the inverses of the arrows denote the node id mapping $\text{idM()}$. Intuitively, given any $T \in I(S_1)$, an instance $\sigma_d(T)$ is constructed such that its
id mapping \( \text{idM}() \) maps (a) the id of the root \( r_2 \) of \( \sigma_d(T) \) to the id of the root \( r_1 \) of \( T \); (b) the id of the \( A \) child of \( r_2 \) to the \( A \) child of \( r_1 \); and inductively, (c) if the id of element \( v' \) in \( \sigma_d(T) \) is mapped to the id of an \( A \) element \( v \) in \( T \), then the ids of the child and the grandchild of \( v' \) are mapped to the ids of the \( B, C \) children of \( v \), respectively, and the id of the great grandchild of \( v' \) is mapped to the id of the \( A \) child of the \( B \) child of \( v \).

Consider an XPath query \( Q = A/B \) posed at the root \( r_1 \) of \( T \), and \( Q' = A/A \) at the root \( r_2 \) of \( \sigma_d(T) \). Then \( Q \) and \( Q' \) are equivalent \( w.r.t. \) \( \text{idM}() \). Indeed, \( Q(T) \) returns a single node id \( o \), and \( Q'(\sigma_d(T)) \) returns a single node id \( o' \), where \( \text{idM}(o') = o \).

This semantics of query equivalence can be implemented in, for example, XSLT, as follows. Distinct ids can be generated for distinct nodes in \( T \) via, for example, the \( \text{generate-id}() \) function of XSLT, which returns a (printable) string value as the unique id of a node. As will be seen in Section 4.3, a mapping \( \sigma_d() \) can be expressed in XSLT, which can be easily extended such that given \( T \), \( \sigma_d() \) also creates a unique id for each node in \( T \) and furthermore, associates the id of each node in \( T \) with the id of the corresponding node in \( \sigma_d(T) \). This produces the definition of \( \text{idM}() \). This can also be used to display ids in query result, that is, for each id in the query result, we can simply return its string representation generated by \( \text{generate-id}() \), a printable string.

To simplify the discussion and due to the space constraint, in the sequel, we omit the construction of the id mapping \( \text{idM}() \) when it is clear from the definition of \( \sigma_d \), and simply write \( Q'(T) = \text{idM}(\text{Tr}(Q)(\sigma_d(T))) \) as \( Q(T) = \text{Tr}(Q)(\sigma_d(T)) \). By mapping a node \( v \) in \( T \) to a node \( v' \) in \( \sigma_d(T) \), or copying \( v \) to \( v' \), we mean that we create a node \( v' \) such that \( \text{idM}() \) maps the id of \( v \) to the id of \( v' \).

3. INFORMATION PRESERVATION

In this section we establish basic results for the separation and equivalence of the invertibility and query preservation of XML mappings, as well as the complexity of determining whether a given XML mapping is information preserving.
Invertibility and Query Preservation: Separation. It was shown [Hull 1986] that calculus dominance and query dominance are equivalent for relational mappings. In contrast, invertibility and query preservation do not necessarily coincide for XML mappings and query languages. Recall the class $\mathcal{X}$ of XPath queries defined in Section 2, which does not support query composition, identity mapping (from XML documents to XML documents), or the ability to navigate a recursive DTD based on certain patterns that are expressible in terms of the Kleene closure $p^*$.  

Theorem 3.1. There exists an invertible XML mapping that is not query preserving w.r.t. $\mathcal{X}$; and there exists an XML mapping that is not invertible but is query preserving w.r.t. the class of $\mathcal{X}$ queries without position() qualifier.

Proof. The proof consists of two parts.

1. We first show that invertibility does not entail query preservation w.r.t. the XPath fragment $\mathcal{X}$. Recall the source DTD $S_1$ and the target DTD $S_2$ shown in Figure 2:

   $S_1 = ((r, A, B, C), P_1, r)$, where $P_1$ consists of the following productions:
   
   $r \rightarrow A$, $A \rightarrow B, C$, $B \rightarrow A + \epsilon$, $C \rightarrow \epsilon$,

   $S_2 = ((r, A), P_2, r)$, where $P_2$ consists of:
   
   $r \rightarrow A$, $A \rightarrow A + \epsilon$.

The mapping $\sigma_d : \mathcal{T}(S_1) \rightarrow \mathcal{T}(S_2)$ given in Example 2.1 can be expressed by the function $\text{path}()$ (see Section 4.1) from the edges of $S_1$ to paths of $S_2$ as follows:

   $\text{path}(r, A) = A$ \hspace{1em} $\text{path}(A, B) = A$ \hspace{1em} $\text{path}(A, C) = A/A$ \hspace{1em} $\text{path}(B, A) = A/A$

For instance, given a $B$ node $v_1$ and its $A$ child $v_2$ in $T$, $\text{path}(B, A)$ maps the edge $(v_1, v_2)$ in $T$ to a path $(v'_1, v', v'_2)$ in $\sigma_d(T)$, where $v'_1, v', v'_2$ are all labeled with $A$, and $v'_1, v'_2$ are mapped from $v_1, v_2$, respectively. That is, if $v_1$ in $T$ is mapped to $v'_1$ in $\sigma_d(T)$, then the child $v_2$ of $v_1$ in $T$ is mapped to the node $v'_2$ in $\sigma_d(T)$ that is reachable from $v'_1$ by following $\text{path}(B, A) = A/A$. In other words, $\text{path}(B, A)$ is relative to node $v'_1$.

Obviously $\sigma_d$ is invertible: one can restore the original $T$ from $\sigma_d(T)$ by generating $T$ inductively top-down starting from the root $r_1$ of $T$.

Now consider an $\mathcal{X}$ query $Q = //B$. An equivalent translation of $Q$ over $\sigma_d(T)$ is to find all the elements in the $A$-chain of $\sigma_d(T)$ that are reachable from $r_2$ via $A^{3k+2}$. It is easy to prove by contradiction that $A^{3k+2}$ is not expressible in $\mathcal{X}$, even with the position() qualifier. Thus $\sigma_d$ is not query preserving w.r.t. $\mathcal{X}$.

2. We next show that query preservation w.r.t. the XPath fragment $\mathcal{X}$ without position() qualifiers does not entail invertibility. Consider a source DTD $S_1$:

   $S_1 = ((r, A), P_1, r)$, where $P_1$ consists of:
   
   $r \rightarrow A^*$, \hspace{1em} $A \rightarrow \text{str}$.

and assume that the target DTD $S_2$ is identical to $S_1$.

The mapping $\sigma_d : \mathcal{T}(S_1) \rightarrow \mathcal{T}(S_2)$ is such defined that for any $T \in \mathcal{T}(S_1)$, the root $r_1$ of $T$ is mapped to the root $r_2$ of $\sigma_d(T)$, the $A$ children of $r_1$
are mapped to the $A$ children of $r_2$ such that there is a bijection from the $A$ children of $r_1$ to the $A$ children of $r_2$; however, the $A$-children of $r_2$ are ordered based on their string values (str).

All the $X$ queries posed over $T \in \mathcal{I}(S_1)$ are equivalent to one of the following forms of $X$ queries: $\epsilon, A, A[q]$, where $q$ is a Boolean formula defined in terms of atomic formulas of the form $\text{text}() = 'c'$. Since the identity mapping from $X$ to $X$ yields equivalent queries over $\sigma_d(T)$ for these queries, the mapping $\sigma_d$ is query preserving w.r.t. $X$. However, $\sigma_d$ is not invertible: one cannot recover the original order of the $A$ elements of $r_1$ based on $\sigma_d$. □

**Invertibility and Query Preservation: Equivalence.** We next identify sufficient conditions for the two to coincide: the definability of the identity mapping from XML documents to XML documents, and query composability (i.e., for any $Q_1, Q_2$ in $L$, $Q_1 \circ Q_2$ is also in $L$). Recall that the identity mapping is definable in neither regular XPath nor XPath, because (regular) XPath does not return XML trees.

**Theorem 3.2.** Let $L$ be any XML query language and $\sigma_d$ be a mapping: $\mathcal{I}(S_1) \rightarrow \mathcal{I}(S_2)$.

—If the identity mapping id is definable in $L$ and $\sigma_d$ is query preserving w.r.t. $L$, then $\sigma_d$ is invertible.

—If $L$ is composable, $\sigma_d$ is invertible and $\sigma_d^{-1}$ is expressible in $L$, then $\sigma_d$ is query preserving w.r.t. $L$.

**Proof.** We prove the two statements as follows.

(1) Suppose that $\sigma_d$ is query preserving w.r.t. $L$. Then there exists a computable function $\text{Tr} : L \rightarrow L$ such that for any $Q \in L$ and any $T \in \mathcal{I}(S_1)$, $Q(T) = \text{Tr}(Q)(\sigma_d(T))$. Since id is in $L$, we have $T = id(T) = \text{Tr}(id)(\sigma_d(T))$ for any $T \in \mathcal{I}(S_1)$). That is, $\sigma_d^{-1} = \text{Tr}(id)$, and thus $\sigma_d$ is invertible.

(2) Suppose that $L$ is composable, $\sigma_d$ is invertible and $\sigma_d^{-1}$ is in $L$. Then define $\text{Tr} : L \rightarrow L$ to be $\text{Tr}(Q) = Q \circ \sigma_d^{-1}$ for any $Q \in L$. Obviously $\text{Tr}$ is computable, and $\text{Tr}(Q)$ is in $L$ since $L$ is composable. Furthermore, for any $Q \in L$ and $T \in \mathcal{I}(S_1)$, $Q(T) = Q(\sigma_d^{-1}(\sigma_d(T))) = \text{Tr}(Q)(\sigma_d(T))$. Thus $\text{Tr}$ is an effective query translation function for $L$. □

Recall the class $X_R$ of regular XPath queries defined in Section 2. Although the identity mapping id is not definable in $X_R$, we show below that query preservation w.r.t. $X_R$ is a stronger property than invertibility: every node in a source document can be uniquely identified by an $X_R$ query on the target document, and thus can be recovered.

**Theorem 3.3.** If an XML mapping $\sigma_d$ is query preserving w.r.t. $X_R$, then $\sigma_d$ is invertible. Conversely, there exists $\sigma_d$ that is invertible but is not query preserving w.r.t. $X_R$.

**Proof.** Suppose that $\sigma_d : \mathcal{I}(S_1) \rightarrow \mathcal{I}(S_2)$ is query preserving w.r.t. $X_R$. We show that $\sigma_d$ is invertible by providing an algorithm for computing $\sigma_d^{-1}$. Given $\sigma_d(T)$, the algorithm recovers $T$ as follows. It first creates the root $r_1$ of $T$, with id $o$ given in $\text{idM}(o, o')$, where $o'$ is the id of the root $r_2$ of $\sigma_d(T)$. It then recursively expands $T$ top-down as follows, until $T$ cannot be expanded further.
To expand $T$, for each node $v$ created for $T$, it recovers the children of $v$ based on its type $A$, the production $A \to \alpha$ of $A$ in $S_1$, and the query translation function $\Tr : \mathcal{X}_R \to \mathcal{X}_R$. To do so it makes use of a subclass of $\mathcal{X}_R$, referred to as $\mathcal{X}_R$ paths, which are of the form $\rho = \eta_1/\ldots/\eta_k$, where $k \geq 1$, $\eta_i$ is of the form $A[q]$, and $q$ is either true or a position() qualifier. By induction on the length of the path from $r_1$ to $v$, one can easily verify that there is a unique $\mathcal{X}_R$ path $\rho$ such that $r_1[\rho]$ is a singleton set $\{v\}$. The process of recovering the children of $v$ is based on the structure of $\alpha$:

1. $\alpha = A_1, \ldots, A_n$. For each $A_i$, define an $\mathcal{X}_R$ query $Q_i = \Tr(\rho/A_i[\text{position()} = k])$, where $k$ indicates the $k$-th occurrence of $A_i$ element in $\alpha$ if it has multiple $A_i$ elements. Note that evaluating $\rho/A_i[\text{position()} = k]$ at the root $r_1$ of $T$ is equivalent to evaluating the query $A_i[\text{position()} = k]$ at the context node $v$ in $T$, which would return the $k$-th $A_i$ child of $v$. Since $\sigma_d$ is query preserving, evaluating $Q_i(\sigma_d(T))$ at the root $r_2$ of $\sigma_d(T)$ yields the same answer as evaluating $\rho/A_i[\text{position()} = k]$ at the root $r_1$ in $T$. Let $v_i$ be the single node returned by $Q_i(\sigma_d(T))$ at the root $r_2$. Copy $v_1, \ldots, v_n$ to $T$ as the children of $v$, and for each $i \in [1, n]$, proceed to expand the subtree at $v_i$ in the same way.

2. $\alpha = A_1 + \cdots + A_n$. For each $A_i$, let $Q_i = \Tr(\rho/A_i)$. Evaluate $Q_i(\sigma_d(T))$ at the root $r_2$ of $\sigma_d(T)$ as in (1). Since $\sigma_d$ is query preserving and $T$ is an XML tree that conform to $S_1$, there exists one and only one position $i \in [1, n]$ such that $Q_i(\sigma_d(T))$ returns a single note $v_i$ (and the $Q_j$’s return empty for $j \neq i$). Copy $v_1$ to $T$ as the only child of $v$ and proceed to expand the subtree at $v_i$ in the same way.

3. $\alpha = B^\ast$. For each natural number $k$, evaluate $Q_k(\sigma_d(T))$ at the root $r_2$ of $\sigma_d(T)$ as in (1), where $Q_k = \Tr(\rho/B[\text{position()} = k])$, until it reaches a $k_0$ such that $Q_{k_0}(\sigma_d(T)) = \emptyset$. Since $\sigma_d$ is query preserving and $\sigma_d(T)$ is mapped from an XML tree $T$ that conforms to $S_1$, $Q_{k_0}(\sigma_d(T))$ at $r_2$ of $\sigma_d(T)$ yields the same answer as evaluating the query $B[\text{position()} = k]$ at the context node $v$ in $T$, that is, there exists one and only one node $v_k$ returned by $Q_k(\sigma_d(T))$ at $r_2$ for each $k < k_0$, and for any $k \geq k_0$, $Q_k(\sigma_d(T)) = \emptyset$. Copy $v_k$ to $T$ as the $k$-th child of $v$ for all $k < k_0$, and proceed to expand the subtree at each $v_k$ in the same way.

4. $\alpha = \text{str}$. Find the string value by evaluating $\Tr(\rho/\text{str()}(i))$ at the root $r_2$ of $\sigma_d(T)$ as in (1).

5. $\alpha = \varepsilon$. Nothing needs be done here.

The children of $v$ generated above have different identities from $v$ because no distinct nodes in $T$ have the same identity and $\sigma_d$ is query preserving. This process terminates. Indeed, each step of the process expands $T$ by copying distinct nodes from $\sigma_d(T)$, and $\sigma_d(T)$ is a (finite) XML tree. One can verify that $T = \sigma_d^{-1}(\sigma_d(T))$, i.e., the algorithm above indeed computes $\sigma_d^{-1}$. Thus $\sigma_d^{-1}$ is computable and $\sigma_d$ is invertible.

To show that invertibility does not necessarily lead to query preservation w.r.t. $\mathcal{X}_R$, recall the $\mathcal{D}\mathcal{T}\mathcal{D}_R$ $S_1$ and $S_2$ defined in the proof of Theorem 3.1 (1). Consider a mapping $\sigma_d : \mathcal{I}(S_1) \to \mathcal{I}(S_2)$ such that for any $T \in \mathcal{I}(S_1)$, the root $r_1$ of $T$ is mapped to the root $r_2$ of $\sigma_d(T)$, the $A$ child of $r_1$ is mapped to the $A$ child of $r_2$, and inductively, if an $A$ element $v$ in $T$ is mapped to an $A$ element $v'$ in $\sigma_d(T)$, then the $B, C$ children of $v$ are also mapped to $v'$, and the $A$ child of the $B$ node is mapped to the $A$ child of $v'$, such that the number of $A$ nodes in $T$ is the same as that in $\sigma_d(T)$. Obviously, $\sigma_d$ is invertible: given any $\sigma_d(T)$ one can recover $T$. 


such that the number of $A$ nodes in $T$ is the same as that in $\sigma_d(T)$, and each $A$ node in $T$ has a $B$ child followed by a $C$ child. However, one cannot translate an $\lambda_R$ query $(A/(B \cup C))^*$ over $S_1$ to an equivalent $\lambda_R$ query over $S_2$. \qed

**Complexity.** It is common to find XML mappings defined in XQuery or XSLT. A natural and important question is to decide whether or not an XML mapping in XQuery or XSLT is invertible or query preserving w.r.t. a query language $\mathcal{L}$. Unfortunately, this is impossible for XML mappings defined in any language that subsumes first-order logic (FO), such as XQuery, XSLT, even when $\mathcal{L}$ consists of projection queries only. Thus it is beyond reach in practice to answer the question for XQuery or XSLT mappings. That is, it is impossible to find a systematic method to determine an XML mapping defined in one of these languages is information preserving or not.

**Theorem 3.4.** *It is undecidable to determine, given an XML mapping $\sigma_d$ defined in any language subsuming FO, whether or not (a) $\sigma_d$ is invertible; and (b) $\sigma_d$ is query preserving w.r.t. projection queries.*

These negative results are not surprising: as indicated by the proof below, the undecidability results already hold for relational data transformations expressed in relational algebra (FO), and for relational projection queries. Similar undecidability results have been established for relational and object-oriented models [Hull 1986; Miller et al. 1994], and recently for mappings from XML to relations [Barbosa et al. 2005], although query preservation was not investigated there.

**Proof.** It suffices to show that these problem are undecidable for relational mappings defined in relational algebra (RA). For if it holds, the undecidability carries over to XML mappings defined in FO since relational data can be coded in XML and RA queries can be expressed in FO over XML trees.

We verify the undecidability by reduction from the equivalence problem for RA queries. That is the problem to decide, given two RA queries $Q_1, Q_2 : \mathcal{R}_1 \rightarrow \mathcal{R}_2$, whether or not $Q_1 \equiv Q_2$, that is, whether or not for any relational database $I$ of $\mathcal{R}_1$, $Q_1(I) = Q_2(I)$. This equivalence problem is undecidable [Abiteboul et al. 1995].

(a) We first show that the invertibility problem is undecidable. Given two RA queries $Q_1, Q_2 : \mathcal{R}_1 \rightarrow \mathcal{R}_2$, we define a RA mapping $V : \mathcal{R}_1 \times \mathcal{R}_2 \rightarrow \mathcal{R}_1 \times \mathcal{R}_2$, as follows:

$$V = \pi_{R_1} \times (\pi_{R_2} \cup \Delta(Q_1, Q_2)), \quad \Delta(Q_1, Q_2) = (Q_1 \setminus Q_2) \cup (Q_2 \setminus Q_1).$$

Note that $Q_1 \equiv Q_2$ iff $\Delta(Q_1, Q_2) = \emptyset$, that is, when $\Delta(Q_1, Q_2)$ always returns an empty set.

We show that $V$ is invertible iff $Q_1 \equiv Q_2$. If $Q_1 \equiv Q_2$, then $\Delta(Q_1, Q_2) = \emptyset$. Then $V$ is the identity query and is certainly invertible. Conversely, if $Q_1 \not\equiv Q_2$, then there exists an instance $I$ of $\mathcal{R}_1$ such that $\Delta(Q_1, Q_2)(I)$ is nonempty. Consider two distinct instances of $\mathcal{R}_1 \times \mathcal{R}_2$: $I_1 = (I, \Delta(Q_1, Q_2)(I))$ and $I_2 = (I, \emptyset)$. Since $V(I_1) = V(I_2) = (I, \Delta(Q_1, Q_2)(I))$, $V$ is not injective and thus is not invertible (there exists no inverse function for $V$).
(b) We now show that query preservation for projection queries is undecidable. Given two RA queries \( Q_1, Q_2 : \mathcal{R}_1 \rightarrow \mathcal{R}_2 \), we use the same RA mapping \( V \) given above to show that \( V \) is query preserving w.r.t. a fixed query iff \( Q_1 \equiv Q_2 \). Consider a fixed query \( Q = \pi_{R_2} \). First, suppose that \( Q_1 \equiv Q_2 \). Then one can define \( \mathcal{V} \) such that \( \mathcal{V}(Q) = Q \). This shows that \( V \) is query preserving w.r.t. \( Q \). Conversely, suppose that \( Q_1 \not\equiv Q_2 \). Suppose, by contradiction, that there is a computable query translation function \( \mathcal{V} \) such that \( \mathcal{V}(Q) = Q \). Recall \( I_1, I_2 \) given above. Obviously, \( \mathcal{V}(I_1) \neq \mathcal{V}(I_2) \), while \( \mathcal{V}(\mathcal{V}(I_1)) = \mathcal{V}(\mathcal{V}(I_2)) \) since \( V(I_1) = V(I_2) \). Thus either \( \mathcal{V}(I_1) \neq \mathcal{V}(\mathcal{V}(I_1)) \) or \( \mathcal{V}(I_2) \neq \mathcal{V}(\mathcal{V}(I_2)) \); that is, \( \mathcal{V} \) does not translate \( Q \) to an equivalent query over the target, which contradicts the assumption above. Thus \( V \) is not query preserving w.r.t. \( Q \). \( \square \)

The undecidability suggests that we start with languages simpler than XQuery and XSLT when studying information preserving XML mappings. Indeed, understanding (regular) XPath query preservation is a necessary step toward a full treatment of XML mappings defined in XQuery or XSLT, in which XPath is embedded. The extension to regular XPath is particularly natural for studying XSLT, where the recursive semantics of rule processing makes it straightforward to express regular XPath queries in small stylesheets. Thus in the remainder of the paper we shall focus on (regular) XPath, both for defining XML mappings and for querying XML data.

4. SCHEMA EMBEDDINGS FOR XML

The negative results in Section 3 tell us that it is already hard to determine whether or not an XML mapping is information preserving, not to mention finding one. As remarked in Section 1, it is also nontrivial to check the type safety of XML mappings. This motivates us to look for a class of XML mappings that are guaranteed to be both information preserving and type safe.

We approach this problem by specifying XML mappings in terms of schema level embeddings, and providing an automated derivation of instance-level mappings from these embeddings. Our notion of schema embeddings is novel: it extends the conventional notion of graph similarity by allowing an edge in a source DTD to be mapped to a path in a target DTD. Intuitively, this allows a “smaller” DTD to be embedded in a “larger” one.

In this section we define XML schema embeddings, present an algorithm for deriving an instance-level mapping from a schema embedding, provide XSLT coding of these instance-level mappings as well as their inverse, and verify that the resulting mappings indeed ensure both type safety and information preservation.

4.1 Schema Level Embeddings

Consider a source XML DTD schema \( S_1 = (E_1, P_1, r_1) \) and a target DTD \( S_2 = (E_2, P_2, r_2) \). In a nutshell, a schema embedding \( \sigma \) is a pair of functions \((\lambda, \text{path})\) that maps each \( A \) type in \( E_1 \) to a \( \lambda(A) \) type in \( E_2 \), and each edge \((A, B)\) in \( S_1 \) to a unique path, \( \text{path}(A, B) \) in \( S_2 \), from \( \lambda(A) \) to \( \lambda(B) \). Intuitively, if an \( A \) node \( u \) in the source is mapped to a \( \lambda(A) \) node \( v \) in the target, then we map the \( B \) child of \( u \) to a \( \lambda(B) \) descendant of \( v \) identified by the unique path\((A, B)\) emanating from \( v \). The
mapping must obey three correctness properties: (1) \( \lambda(A) \) must be semantically compatible with \( A \), i.e., \( \lambda(A) \) and \( A \) belong to the same “domain”, (2) \( \text{path}(A, B) \) must have a “larger information capacity” than the edge \( (A, B) \)—for example, a \text{STAR} edge can only be mapped to a path with at least one \text{STAR} edge, and (3) the \( S_2 \) paths mapped from sibling edges in \( S_1 \) must be sufficiently distinct to allow information to be preserved. To formally define these correctness conditions, we first introduce some notation.

\( \mathcal{X}_R \) Paths. An \( \mathcal{X}_R \) path over a \text{DTD} \( S = (E, P, r) \) is an \( \mathcal{X}_R \) query of the form \( \rho = \eta_1/\ldots/\eta_k \), where \( k \geq 1 \), \( \eta_i \) is of the form \( A[q] \), and \( q \) is either true or a position() qualifier, such that \( \rho \) represents a label path in \( S \), carrying all the position labels on the path. An \( \mathcal{X}_R \) path is called an \text{AND} path (resp. \text{OR} path, and \text{STAR} path) if it is nonempty and consists of only solid or star edges (resp. of solid edges and at least one dashed edge, and of solid edges and at least one edge labeled \( * \)). Referring to Figure 1(c), for example, \text{basic/class/semester} is an \text{AND} path and a \text{STAR} path, and \text{mandatory/regular} is an \text{OR} path.

An \( \mathcal{X}_R \) path \( \rho_1 \) is called a prefix of another \( \mathcal{X}_R \) path \( \rho_2 \) if \( \rho_2 = \rho_1/\eta_j/\ldots/\eta_k \).

Schema Element Similarity. A similarity matrix for \( S_1 \) and \( S_2 \) is an \( |E_1| \times |E_2| \) matrix \( \text{att} \) of numbers in the range \([0, 1] \). For any \( A \in E_1 \) and \( B \in E_2 \), \( \text{att}(A, B) \) indicates the suitability of mapping \( A \) to \( B \) as determined by human domain experts or computed by an existing schema matching algorithm, e.g., [Athitsos et al. 2005; Doan et al. 2001; Li and Clifton 2000]. We note that most previous work on mapping construction has assumed an accurate set of attribute correspondences; that is, \( \text{att}(A, B) \in \{0, 1\} \). Supporting non-Boolean quality measures accrues several advantages with minimal increased complexity, since a candidate embedding can be computed based on a machine-generated similarity measure. First, the algorithm can be used in “best-effort” applications, and second, attribute matches that participate in information-preserving mappings can be preferred over others, even if resulting matching will be hand-checked by a domain expert. Leveraging this, in the next section we shall formalize the problem of finding a schema embedding as an optimization problem as commonly encountered in “best-effort” applications.

Type Mapping. A type mapping \( \lambda \) from \( S_1 \) to \( S_2 \) is a (total) function from \( E_1 \) to \( E_2 \); in particular, it maps the root of \( S_1 \) to the root of \( S_2 \), i.e., \( \lambda(r_1) = r_2 \). A type mapping \( \lambda \) is valid w.r.t. a similarity matrix \( \text{att} \) if for any \( A \in E_1 \), \( \text{att}(A, \lambda(A)) > 0 \). Note that in general one could define validity in terms of a threshold \( \theta \), i.e., \( \lambda \) is valid if \( \text{att}(A, \lambda(A)) > \theta \); we assume \( \theta = 0 \) in this paper to simplify the discussion.

Path Mapping. A path mapping from \( S_1 \) to \( S_2 \), denoted by \( \sigma : S_1 \rightarrow S_2 \), is a pair \( (\lambda, \text{path}) \), where \( \lambda \) is a type mapping and \( \text{path} \) is a function that maps each edge \( (A, B) \) in \( S_1 \) to an \( \mathcal{X}_R \) path, \( \text{path}(A, B) \), that is from \( \lambda(A) \) to \( \lambda(B) \) in \( S_2 \).

For a particular element type \( A \) in \( E_1 \), we say that \( \sigma \) is valid for \( A \) if the following conditions hold, referred to as the path type condition and the prefix-free condition on \( \text{path}(A, B) \), based on the production \( A \rightarrow P_1(A) \) in \( S_1 \):

— if \( P_1(A) = B_1, \ldots, B_l \), then for each \( i \), \( \text{path}(A, B_i) \) is an \text{AND} path from \( \lambda(A) \) to \( \lambda(B_i) \) that is not a prefix of \( \text{path}(A, B_j) \) for any \( j \neq i \);
— if $P_1(A) = B_1 + \cdots + B_l$, then for each $i$, $\text{path}(A, B_i)$ is an OR path from $\lambda(A)$ to $\lambda(B_i)$ that is not a prefix of $\text{path}(A, B_j)$ for any $j \neq i$;
— if $P_1(A) = B^*$, then $\text{path}(A, B_i)$ is a STAR path;
— if $P_1(A) = \text{str}$, then $\text{path}(A, \text{str})$ is an AND path ending with $\text{text()}$.

The following example illustrates why these conditions are necessary to impose for deriving an instance-level mapping from $\sigma$.

**Example 4.1.** In Figure 3 a number of simple schema mapping examples are presented to illustrate the validity conditions for schema embeddings. The figure shows five scenarios, labeled “a” through “e.” Each scenario consists of a source and a target DTD, with the schema graph of the source DTD on the left and the target on the right. Except for Figure 3(c), types in the source are mapped (by the type mapping $\lambda$) to types with the same name in the target, for example, $A$ is mapped to $A'$. In Figure 3(c), two source types are mapped to one target type, in that both $\lambda(B) = B'$ and $\lambda(C) = B'$.

For Figure 3(a), there is no valid path mapping from the source DTD to the target, since $\text{path}(A, B)$ and $\text{path}(A, C)$ violate the path type condition; intuitively, $B$ and $C$ must coexist in a source document while only one of $B'$ and $C'$ exists in the target. Similarly, for Figure 3(b), the source cannot be mapped to the target since the target cannot accommodate possibly multiple $B$ elements in the source. For Figure 3(c), a valid embedding is $\text{path}(A, B) = B'[\text{position()} = 1]$ and $\text{path}(A, C) = B'[\text{position()} = 2]$. For Figure 3(d), there is no valid embedding since $\text{path}(A, B)$ is a prefix of $\text{path}(A, C)$, violating the prefix-free condition. For Figure 3(e), a valid embedding is $\text{path}(A, B) = A'/B'$ (by unfolding the cycle once) and $\text{path}(A, C) = B'/C'$.

Finally, we define XML schema embeddings as follows.

**Schema Embedding.** A schema embedding from $S_1$ to $S_2$ w.r.t. a similarity matrix $\text{att}$ is a path mapping $\sigma = (\lambda, \text{path})$ from $S_1$ to $S_2$ such that $\lambda$ is valid w.r.t. $\text{att}$, and $\sigma$ is valid for every element $A$ in $E_1$.

Note that schema embedding takes into account the semantics of the source and target schemas by means of the similarity matrix, on top of the syntactic and structural correspondences between the two schemas.

---

Abusing our normal form of DTDs, an optional type $B$ can be specified as, for example, $A \rightarrow B + \epsilon$; here $\text{path}(A, B)$ simply needs to be an OR path since $\epsilon$ is not an element type and thus $\text{path}(A, \epsilon)$ is undefined.
Example 4.2. Assume a similarity matrix $\text{att}$ such that $\text{att}(X, X') = 1$ for all $X$ in the DTD $S_0$ of Figure 1(a) and $X'$ in $S$ of Figure 1(c). Here the similarity matrix $\text{att}$ imposes no restrictions: any name in the source can be mapped to any name in the target; thus the embedding here is decided solely on the DTD structures. The source DTD $S_0$ can be embedded in the target $S$ via $\sigma_1 = (\lambda_1, \text{path}_1)$ defined as follows:

$$
\lambda_1(\text{db}) = \text{school}, \quad \lambda_1(\text{class}) = \text{course}, \quad \lambda_1(\text{type}) = \text{category}, \\
\lambda_1(A) = A /* A: cno, title, regular, project, prereq, str */ \\
\text{path}_1(\text{db}, \text{class}) = \text{courses/current/course} \\
\text{path}_1(\text{class}, \text{cno}) = \text{basic/cno} \\
\text{path}_1(\text{class}, \text{title}) = \text{basic/class/semester[position()=1]/title} \\
\text{path}_1(\text{class}, \text{type}) = \text{category} \\
\text{path}_1(\text{type}, \text{regular}) = \text{mandatory/regular} \\
\text{path}_1(\text{type}, \text{project}) = \text{advanced/project} \\
\text{path}_1(\text{regular}, \text{prereq}) = \text{required/prereq} \\
\text{path}_1(\text{prereq}, \text{class}) = \text{course} \\
\text{path}_1(A, \text{str}) = \text{text()} /* A for cno, title */
$$

Note that $\text{path}_1(A, B)$ is a path in $S$ denoting how to reach $\lambda_1(B)$ from $\lambda_1(A)$; that is, the path is relative to $\lambda_1(A)$ rather than starting from the root. For example, $\text{path}_1(\text{type}, \text{project})$ indicates how to reach $\text{project}$ from a $\text{category}$ context node in $S$, where $\text{category}$ is mapped from $\text{type}$ in $S_0$ by $\lambda_1$.

In contrast, one cannot map $S_0$ to $S$ by graph similarity, which requires that node $A$ in the source is mapped (similar) to $B$ in the target only if all children of $A$ are mapped (similar) to children of $B$. In other words, graph similarity maps an edge in the source to an edge in the target.

The definition of schema embedding can be extended to support further restructuring “across hierarchies” such that a child $B$ of a source type $A$ is not necessarily mapped to a descendant of $\lambda(A)$ in the target; this can be achieved via, for example, upward modality in $\text{path}(A, B)$. It is also possible that an AND edge does not have to be mapped to an AND path. We focus on the main idea of schema embeddings in this paper and defer the extension to a later study.

Embedding Quality. There are many possible metrics. In this paper we consider only a simple one: the quality of a schema embedding $\sigma = (\lambda, \text{path})$ w.r.t. $\text{att}$ is the sum of $\text{att}(A, \lambda(A))$ for $A \in E_1$, and we say that $\sigma$ is invalid if $\lambda$ is invalid w.r.t. $\text{att}$. We refer to this metric as $\text{qual}(\sigma, \text{att})$.

4.2 Instance Level Mapping

For a valid schema embedding $\sigma = (\lambda, \text{path})$ from $S_1$ to $S_2$, we give its semantics by defining a (data) instance-level mapping $\sigma_d : T(S_1) \rightarrow T(S_2)$, referred to as the XML mapping of $\sigma$. We define $\sigma_d$ by presenting an algorithm that, given an instance $T_1$ of $S_1$, computes an instance $T_2 = \sigma_d(T_1)$ of $S_2$.

Before presenting the full algorithm, we introduce two notions, the minimum default instance of a target schema tag and the mapping fragment of a source node. In a nutshell, the mapping fragment of a source node $v$ is the subtree in
the target $T_2$ that is “mapped” from the subtree of $v$ in $T_1$. The minimum default instance of a target schema tag $A$ is a fixed default instance of $A$, which will be added to $T_2$ by the instance-level mapping $\sigma_d$ such that $T_2$ is guaranteed to conform to $S_2$.

**Minimum Default Instances.** For a DTD $S_1 = (E_1, P_1, r_1)$ and a particular element type $A \in E_1$, we fix a default instance of $A$. Recall from Section 2 that we consider consistent DTDs only; as a result, instances of $A$ exist. Among these instances of $A$ one can fix an arbitrary one and treat it as the default instance. In other words, the default instance is a constant property of a single schema. Below we present how we fix a default instance.

Assume a fixed order on the types (XML tags) of $E_1$, and a fixed string value $\#s$. We compute the minimum default instance of $A$, denoted by $\text{mindef}(A)$, inductively based on the definition of $A$ as follows. We associate a variable $\text{rank}(A)$ with $A$, having an initial value 1. (1) If $P_1(A)$ is $\text{str}$, then $\text{mindef}(A)$ is a node with label $A$ carrying a $\text{str}$ child with $\#s$ as its value, and we set $\text{rank}(A) = 0$. (2) If $P_1(A)$ is $B^*$, then $\text{mindef}(A)$ is a single $A$-node without any children, and we set $\text{rank}(A) = 0$. We then repeat the following process until for all $A \in E_1$, $\text{rank}(A) = 0$. For each $A \in E_1$ with $\text{rank}(A) = 1$, (3) if $P_1(A)$ is $B_1, \ldots, B_n$ and $\text{rank}(B_i) = 0$ for all $i \in [1, n]$, we let $\text{mindef}(A)$ be a node with label $A$ and children consisting of $\text{mindef}(B_1), \ldots, \text{mindef}(B_n)$; or (4) if $P_1(A)$ is $B_1 + \cdots + B_n$ and one of $B_i$ has $\text{rank}(B_i) = 0$, we let $\text{mindef}(A)$ be $\text{mindef}(B_j)$ such that $B_j$ is the smallest among all $B_i$’s with $\text{rank}(B_i) = 0$ w.r.t. the order on the types in $E_1$. In both cases we set $\text{rank}(A) = 0$. Since $S_1$ is consistent, in each iteration there must exist some $A$ satisfying (3) or (4) above. Upon the termination of the process we have $\text{mindef}(A)$ defined for all $A \in E_1$.

**Example 4.3.** Given the XML mapping $\sigma_d$ of the embedding defined in Example 4.2, some example values of $\text{mindef}$ might be:

\[
\text{<student>}
\quad \text{<ssn> $\#s$ </ssn>}
\quad \text{<name> $\#s$ </name>}
\quad \text{<gpa> $\#s$ </gpa>}
\quad \text{<taking> </taking>}
\text{</student>}
\]

\[
\text{\text{mindef(prereq) = <prereq> </prereq>}}
\quad \text{<category>}
\quad \text{<advanced>}
\]

\[
\text{\text{mindef(category) = <project> $\#s$ </project>}}
\quad \text{<advanced>}
\quad \text{</category>}
\]

**Production Fragments.** For a source node $v$ with type $A$ in $S_1$, we define $t = \text{pfrag}_\lambda(v)$ to be an XML fragment, referred to as the production fragment of $v$ with respect to $\sigma_d$. The root $r_t$ of $t$ is a node with label $\lambda(A)$ and carrying the same node identity as $v$. In addition, a set of “hot” leaf nodes $\text{hleaf}(t)$ is defined,
and with each such leaf, $h$, is associated a node from $T_1$, $\text{src}(h)$. Finally, during the production of $t$, position information is associated with each node $v \in t$ by $\text{pos}(v)$ (with the first child of a node numbered “1”). For example, nodes of type $\text{class}$ in Example 4.2 will have production fragments, as shown in Figure 4. Here $\text{hleaf}(t) = \{\text{category}, \text{cno}, \text{title}\}$, shown in rectangles in the figure. Other nodes correspond to the minimum definition of $\text{str}$ nodes. Finally, $\text{pos}(v)$ for each node is shown as a number under the node.

Constructing Production Fragments. We now give the details of computing the XML fragment $t = \text{pfrag}_A(v)$, for a source node $v$ of type $A$. First, the root $r_t$ is created and set as the root of $t$, and $\text{pos}(r_t)$ is set to 1. Second, for each child $v'$ of $v$ in $T_1$, we add $\rho = \text{path}(A, B)$ to $t$, where $v'$ is of type $B$. In general, this is accomplished by dividing $\rho$ into a prefix $\rho_1$ and a suffix $\rho_2$, such that $\rho_1$ is the longest prefix of $\rho$ that matches a path $\rho'$ in $t$. Nodes $u_1, \ldots, u_k$ are created for each of the $k$ steps in $\rho_2$ ($|\rho_2| = k$), and $\text{pos}(u_i)$ is set to one of a) $j$ where the predicate $\{\text{position}() = j\}$ appeared on the corresponding step of $\rho_2$ or b) $j$ where the parent of $u_i$ is of type $C$ in $S_2$, $u_i$ is of type $C_j'$, and $P_2(C)$ is of the form $C_{i_1}', \ldots, C_{j_1}', \ldots, C_{m_1}'$, and c) if neither (a) nor (b) holds, $j$ where $v'$ is the $j$-th child of $v$. Node $u_1$ is then added as a child of $u_0$, which is the lowest node $t$ matching $\rho'$. Finally, $u_k$ is added to $\text{hleaf}(t)$, and $\text{src}(u_k)$ is set to $v'$. (Note that $u_0$ cannot be in $\text{hleaf}(t)$ due to the prefix-free property of valid schema embeddings.)

Once this process completes, the embedded nodes needed are present, but ordering may be incorrect and some required nodes may be missing. To deal with this, if any node $u$ in $t$ but not in $\text{hleaf}(t)$ requires a child $u'$ of type $C$ at position $i$, but no such $u'$ exists with $\text{pos}(u') = i$, then a copy of $\text{mindef}(C)$ is added as a child of $u$, and $\text{pos}(m)$ where $m$ is the root of the copy of $\text{mindef}(C)$ is set to $i$. Note that such a child can be required for a parent $u$ that is associated with an $\text{AND}$ node in the schema, or a parent that is associated with a $\text{STAR}$ node if some child $u''$ with $\text{pos}(u'') > i$. Finally, the children of nodes in $t$ not copied from some $\text{mindef}$ are sorted into the $\text{pos}$ order.

Instance Construction Algorithm. A construction algorithm, $\text{InstMap}$, for $\sigma_d$ is shown in Figure 5. In a nutshell, $\text{InstMap}$ constructs $T_2$ in a top down fashion, by repeatedly replacing a hot node with the appropriate production fragment. In the process, the node id mapping $\text{idM}(\cdot)$ is generated at line 6 to map the ids of the nodes in $T_2$ to the ids of the corresponding nodes in $T_1$. Note that a node
Fig. 5. Algorithm InstMap.

function InstMap (T₁)
Input: XML tree T₁ conforming to DTD S₁
Output: σd(T₁)
1. initialize T₂ to be a single root node r₂;
2. H := {r₂}; // set of hot nodes
3. while H ≠ ∅ do
4.   select some h in T₂ from H
        where src(h) is a node of type B;
5.   replace h in T₂ with pfag_H(src(h));
6.   idM(r) := src(h) where r is the root of pfag_H(src(h));
7.   H := (H \ hleaf(t)) \ {h};
8. return T₂;

in T₁ is in H exactly once, and thus the algorithm trivially terminates in time linearly proportional to the size of the larger of T₁ and T₂.

Example 4.4. Consider the XML mapping σd of the embedding defined in Example 4.2. Given an instance T₁ of S₀ of Figure 1(a) and σd, algorithm InstMap generates a tree T₂ of S of Figure 1(c) as follows: InstMap first creates the root school of T₂, as a copy of the root db of T₁, and marks school as a “hot” node by adding it to H at line 2. The first time through the loop at lines 4–7, the new root is chosen as h, and replaced with the production fragment of the db node from T₁. This fragment is rooted at a school node, and has a history child and a current child. Since history is not involved in any path, the minimum default instance of the history node is used in this production fragment. Since history has an outgoing STAR edge, this minimum default instance is in fact a single history node. For the current node, the construction of the production fragment is more complicated. In fact, it produces a child of current with label course for each class child of the original root of T₁. Since these nodes terminate a path in the mapping, they are in the hleaf set for the production fragment just added to the tree, and thus they are added to H at line 7 (and db is removed). The algorithm continues by selecting one of the newly-created course nodes as h and replacing it with the production fragment of the class node in T₁. Note that at line 6 the node id mapping idM() is generated accordingly to map the ids of the nodes in T₂ to the ids of the corresponding nodes in T₁, in this case mapping the newly created course node back to the source class node. The new production fragment for class follows the form shown in Figure 4, and includes a basic subtree with cno as a “hot node,” credit as a minimum default instance and a subtree under class of a single semester. Under this node, title is again added to H as a “hot node,” while year, term and professor are filled in with their respective minimum default instances. The algorithm continues until the entire tree is created.

Correctness. We next show that σd is well defined. That is, given any T₁ in T(S₁), σd(T₁) is an XML tree and moreover, it is type safe; that is, it conforms to S₂. This is nontrivial due to the interaction between different paths defined for
disjunction types in the schema mapping \( \sigma \), among other things. Consider, for example, \texttt{path(type, regular)} in Example 4.2. The path requires the existence of a \textit{regular} child under a \textit{mandatory} element \( m \), which is in turn a child under a \textit{category} element \( c \) in an instance of \( S \). Thus it rules out the possibility of adding an \textit{advanced} child under \( c \) or a \textit{lab} child under \( m \), perhaps requested by a conflicting path in \( \sigma \). However, Theorem 4.1 shows that the prefix-free condition in the definition of valid \texttt{path} functions ensures that conflicting paths do not exist. Theorem 4.1 also shows that \( \sigma_d \) is \textit{injective}: it maps distinct nodes in \( T_1 \) to distinct nodes in \( \sigma_d(T_1) \), a property necessary for information preservation.

**Theorem 4.1.** The XML mapping \( \sigma_d \) of a valid schema embedding \( \sigma : S_1 \rightarrow S_2 \) is well defined and injective.

**Proof.** The proof consists of three parts. We first show that \( \delta \) maps distinct \( \mathcal{X}_R \) paths in \( S_1 \) from \( r_1 \) to distinct \( \mathcal{X}_R \) paths in \( S_2 \) from \( r_2 \). Then, using this we show that \( \sigma_d \) is injective. Based on this we finally show that \( \sigma_d \) is well defined.

(1) We first define a function \( \delta \) that maps \( \mathcal{X}_R \) paths from the root \( r_1 \) in \( S_1 \) to \( \mathcal{X}_R \) paths from the root \( r_2 \) in \( S_2 \). Given an \( \mathcal{X}_R \) path \( \rho = A_1[q_1]/\ldots/A_k[q_k] \) in \( S_1 \) from \( r_1 \), \( \delta(\rho) \) is defined to be \texttt{path(r_1, A_1[q_1]/\ldots/path(A_{k-1}, A_k[q_k])} \), an \( \mathcal{X}_R \) path in \( S_2 \) from \( r_2 \), by substituting \texttt{path(A_i, A_{i+1})} for each \( A_{i+1} \) in \( \rho \).

We show that \( \delta \) maps distinct \( \mathcal{X}_R \) paths in \( S_1 \) from \( r_1 \) to distinct \( \mathcal{X}_R \) paths in \( S_2 \) from \( r_2 \). Let \( \rho_1, \rho_2 \) be distinct \( \mathcal{X}_R \) paths from \( r_1 \) in \( S_1 \). Consider the following two cases. First, \( \rho_1 \) is a prefix of \( \rho_2 \). That is, \( \rho_2 = \rho_1/\rho \) where \( \rho \) is nonempty since \( \rho_1 \) and \( \rho_2 \) are distinct. Then \( \rho \) is mapped to a nonempty \( \mathcal{X}_R \) path in \( S_2 \) by the definition of \( \delta \), and thus \( \delta(\rho_1) = \delta(\rho_2) \); similarly if \( \rho_2 \) is a prefix of \( \rho_1 \). Second, neither is \( \rho_1 \) a prefix of \( \rho_2 \) nor \( \rho_2 \) is a prefix of \( \rho_1 \). Then there exist \( \rho, \rho', A[q], B_1[q_1] \) and \( B_2[q_2] \) such that \( \rho_1 = \rho/A[q]/B_1[q_1]/\rho' \), \( \rho_2 = \rho/A[q]/B_2[q_2]/\rho' \), and \( B_1[q_1], B_2[q_2] \) are the first labels that differ in \( \rho_1 \) and \( \rho_2 \). Then \( B_1, B_2 \) are child types of \( A, A \) is either a concatenation type or a disjunction type, and moreover, either \( B_1, B_2 \) are distinct labels, or \( q_1, q_2 \) indicate different positions of the same label. By the definition of schema embedding, neither is \texttt{path(A, B_1)} a prefix of \texttt{path(A, B_2)} nor the other way around. That is, \texttt{path(A, B_1) = q/q_1/q_1} and \texttt{path(A, B_2) = q/q_2/q_2} such that \( q_1 \) and \( q_2 \) are distinct. Thus \( \delta(\rho_1) \neq \delta(\rho_2) \).

(2) From (1) and the definition of \( \sigma_d \) it follows that \( \sigma_d \) is injective. Indeed, any node in an XML tree is uniquely determined by an \( \mathcal{X}_R \) path from the root. Thus by the definition of \( \sigma_d \), any node \( v \) in \( T \in \mathcal{T}(S_1) \) is mapped to a distinct node in \( \sigma_d(T) \). Indeed, this obviously holds if the parent of \( v \) is of a concatenation or disjunction type or \( \texttt{str} \); and moreover, if the type of the parent \( v' \) of \( v \) is defined with a Kleene star, the children of \( v' \) are mapped to distinct nodes preserving the original order, by the definition of \( \sigma_d \).

(3) We next show that \( \sigma_d \) is type safe; that is, for any \( T \in \mathcal{T}(S_1) \), \( \sigma_d(T) \) conforms to \( S_2 \). One possible violation of \( S_2 \) may occur when there exists an \( A \)-node \( u \) in \( \sigma_d(T) \) such that \( A \) is a disjunction type \( A \rightarrow B_1 + \ldots + B_k \), and \( \sigma_d(T) \) forces the presences of both \( B_i \) and \( B_j \) children of \( u \). Then there must be two nodes \( v_1, v_2 \) in \( T \) identified by \( \mathcal{X}_R \) paths \( \rho_1, \rho_2 \) from the root of \( T \) such that \( v_1, v_2 \) are mapped to the \( B_i, B_j \) children of \( u \), respectively; furthermore,
\[ \rho_1 = \rho / A[q] / \rho_1', \rho_2 = \rho / A[q] / \rho_2', \text{ and } v_1, v_2 \text{ have the lowest common ancestor } u \text{ that is identified by } \rho / A[q] \text{ and is mapped to either } u \text{ or an ancestor } u' \text{ of } u \text{ by } \sigma_d. \text{ If } v \text{ is mapped to } u \text{ then } v \text{ must have a disjunction type by the definition of schema embedding, and thus } v_1, v_2 \text{ cannot coexist. This contradicts the assumption. Now assume that } v \text{ is mapped to } u'. \text{ Consider the following cases of the production of } A', \text{ where } A' \text{ is the element type of } v. \text{ (i) Obviously if } A' \to \epsilon \text{ or } A' \to \text{str}, \text{ it is impossible for } v \text{ to have descendants } v_1 \text{ and } v_2. \text{ (ii) If } A' \to B'_1, \ldots, B'_n, \text{ then both } \text{path}(A', B'_i) \text{ and } \text{path}(A', B'_j) \text{ must be suffixes of the same } \chi_R \text{ path that is mapped from } \rho / A[q], \text{ ending with } A, \text{ since otherwise it would violate the path type condition given that } A \text{ is a disjunction type. However, this contradicts the prefix-free condition of schema embedding since either } \text{path}(A', B'_i) \text{ is a prefix of } \text{path}(A', B'_j) \text{ or the other way around. (iii) If } A' \to B'_1 + \cdots + B'_n, \text{ then either } v_1, v_2 \text{ cannot exist at the same time, or } v \text{ cannot be the lowest common ancestor of } v_1 \text{ and } v_2, \text{ since } v \text{ has one and only one child. Again this leads to contradiction. (iv) If } A' \to B', \text{ then by the definition of } \sigma_d, v_1, v_2 \text{ cannot be mapped to nodes that have a common ancestor } u \text{ without violating the path type condition, given that } A \text{ has a disjunction type. This again contradicts the assumption. Putting these together, the violation of } S_2 \text{ by OR paths cannot happen. Similarly, it can be verified that violations cannot be caused by AND and STAR paths either. } \square \]

4.3 Instance Level Mapping with XSLT

While the given procedure clearly demonstrates that instance-level schema embeddings can be computed in a straightforward and efficient manner, it requires an implementation effort on the part of the user. In fact, the top-down rule-driven style of computation on which instance-level embedding is based is quite compatible with the widely used XML Stylesheet Language for Transformations (XSLT) [Clark 1999]. In this section, we sketch the construction of XSLT stylesheets to effect both \( \sigma_d \) and \( \sigma_d^{-1} \), the construction of the original document. To simplify the discussion we omit the concrete construction of node id mapping idM(), which, as remarked earlier, can be easily incorporated.

**XSLT Overview.** We now present a (somewhat simplified) model of XSLT stylesheet processing. In our model, an XSLT stylesheet \( X \) is a set of template rules \( \{ r_i \} \). Each rule, \( r_i \in X \), is a 3-tuple \( (\text{match}(r_i), \text{mode}(r_i), \text{output}(r_i)) \), where \( \text{match}(r_i) \) is the match pattern of \( r_i \), \( \text{mode}(r_i) \) is the mode of \( r_i \), and \( \text{output}(r_i) \) is the output-tree fragment of \( r_i \). The match pattern of a template rule, \( \text{match}(r_i) \), is a pattern [Clark 1999] and is essentially a subset of XPath expressions containing only child, descendant, and attribute axes. The mode of a rule, \( \text{mode}(r_i) \), is a symbol that allows rules to be partitioned; that is, rule invocations must match in mode as well as match pattern. If there is no mode attribute, the XSLT processor will set it to a default value.

The output tree fragment for a rule, \( \text{output}(r_i) \), controls the structure of the rule’s output. Essentially, \( \text{output}(r_i) \) is a well-formed fragment of XML, except that some leaf-nodes of the fragment may be apply-template nodes. We use \( \text{apply}(r_i) \) to denote the set of apply-template nodes in the output fragment of
An apply-templates node, $a_j$, is a 2-tuple of the form $(\text{select}(a_j), \text{mode}(a_j))$, where $\text{select}(a_j)$ is the select expression of $a_j$, and $\text{mode}(a_j)$ is the mode of $a_j$.

**XSLT Processing Model.** We will now informally describe the processing model of XSLT; for a formal discussion see Wadler [2000]. An XSLT stylesheet is executed against a source document $T_s$ to produce a target document $T_t$. Document processing revolves around a set $C$ of source nodes in $T_s$, referred to as context nodes. Associated with each node $c \in C$ is a node $t(c)$ in the (partially constructed) $T_t$. Processing of $T_s$ with XSLT stylesheet $X$ proceeds in general by selecting a node $c$ from $C$ and a processing rule $r_i \in x$ that matches $c$, then replacing $t(c)$ in $T_t$ with a copy $o_i$ of $\text{output}(r_i)$. Each apply-template node $a_j \in \text{output}(r_i)$ is then visited, and the XPath expression $\text{select}(a_j)$ evaluated on $T_s$, using $c$ as the start node, to yield a sequence of source nodes, $R_j$. For each node $u$ in $R_j$ (in order), a new dummy node $t(u)$ is created, forming a sequence of dummy target nodes, $G_j$. The apply-template node $a_j$ in $o_i$ is then replaced by the sequence $G_j$, and $R_j$ is added to $C$. This process continues until $C$ is empty.

An XSLT Template for $\sigma_d^{-1}$. Consider computing $\sigma_d^{-1}(T)$ for a source DTD $S_1 = (E_1, P_1, r_1)$, target DTD $S_2 = (E_2, P_2, r_2)$, mapping $\sigma = (\lambda, \text{path})$, and a particular element type $C = \lambda(A)$, where $A \in E_1$ and $C \in E_2$. We define $\text{invt}(C)$ to be one or more XSLT templates. The idea is to define a stylesheet comprised of templates for each element in the image of $S_1$ under $\lambda$, such that when the stylesheet is run on an instance produced by the instance-level mapping function $\sigma_d$ applied to a tree, $T_1$, it will compute the inverse, $\sigma_d^{-1}$, recovering $T_1$. We now give the definition of each such template. For each such template $r_C = \text{invt}(C)$, recall that we must define $(\text{match}(r_C), \text{mode}(r_C), \text{output}(r_C))$. In this construction $\text{match}(r_C)$ will be $C$, and $\text{mode}(r_C)$ will always be $\text{MDATA}$, a fixed mode picked for the templates in $\sigma_d^{-1}$. The output tree fragment, $\text{output}(r_C)$, always has a root element $e_r$, labeled $A$, where $C = \lambda(A)$. The sequence of children of this node differs based on the form of $P_t(A)$, as follows:

1. $P_t(A)$ is $B_1, \ldots, B_n$, then the children of $e_r$ will be a sequence of apply-template nodes, $a_1, \ldots, a_n$. For $a_i$, $\text{select}(a_i) = \text{path}(A, B_i)$.
2. $P_t(A)$ is $B_1 + \ldots + B_n$, then instead of a single template for $\text{invt}(C)$, we create $n$ templates, $r_{C_1}, \ldots, r_{C_n}$. Each $r_{C_i}$ has as the match condition $\text{match}(r_{C_i}) = C[\text{path}(A, B_i)]$, which will match any $C$ node with $\text{path}(A, B_i)$ as an outgoing path. Each of these rules has for its output tree a node $e_r$ with label $A$, and $e_r$ will have a single child node that is an apply-template node, $a$, with $\text{select}(a) = \text{path}(A, B_i)$.
3. $P_t(A) = B^*$, then a single rule $r_C$ will be created. The root node of $\text{output}(r_C)$ will be labeled $A$, and it will have a single child node that is an apply-template node, $a$. The mode of $a$ will be $\text{MDATA}$, and $\text{select}(a) = \text{text}()$.
4. $P_t(A)$ is $\text{str}$, then a single rule $r_C$ will be created. The root node of $\text{output}(r_C)$ will be labeled $A$, and it will have a single child node that is an apply-template node, $a$. The mode of $a$ will be $\text{MDATA}$, and $\text{select}(a) = \text{text}()$. 
Note that \texttt{text()} is an XPath function that returns true when applied to a \texttt{str} node.

Finally, we add a template that matches a text node and generates an output tree that is a copy of that node.

Example 4.5. Consider the target type \texttt{course} in Example 4.2 mapped to source type \texttt{class} under \(\sigma_d^{-1}\). The \texttt{XSLT} template generated for \texttt{course} in the implementation of \(\sigma_d^{-1}\) would be:

```xml
<xsl:template match="course">
  <class>
    <xsl:apply-templates select="basic/cno"/>
    <xsl:apply-templates select="class/semester/title"/>
    <xsl:apply-templates select="category"/>
  </class>
</xsl:template>
```

Note that this template follows closely the tree shown in Figure 4, with each node in \(\texttt{hleaf}\) replaced with an apply-templates node. However, the form of production fragments is not as simple with other nodes, and we now show the two templates that are generated for \texttt{category}, since it is mapped to \texttt{type} which is a disjunctive node with two children in \(S_0\):

```xml
<xsl:template match="category[mandatory/regular]">
  <category>
    <xsl:apply-templates select="mandatory/regular"/>
  </category>
</xsl:template>

<xsl:template match="category[advanced/project]">
  <category>
    <xsl:apply-templates select="advanced/project"/>
  </category>
</xsl:template>
```

Before defining an \texttt{XSLT} template for the instance-level mapping, \(\sigma_d\), we introduce template rules to generate default values for elements:

**Minimum Default Templates.** For a DTD \(S_1 = (E_1, P_1, r_1)\), and a particular element type \(A \in E_1\), we define \(\text{mint}(A)\) to be the minimum default template, an \texttt{XSLT} template \(r_A\) with \(\text{match}(r_A) = \epsilon\), which will match any node, with \(\text{mode}(r_A) = \text{MDATA}\), and with \(\text{output}(r_A) = \text{mindef}(r_A)\).

**An XSLT Template for \(\sigma_d\).** We now outline the construction of an \texttt{XSLT} stylesheet to compute \(\sigma_d\). The general idea is to follow the construction algorithm very closely, by providing one or more \texttt{XSLT} template rules for each production in \(S_1\). The form of these rules takes advantage of regularities in the form taken by \(\text{pfrag}_A(v)\) depending on the type of the production, \(P_1(A)\). In particular, the body of each rule will be one form taken by \(\text{pfrag}_A(v)\), and each “hot” node in this form will be replaced by an apply-templates node. We now describe the production of \(\text{pfrag}_A(v)\) in each case:
(1) \( P_1(A) = B_1, \ldots, B_n \). Note that, except for the node identity of the root node, 
\( pfrag_A(u) \) is a constant tree, say \( t_A \), w.r.t. \( v \). Accordingly, an XSLT template rule 
\( r_A \) can be constructed with \( \text{match}(r_A) = \{A\} \) and \( \text{output}(r_A) = t_A \) modified by 
substituting an apply-templates node in \( \text{output}(r_A) \) for each node in \( \text{hleaf}(t_A) \). 
In particular, for \( u \in \text{hleaf}(t_A) \), we construct an apply template node \( a_u \), with 
\( \text{select}(a_u) = B_i \) if the type of \( \text{src}(u) \) would be \( B_i \) in an instantiation of this 
fragment. (Default values for \( \text{mode}(r_i) \) are used unless specified otherwise.)

(2) \( P_1(A) = B_1 + \cdots + B_n \). In this case, \( n \) template rules, \( r_{A,1}, \ldots, r_{A,n} \) can be 
constructed. The \( i \)-th template rule, \( r_{A,i} \), is constructed as follows. First, 
we ensure that the variant is only fired when the correct child appears 
in \( T_1 \) by setting \( \text{match}(r_{A,i}) = A[B_i] \). The output fragment \( \text{output}(r_{A,i}) \) is 
then based on the single path \( \text{path}(A, B_i) \), and the single leaf node becomes 
the only apply-templates node, \( a_{A,i} \), of \( r_{A,i} \). For this apply-templates node, 
\( \text{select}(a_{A,i}) = B_i \).

(3) \( P_1(A) = B^* \). Since the number of children of \( v \) may vary, \( pfrag_A \) cannot be 
precomputed in general. Note however, that by the definition of a valid path function, 
\( \rho = \text{path}(A, B) \) is of the form \( \lambda(A)/C_1/\ldots/C_k/\lambda(B) \), where \( C_k \) is the first type defined in terms of Kleene star in \( P_2 \), i.e., \( P_2(C_k) = C_k^* \) and no element type on \( \lambda(A)/C_1/\ldots/C_k \), except \( C_k \), has production of 
this form. Accordingly, \( pfrag_A \) will have a constant prefix corresponding to 
\( \lambda(A)/C_1/\ldots/C_k \) regardless of the number of children of \( v \), and this fact can 
be used to construct a pair of XSLT template rules \( r_{A,p} \) (\( p \) for “prefix”) and \( r_{A,s} \) 
(\( s \) for “suffix”) for \( P_1(A) \) as follows: For \( r_{A,p} \), \( \text{match}(r_{A,p}) = A \), and the body 
\( \text{output}(r_{A,p}) \) is a tree corresponding to the path \( \lambda(A)/C_1/\ldots/C_k \). A single 
apply-templates node \( a_{A,p} \) is added as a child of \( C_k \), with \( \text{select}(a_{A,p}) = B, \) 
and unlike the other rules for a new mode, \( \text{mode}(a_{A,p}) = M_A \). The sec-
ond template rule, \( r_{A,s} \) has that \( \text{match}(r_{A,s}) = B \), \( \text{mode}(r_{A,s}) = M_A \), and 
\( \text{output}(r_{A,s}) \) is a tree corresponding to the path \( C_{k+1}/\ldots/C_n \) (note it is the 
responsibility of the next rule to generate the \( \lambda(B) \) node). As a child of the 
final \( C_n \) element in tree, a single apply-templates node \( a_{A,s} \) is added, with 
\( \text{select}(a_{A,s}) = B \). Each node \( v \) of type \( B \) in the source document will be pro-
cessed by the rest of the stylesheet, and the result placed as a subtree, as 
required.

(4) \( P_1(A) \) is \( \text{str} \). The treatment is the same as (1) except the last node of 
\( \text{path}(A, \text{str}) \) in \( T_2 \) is a text node holding the same value as the text node 
in \( T_1 \).

Example 4.6. Consider the source type \textit{class} in Example 4.2 mapped to 
target type \textit{course} under \( \sigma_d \). The XSLT template generated to effect \( \sigma_d \) for \textit{course} 
would be:

\[
<xsl:template match="\textit{class}" >
  <\textit{course}>
    <\textit{basic}>
      <xsl:apply-templates select="\textit{cno}" />
    </\textit{basic}>
    <\textit{credit}> #<\textit{credit}> </\textit{credit}>
    <\textit{class}>
\]

Two templates are generated for type since it is a disjunctive node with two children:

```
<xs:template match="type[regular]" >
  <category>
    <mandatory>
      <apply-templates select="regular" />>
    </mandatory>
  </category>
</xs:template>

<xs:template match="type[project]" >
  <category>
    <advanced>
      <apply-templates select="project" />>
    </advanced>
  </category>
</xs:template>
```

Finally, the prefix and suffix templates for db illustrate the handling of star edges. Note that these templates use mode to ensure that no spurious matches are made.

```
<xs:template match="db" > <!-- prefix template >
  <school>
    <courses>
      <current>
        <apply-templates mode="M-db" select="class" />
      </current>
    </courses>
  </school>
</xs:template>

<xs:template match="class" mode="M-db" > <!-- suffix template >
  <xs:apply-templates select="." />
</xs:template>
```
4.4 Translation of Regular XPath Queries

In this section, we introduce techniques for translating \( \mathcal{X}_R \) queries expressed against the source schema \( S_1 \) into queries against the target schema \( S_2 \). In particular, if \( Q \) is an \( \mathcal{X}_R \) query on \( S_1 \), and \( \sigma \) is an embedding of \( S_1 \) into \( S_2 \) then we would like to find a query \( Q' \) such that \( Q'(\sigma_d(T)) = Q(T) \) for any instance \( T \) of \( S_1 \). We define next a query translation function \( \text{Tr} \) with just this property. The approach we take is to translate \( Q \) into an automaton representation, and use this representation as the basis for the translation.

To motivate the use of an automaton framework for query translation, consider an apparently simpler translation based directly on the parse tree of \( Q \). Recall that \( \mathcal{X}_R \) queries use only the “child::” axis of XPath, albeit possibly in the context of a Kleene-star. An appealing idea is to replace a step “child::A” in a query with \( \text{path}(B, A) \) where \( B \) is \( A \)'s parent in \( S_1 \). However, this simple translation is not generally correct. First, tags in a DTD do not have a unique parent, and \( A \) might appear in the production of a number of elements, say \( B \) and \( C \). In this case, simple edge substitution is not sufficient to translate \( (B \cup C)/A \), since in general \( \text{path}(B, A) \neq \text{path}(C, A) \). Second, consider translating a query \( (A_1 \cup A_2 \cup A_3)/(B_1 \cup B_2 \cup B_3) \). Since each \( \text{path}(A_i, B_j) \) is distinct, and may or may not be defined, it is clear that nine paths may need to be matched when this query is translated to \( S_2 \), and thus simple textual substitutions will not effectively map this query across \( \sigma \). Simply substituting \( \text{path}(A, B) \) for \( A \) may lead to incorrect translation.

Finally, we note that keeping the output in automata form is important to the overall complexity of query translation. If the translated query \( \text{Tr}(Q) \) is explicitly represented as an \( \mathcal{X}_R \) query, in the worst case it is of exponential size. Indeed, the query translation problem subsumes the problem for translating finite state automata to regular expressions, which is known to be exponential-time complete [Ehrenfeucht and Zeiger 1976]. To overcome these difficulties, we adopt a simple automaton (graph) representation of the translated queries, along the same lines as solutions for traditional path problems [Tarjan 1981]. This allows us to translate \( \mathcal{X}_R \) queries on \( S_1 \) to equivalent queries, represented as automata, against \( S_2 \) as embedded by \( \sigma \) in low polynomial time.

We now define a simple automaton representation of \( \mathcal{X}_R \) queries. We refer to such an automaton as an annotated nondeterministic finite state automaton (ANFA). As will be seen shortly, for each \( \mathcal{X}_R \) query \( Q \) posed on instances \( T \) of \( S_1 \), there exists an ANFA characterizing the equivalent \( \mathcal{X}_R \) query \( \text{Tr}(Q) \) on corresponding target documents \( \sigma_d(T) \); furthermore, the size of the ANFA is bounded by \( O(|Q| |\sigma| |S_1|) \). Leveraging ANFA’s, we will then provide the definition of \( \text{Tr} \).

**Automaton Representation of \( \mathcal{X}_R \) Queries.** We represent an \( \mathcal{X}_R \) query \( Q \) in terms of a mild extension of non-deterministic finite state automaton (NFA), by annotating states in a NFA with ANFA’s that represent qualifiers in \( Q \). Formally, the ANFA representing \( Q \) is defined to be \( M_Q = (M, \nu) \), where \( \nu \) and \( M \) are given as follows. (i) \( \nu \) is a mapping, referred to as the annotation of \( M_Q \), from a set of names \( \{X_i \mid i \in [1, m]\} \) to a set of ANFA’s \( \{M_i \mid i \in [1, m]\} \), and \( M_i \) is an ANFA representing a subqualifier. Here a subquery of \( Q \) denotes a descendant in \( Q \)'s parse tree, and a subqualifier denotes a descendant in the parse tree of
a qualifier of \( Q \). Note that \( m \) is the number of subqualifiers in \( Q \), and thus is no larger than the size \( |Q| \) of \( Q \). (ii) \( M = (K, \Sigma, \delta, s, F, \theta) \), where \( K, \Sigma, \delta, s, F \) are the states, alphabet (the labels in \( Q \)), transition function, start state and final states as in the standard NFA definition; and \( \theta \) is a partial mapping from \( K \) to “qualifiers” defined as

\[
q_x := X \mid X/text() = 'c' \mid position() = k \mid \neg X \mid X \wedge X \mid X \vee X ,
\]

where \( X \) is a name. That is, \( \theta \) annotates a state in \( M \) with a qualifier \( q_x \).

Example 4.7. Consider a query \( Q' = \text{courses/current/course[basic/cno/ text()=CS331]/(category/mandatory/regular/required/prereq/course} \). This \( \lambda_R \) query is represented by the ANFA \( M \) shown in Figure 6, where \( M = (M, \nu) \) and \( \nu(X) = M1 \).

More specifically, we define \( M_Q \) based on the structure of \( Q \) as follows.

(a) If \( Q \) is \( \epsilon \), then \( M = ([s], \Sigma, \delta, s, \{s\}, \theta) \), where \( \delta(s, \epsilon) \) is the only defined transition (\( \epsilon \)-transition). The mappings \( \theta() \) and \( \nu() \) are undefined.

(b) If \( Q \) is a label \( B \), then \( M = ([s, f], \Sigma, \delta, s, \{f\}, \theta) \), where \( \delta(s, B) = \{f\} \) is the only defined transition. The mappings \( \theta() \) and \( \nu() \) are undefined.

(c) If \( Q \) is \( Q_1 \cup Q_2 \), assume that \( M_{Q_i} = (M_{Q_i}, \nu_{Q_i}) \) is the ANFA representing \( Q_i \) for \( i \in [1, 2] \). We define \( M_Q \) as the union of \( M_{Q_1} \) and \( M_{Q_2} \) as for standard NFAs [Yu 1996], and \( \theta() \) as the union of \( \theta_1() \) in \( M_{Q_1} \) and \( \theta_2() \) in \( M_{Q_2} \); similarly for \( \nu() \). We assume w.l.o.g. that the name \( X_q \) of a subqualifier \( q \) is uniquely identified by \( q \) in both \( \nu_{Q_1} \) and \( \nu_{Q_2} \).

As for standard NFAs, \( M_Q \) can be defined for \( Q_1/Q_2 \) and \( Q_1^* \) in terms of the concatenation and Kleene closure of ANFA’s, respectively.

Similarly, \( p/text() \) is a special case of \( Q_1/Q_2 \) in which \( Q_2 \) is represented by an ANFA with a single transition defined by \( \text{str} \).

(d) If \( Q \) is \( p[q] \), assume that \( M_{p} = (M_{p}, \nu_{p}) \) and \( M_{q} = (M_{q}, \nu_{q}) \) are the ANFA’s representing \( p \) and \( q \), respectively, where \( M_{p} = \langle K_{p}, \Sigma, \delta_{p}, s_{p}, F_{p}, \theta_{p} \rangle \). We define \( M_{Q} \) to be \( \langle K_{p}, \Sigma, \delta_{p}, s_{p}, F_{p}, \theta \rangle \), where \( \theta() \) is an extension of \( \theta_p() \) by letting \( \theta(f) = X_q \), for all \( f \in F_p \), and \( \nu() \) be an extension of the union of \( \nu_p \) and \( \nu_q \) by letting \( \nu(X_q) = M_{q} \).

The remaining cases cover the translation of a qualifier (Boolean expression) \( q \) in an \( \lambda_R \) query (e.g., \( p[q] \)) to an ANFA form. Recall from Section 2.2 the definition of qualifiers. The translation of \( q \) is inductive based on the structure of \( q \), in which the ANFA for a subexpression of \( q \) may be constructed by one of the cases (a)-(d) and the cases below.
(e) If \( q \) is \( p \), assume that \( M_p = (M_p, \nu_p) \) is the ANFA representing \( p \). Then \( M \) is defined as in (a), except that \( \theta(s) = X_p \) and \( \nu(X_p) = M_p \).

(f) If \( q \) is \( p/text() = c \), assume that \( M_p = (M_p, \nu_p) \) is the ANFA representing \( p \). Then \( M_q \) is defined as in case (a), except that \( \theta(s) = [X_p/text() = c] \) and \( \nu(X_p) = M_p \).

(g) If \( q \) is \( position() = k \), then \( M \) is defined as in case (a), except that \( \theta(s) = [position() = k] \).

(h) If \( q \) is \( \lnot q_1 \), assume that \( M_{q_1} = (M_{q_1}, \nu_{q_1}) \) is the ANFA representing \( q_1 \). Then \( M \) is defined as in case (a), except that \( \theta(s) = [\lnot X_{q_1}] \), and \( \nu() \) is an extension of \( \nu_{q_1} \) by letting \( \nu(X_{q_1}) = M_{q_1} \).

(i) If \( q \) is \( q_1 \land q_2 \), assume that \( M_{q_i} = (M_{q_i}, \nu_{q_i}) \) is the ANFA representing \( q_i \) for \( i \in \{1, 2\} \). We define \( M_q \) as in case (a), except that \( \theta(s) = [X_{q_1} \land X_{q_2}] \) and \( \nu() \) is an extension of the union of \( \nu_{q_1} \) and \( \nu_{q_2} \) by letting \( \nu(X_{q_i}) = M_{q_i} \).

Similarly for the case when \( q \) is \( q_1 \lor q_2 \).

Along the same lines as the translation from standard \( NFA \)'s to regular expressions [Yu 1996], one can restore an \( \lambda_R \) query \( Q \) from its ANFA representation \( M_Q \). In fact it is easy to develop an algorithm for directly evaluating the ANFA \( M_Q \) on an XML tree following the semantics of \( \lambda_R \) query evaluation on XML trees [Marx 2004]. Indeed, evaluation algorithms and optimization techniques have been developed for a similar automaton representation of regular XPath queries [Fan et al. 2007], which have shown to outperform several commercial systems for evaluating XPath queries (to the best of our knowledge, a commercial system for regular XPath is not yet in place). We do not elaborate the evaluation algorithms as they are beyond the scope of this paper.

**Schema-Directed Query Translation.** We now present the definition of \( \text{Tr} \). Recall that \( \text{Tr} \) is a mapping from \( \lambda_R \) queries to ANFA’s that, given any XML query \( Q \in \lambda_R \), yields an ANFA \( \text{Tr}(Q) \) representing an \( \lambda_R \) query \( Q' \) such that for any \( T \in \mathcal{T}(S_1) \), \( Q(T) = Q'(\sigma_d(T)) \). The translation function \( \text{Tr} \) combines the definition of ANFA’s \( M_Q \) for a query \( Q \) with the mapping \( \delta \) on \( \lambda_R \) paths given in Section 4.2.

This translation is schema-directed in that a translation of each subexpression \( q \) of \( Q \) is made relative to each element type \( A \) appearing in schema \( S_1 \). To see why a schema-directed translation is required, consider the source and target schemas of Figure 7. In this figure, a very simple schema embedding is considered in which, for all tags \( X, Y, \lambda(X) = X \) and \( \text{path}(Y, X) = X \) (if \( (Y, X) \) is an edge in the source schema), when \( X, Y \) range over \( r, A, B \) and \( C \). One
might be tempted to think that query translation would be simple in this case, and that \( Q \) itself would work on the target schema. Indeed, simply substituting \( \text{path}(Y, X) \) for each edge \((Y, X)\) in the source schema would yield the same query \( Q \) on target documents specified by the schema shown in Figure 7(b).

However, consider a query \( Q = r/(A \cup B \cup C)^* \). Clearly, such a query does not return any \( C \) children of \( B \) elements when run on \( S_1 \), but will return such nodes when run on \( \sigma_d(T) \), since the \( C \)-child of \( B \) is a required node and will be added by the instance level mapping of Section 4.2. It is thus evident that the simple translation strategy by substituting \( \text{path}(Y, X) \) for \((Y, X)\) does not work. Our schema-directed construction avoids such problems by matching target nodes only when they will be generated by nodes in the source schema by \( \sigma_d() \).

More specifically, given an \( \chi_R \) query \( Q \) over \( S_1 \), \( \text{Tr}(Q) \) is computed by using the following functions. (i) For each element type \( A \) in \( E_1 \) and each subquery \( Q_1 \) of \( Q \), the local translation \( \text{Tr}_l(Q_1, A) = (M, \nu) \) is the \( \text{ANFA} \) presenting an \( \chi_R \) query \( Q_2 \) over \( S_2 \) such that for any instance \( T \) of \( S_1 \) and any element \( a \) of type \( A \) in \( T \), the result of evaluating \( Q_1 \) at \( a \) in \( T \) is the same as the result of evaluating \( Q_2 \) at \( a' \) on \( \sigma_d(T) \), where \( a' \) is mapped from \( a \) by \( \sigma_d \). (ii) For each final state \( f \) in \( M \), the label \( \text{lab}(f, M, A) \) associates an element type of \( S_1 \) with \( f \), which indicates the type of the elements reached via \( Q_1 \) when evaluated at an \( A \) element in an instance \( T \) of \( S_1 \). As will be seen shortly, the construction of the \( \text{ANFA} (M, \nu) \) ensures that each final state \( f \) in \( M \) is associated with a single type of \( S_1 \).

To handle the case that \( \text{Tr}_l(Q_1, A) \) will never return any nodes, we introduce a special automaton \( \text{Fail} \), which can be thought of as consisting of a single start state with no transitions and no final states. Note that any automaton with no final states is equivalent to \( \text{Fail} \), and thus special cases can be introduced in other rules below to handle the case that an automaton for a subexpression is equivalent to \( \text{Fail} \). However, to keep the presentation simple, we assume that a standard useless state removal algorithm is run on each completed automaton, which removes states that cannot reach a final state.

We compute \( \text{Tr}_l(Q_1, A) \) and \( \text{lab}() \) based on the structure of query \( Q_1 \) as follows. (a) If \( Q_1 \) is \( \epsilon \), \( \text{Tr}_l(Q_1, A) \) is the \( \text{ANFA} \) as defined in case (1a), and \( \text{lab}(s, M, A) = A \). (b) If \( Q_1 \) is a label \( B \) and \( \text{path}(A, B) \) is defined (i.e., \( B \in P(A) \)), then \( \text{Tr}_l(Q_1, A) \) is the \( \text{ANFA} \) coding the \( \chi_R \) query \( \text{path}(A, B) \), and \( \text{lab}(f, M, A) = B \), where \( f \) is the (single) final state of \( M \). If \( Q_1 \) is a label \( B \) and \( \text{path}(A, B) \) is not defined, then \( M_{Q_1} \) is \( \text{Fail} \).

(c) If \( Q_1 \) is \( p_1 \cup p_2 \), then \( \text{Tr}_l(Q_1, A) \) is the union of the \( \text{ANFA}'s \) \( \text{Tr}_l(p_1, A) \) and \( \text{Tr}_l(p_2, A) \), and the function \( \text{lab}() \) is the union of labels for the final states (if any) of \( \text{Tr}_l(p_1, A) \) and \( \text{Tr}_l(p_2, A) \). We assume w.l.o.g. that \( \text{Tr}_l(p_1, A) \) and \( \text{Tr}_l(p_2, A) \) have distinct final states.

(d) If \( Q_1 \) is \( p_1/p_2 \), assume that \( \text{Tr}_l(p_1, A) = (M_1, \nu_1) \) and \( L(M_1, A) \) is the set of labels \{\( \text{lab}(f, M_1, A) \mid f \) is a final state of \( M_1 \)\}. For each \( B \in L(M_1, A) \), let \( \text{Tr}_l(p_2, B) = (M_B, \nu_B) \) be the \( \text{ANFA} \) representing the local translation of \( p_2 \) at context type \( B \). Then the \( \text{ANFA} \) \( \text{Tr}_l(Q_1, A) \) is defined to be \((M, \nu)\), where \( M \) is the concatenation of \( M_1 \) and all \( M_B \)'s by connecting via \( \epsilon \)-transition the final state \( f \) of \( M_1 \) and the start state of \( M_B \) if \( \text{lab}(f, M_1, A) = B \), \( \nu \) is the union of \( \nu_1 \) and
all the $v_B$'s. The set $F$ of final states of $M$ is the union of the final states for the $M_B$'s, and similarly the label function for the final states of $M$ is defined to be the union of those label functions for $M_B$'s.

Similarly for the case when $Q_1$ is $p/\text{text()}$, except that here $\text{Tr}(p_2, B)$ represents the $\text{X}_B$ query path $(B, \text{str})$, and all the final states of $\text{Tr}(p_2, B)$'s are merged into a single final state $f_s$, for which $\text{lab}(f_s, M, A) = \text{str}$.

(e) If $Q_1$ is $p[q]$, assume that $\text{Tr}(p, A) = (M_p, v_p)$ and $L(M_p, A)$ is the set of labels $\{\text{lab}(f, M_p, A) \mid f$ is a final state of $M_p\}$. For each $B \in L(M_p, A)$, let $\text{Tr}(l[q], B) = (M_B, v_B)$ be the ANFA representing the local translation of $[q]$ at context type $B$. Then $\text{Tr}(l[q], A)$ is defined to be $(M, v)$, where $M$ is an extension of $M_p$ such that for any final state $f$ of $M_p$, $\theta(f) = X_B$ if $\text{lab}(f, M_p, A) = B$, and $v(X_B) = \text{Tr}(l[q], B)$. The label function of $\text{Tr}(l[q], A)$ is the same as that of $\text{Tr}(p, A)$.

We now present the translation of qualifiers $q$.

(f) If $q$ is $p$, then $\text{Tr}(q, A)$ is defined as in case (2a), except that $\theta(s) = X_p$ and $v(X_p) = \text{Tr}(p, A)$.

(g) If $q$ is $p/\text{text()} = c$, then $\text{Tr}(q, A)$ is defined as in case (2a), except that $\theta(s) = [X/\text{text()} = c]$ and $v(X) = \text{Tr}(p, A)$.

(h) If $q$ is $\text{position()} = k$, then $\text{Tr}(q, A)$ is defined as in case (2a), except that $\theta(s) = [\text{position()} = k]$.

(i) If $q$ is $\neg q_1$, then $\text{Tr}(q, A)$ is defined as in case (2a), except that $\theta(s) = [\neg X]$, and $v()$ is an extension of $v_{q_1}$ by letting $v(X) = \text{Tr}(q_1, A)$, where $v_{q_1}$ is the annotation of $\text{Tr}(q_1, A)$.

(j) If $q$ is $q_1 \land q_2$, $\text{Tr}(q, A)$ is defined as in case (2a), except that $\theta(s) = [X_1 \land X_2]$, and $v()$ is an extension of the union of $v_{q_1}$ and $v_{q_2}$ by letting $v(X_i) = \text{Tr}(q_i, A)$, where $v_{q_i}$ is the annotation of $\text{Tr}(q_i, A)$ for $i \in \{1, 2\}$.

Similarly for the case when $q$ is $q_1 \lor q_2$.

Finally we consider translation of Kleene-star constructs.

(k) If $Q_1$ is $p^*$, the computation of $\text{Tr}(Q_1, A)$ requires an iteration. For each element type $B$ in $S_1$, we define a Boolean flag $\text{visited}(B)$, which is initially set to false. The computation is conducted as follows. We first compute $\text{Tr}(p, A)$ and set $\text{visited}(A)$ to true. Let $M = (M, v)$ be $\text{Tr}(p, A)$. While there exists a final state $f$ in $M$ such that (a) $\text{lab}(f, M, A) = B$, (b) $\text{visited}(B)$ is false for some $B$ in $S_1$ and (c) $\text{Tr}(p, B) \neq \text{fail}$, then assuming that $\text{Tr}(p, B) = (M_B, v_B)$, the following three steps are taken: (i) Concatenate $M$ with $M_B$ by connecting $f$ to the initial state of $M_B$ via $\epsilon$-transition and extend the states, transition function, final states and the $\theta$ function of $M$ by including the counterparts of $M_B$. The initial state of $M$ remains unchanged. (ii) Set $\text{visited}(B)$ to true. (iii) Extend $v$ by including $v_B$. This process is repeated at most $|S_1|$ times since each iteration marks at least one element type in $S_1$ to true. Upon the completion of the process, we extend the final states of $M$ by including its initial state (to capture the case of $p^*$), and define $\text{Tr}(Q, A)$ to be $M$ obtained as above.

Given these, we define $\text{Tr}(Q)$ to be $\text{Tr}(Q, r_1)$. The proof of the following theorem is straightforward by induction on the structure of $Q$. 
Theorem 4.2. The functions \( \text{Tr}_l(Q_1, A) \) and \( \text{lab}(\cdot) \) are well defined, and for any instance \( T \) of \( S_1 \), \( Q(T) = Q'(\sigma_d(T)) \), where \( Q' \) is the \( \lambda_R \) query represented by ANFA \( \text{Tr}(Q) \).

Example 4.8. Consider \( Q = \text{class}[\text{cno}/\text{text()=}’\text{CS331}’] /(\text{type}/\text{regular}/\text{prereq} /\text{class})’ \). Over the DTD \( S_0 \) of Figure 1(a), this \( \lambda_R \) query is to find all the classes that are (direct or indirect) prerequisites of CS331. It is translated to the ANFA shown in Figure 6, which represents the \( \lambda_R \) query \( Q' \) given in Example 4.7. Over the DTD \( S \) of Figure 1(c), \( Q' \) is equivalent to \( Q \) w.r.t. the mapping \( \sigma_d \) given in Example 4.4, i.e. \( Q(T) = Q'(\sigma_d(T)) \) for any \( T \in \mathcal{I}(S_0) \), when evaluated on \( T \) with the root as the context node.

In contrast, the notion of graph similarity ensures neither invertibility nor query preservation w.r.t. \( \lambda_R \). As an example, the source and target schemas in Figure 3(a) are bisimilar by the conventional definition of graph similarity, which does not consider cardinality constraints of different DTD constructs. However, there exists no instance-level mapping from the source to the target with an inverse mapping or a query translation function.

4.5 Properties of Schema Embeddings

Theorem 4.1 has shown that the XML mapping \( \sigma_d \) of a valid schema embedding \( \sigma \) is guaranteed to be type safe. We next show that \( \sigma_d \) and \( \sigma \) have all the other desired properties.

Information Preservation. In contrast to Theorem 3.4, information preservation is guaranteed by schema embeddings. Recall the fragment \( \lambda_R \) of regular XPath from Section 2.

Theorem 4.3. The XML mapping \( \sigma_d \) of a valid schema embedding \( \sigma : S_1 \to S_2 \) is invertible and is query preserving w.r.t. \( \lambda_R \). More precisely, (a) there exists an inverse \( \sigma_d^{-1} \) of \( \sigma_d \) that, given any \( \sigma_d(T) \), recovers \( T \) in \( O(|\sigma_d(T)|^2) \) time; and (b) there is a query translation function \( \text{Tr} \) that given any \( \lambda_R \) query \( Q \) over \( S_1 \), computes an \( \lambda_R \) query \( \text{Tr}(Q) \) equivalent w.r.t. \( \sigma_d \) over \( S_2 \); furthermore, the query \( \text{Tr}(Q) \) has a bounded size \( O(|Q| \cdot |\sigma| \cdot |S_1|) \) and can be computed in \( O(|Q|^2 \cdot |\sigma| \cdot |S_1|^2) \) time if it is represented in an automaton format.

Proof. To show that \( \sigma_d \) is invertible and query preserving w.r.t. \( \lambda_R \), it suffices to define a query translation function \( \lambda_R \to \lambda_R \). For if it holds, then \( \sigma_d \) is query preserving w.r.t. \( \lambda_R \) and in addition, by Theorem 3.3 it is also invertible. By Theorem 4.2, \( \text{Tr} \) is just such a query translation function.

For the complexity of the query translation function \( \text{Tr} \), recall the definition of \( \text{Tr} \) given in Section 4.4. Note that the set of final states in an ANFA is bounded by \( |S_1| \) and that the size of the ANFA \( \text{Tr}(Q_1, A) \) is bounded by \( O(|Q| \cdot |\text{path}| \cdot |S_1|) \), which is less than \( O(|Q| \cdot |\sigma| \cdot |S_1|) \). The computation of \( \text{Tr}(Q_1, A) \) can be conducted by dynamic programming, and it takes at most \( O(|Q|^2 \cdot |\sigma| \cdot |S_1|^2) \) time to compute \( \text{Tr}(Q) \).

The inverse function \( \sigma_d^{-1} \) is defined along the same lines as the function in the proof of Theorem 3.3. Given any \( \sigma_d(T) \) in \( \mathcal{I}(S_2) \), it takes at most \( O(|\sigma_d(T)|^2) \) time to compute the source instance \( T \). □
Multiple Sources. In contrast to graph similarity, it is possible to embed multiple source DTD schemas to a single target DTD, as illustrated by the example below. This property is particularly useful in data integration.

Example 4.9. The embedding \( \sigma_2 = (\theta_2, \text{path}_2) \) below maps the source DTD \( S_1 \) of Figure 1(b) to the target DTD \( S \) of Figure 1(c).

\[
\begin{align*}
\lambda_2(\text{db}) &= \text{school} \\
\lambda_2(A) &= A & \text{/* A: student, ssn, name, taking, cno */} \\
\text{path}_2(\text{db, student}) &= \text{students/student} \\
\text{path}_2(\text{student, B}) &= B & \text{/* B: ssn, name, taking */} \\
\text{path}_2(\text{taking, cno}) &= \text{cno} \\
\text{path}_2(C, \text{str}) &= \text{text()} & \text{/* C: ssn, name, cno */}
\end{align*}
\]

Taken together with \( \sigma_1 \) of Example 4.2, this allows us to integrate a course document of \( S_0 \) and a student document of \( S_1 \) into a single school instance of the target DTD \( S \).

In general, given multiple source DTDs \( S_1, \ldots, S_n \) and a single target DTD \( S \), it is possible to define schema embeddings \( \sigma_i : S_i \to S \) to simultaneously map \( S_i \) to \( S \). In a nutshell, this can be done as follows. Assume that \( S_i = (E_i, r_i, P_i) \), and assume a certain order on \( S_1, \ldots, S_n \). To simplify the discussion, first assume that \( E_i \cap E_j = \emptyset \) for all \( i \neq j \). We can then define a single source DTD \( S' = (E', r', P') \) such that \( E' = E_1 \cup \ldots \cup E_n, r' \to P_1(r_1), \ldots, P_n(r_n) \) (following the order on the source DTDs), and for each \( A \in E' \), \( P'(A) = P_i(A) \) if \( P_i(A) \) is defined. Intuitively, \( S' \) merges multiple sources into a single source. Thus if there exists an embedding \( \sigma \) from \( S' \) to \( S \), \( \sigma \) can be decomposed into \( \sigma_i : S_i \to S \) such that the instance-level mapping \( \sigma'_i \) is invertible and query preserving w.r.t. \( \chi_R \).

In the general setting, if \( E_i \) and \( E_j \) are not disjoint, one can define \( S' \) as a specialized DTD [Papakonstantinou and Vianu 2000] to preserve the element type definitions of \( P_i \) and \( P_j \) on common element types. It is natural to extend the definition of schema embedding to specialized DTDs.

One can treat the target schema \( S \) as a global schema, and the XML mappings \( \sigma_i : S_i \to S \) as the definition of a global view of multiple sources \( S_1, \ldots, S_n \), following the global-as-view approach. The invertibility of \( \sigma_i \) assures that the view is exact [Lenzerini 2002]. The need for the query preservation is evident in this context since one wants to be able to query the source data via the global view. As observed in Fagin [2006], invertibility is also useful in defining new views via mapping compositions, and in data migration where the user may decide to “roll back” to the original data source; furthermore, it is helpful in data provenance, when one needs to recover the original source to trace the origin of certain data [Buneman et al. 2001].

Small Model Property. The result below gives us an upper bound on the length \( |\text{path}(A, B)| \), and allows us to reduce the search space when defining or finding an embedding.

Theorem 4.10. If there exists a valid schema embedding \( \sigma : S_1 \to S_2 \), then there exists one such that for any edge \((A, B)\) in \( S_1 \), \( l = |\text{path}(A, B)| \leq (k + 1)|E_2| \),
where \( S_1 = (E_1, P_1, r_1) \), \( S_2 = (E_2, P_2, r_2) \), and \( k \) is the size of the production \( P_1(A) \). More specifically,

- \( |\text{path}(A, B)| \leq k |E_2| \) if \( A \) is a concatenation type;
- \( |\text{path}(A, B)| \leq (k + 1) |E_2| \) if \( A \) is a disjunction type;
- \( |\text{path}(A, B)| \leq 2 |E_2| \) if \( A \) is a Kleene closure;
- \( |\text{path}(A, B)| \leq |E_2| \) if \( B \) is str.

**Proof.** Suppose that there is a valid embedding \( \sigma : S_1 \rightarrow S_2 \), where \( S_1 = (E_1, P_1, r_1) \) and \( S_2 = (E_2, P_2, r_2) \), and \( \sigma = (\lambda, \text{path}) \). Consider an arbitrary edge \((A, B)\) in \( S_1 \).

1. \( A \) is a concatenation type. Then \( \text{path}(A, B) \) is an \( \text{AND} \) \( \lambda_{R} \) path that can be simplified to one that contains at most \( k \) cycles, where \( k \) cycles may be necessary to ensure that \( \text{path}(A, B) \) is not a prefix of any \( \text{path}(A, B') \) for distinct subelement types \( B, B' \) of \( A \). Any other cycles can be removed, and all of the \( k \) cycles can be made simple cycles (i.e., a cycle that does not contain repeated labels), while the modified \( \sigma \) remains well defined. Thus \( |\text{path}(A, B)| \) is bounded by \( k |E_2| \).

2. \( A \) is a disjunction type. Then \( \text{path}(A, B) \) is a disjunction \( \lambda_{R} \) path that can be simplified to one that contains at most \( k + 1 \) simple cycles: \( k \) cycles to ensure that \( \text{path}(A, B) \) is not a prefix of any \( \text{path}(A, B') \), where \( B' \) is another subelement type of \( A \), and an additional cycle to include a dashed edge. After the simplification, the modified \( \sigma \) remains well defined. Thus \( |\text{path}(A, B)| \leq (k + 1) |E_2| \).

3. \( A \) is defined to be a Kleene closure \( A \rightarrow B^* \). Then \( \text{path}(A, B) \) is a \( \text{STAR} \) \( \lambda_{R} \) path, which can be simplified such that \( \text{path}(A, B) \) contains at most one simple cycle (to include a star edge). Thus \( |\text{path}(A, B)| \leq 2 |E_2| \).

4. \( A \) is defined to be \( A \rightarrow \text{str} \). As in (1), \( \text{path}(A, B) \) is no longer than \( |E_2| \). □

Transformation Language. The nice properties of schema embeddings suggest a language for specifying XML transformations. Given two DTDs \( S_1, S_2 \), one can specify a mapping from \( \mathcal{I}(S_1) \) to \( \mathcal{I}(S_2) \) by defining embedding \( \sigma = (\lambda, \text{path}) \), that is, specifying a mapping \( \lambda \) from types of \( S_1 \) to types of \( S_2 \), and a mapping from edges over \( S_1 \) to \( \lambda_{R} \) paths over \( S_2 \), both at the schema level in a declarative manner. Such an embedding specification \( \sigma \) yields an XML mapping \( \sigma_d \) of \( \sigma \) that guarantees the following: (1) it is type safe, that is, for any \( T \in \mathcal{I}(S_1) \), \( \sigma_d(T) \) conforms to the target schema \( S_2 \); (2) it is invertible, that is, there exists a quadratic time function \( \sigma_d^{-1} \) such that \( \sigma_d^{-1}(\sigma_d(T)) = T \) for any \( T \in \mathcal{I}(S_1) \), and (3) it is query preserving w.r.t. \( \lambda_{R} \), that is, there is a query translation function \( \text{Tr} \) such that for any \( Q \in \lambda_{R} \) and any \( T \in \mathcal{I}(S_1) \), \( Q(T) = \text{Tr}(Q)(\sigma_d(T)) \). This language is able to capture XML DTD mappings commonly found in data migration and integration, and provides a practical approach to defining XML schema mappings. One might want to define a mapping in a richer such as XQuery or XSLT. However, this is hampered by the negative results of Section 3, which tell us that the richer the language is, the more difficult it is to identify information-preserving mappings. In addition, many XML mappings found in practice can be expressed by annotating schemas with (regular) XPath expressions, along the same lines as schema embedding.
In this section, we state the computation problem for schema embeddings and briefly summarize several techniques for computing XML schema embeddings. Details of these techniques, as well as an experimental evaluation, are presented in Bohannon et al. [2005].

The problem of computing XML schema embeddings is formally stated as follows:

**PROBLEM:** Schema-Embedding

**INPUT:** Two DTD schemas $S_1$ and $S_2$ and a similarity matrix $\text{att}.$

**OUTPUT:** A schema embedding $\sigma : S_1 \rightarrow S_2$ valid w.r.t. $\text{att}$ if one exists.

Here $S_1 = (E_1, P_1, r_1)$ and $S_2 = (E_2, P_2, r_2)$.

In practice, it is useful to find an embedding $\sigma : S_1 \rightarrow S_2$ with as high a value for $\text{qual}(\sigma, \text{att})$ as possible (recall from Section 4.1 for the definition of $\text{qual}(\sigma, \text{att})$). The ability to efficiently find good solutions to this problem will lead to an automated tool that, given two DTD schemas, can compute candidate embeddings to recommend to users, or to rank schema matches that are known to participate in an information-preserving embedding higher than those that are not.

It turns out that if $\text{att}$ allows ambiguity, that is, if a single schema element in $S_1$ may map to more than one element of $S_2$, then it is intractable to solve Schema-Embedding. Worse still, it remains NP-hard for nonrecursive DTDs even when they are defined in terms of concatenation types only.

**Theorem 5.1.** The Schema-Embedding problem is NP-complete. It remains NP-hard for nonrecursive DTDs defined with concatenation types only.

**Proof.** An NP algorithm is as follows: guess a mapping, and then check whether it is an embedding. Theorem 4.4 gives maximum sizes that need to be guessed, and thus a mapping can be guessed in polynomial time. Checking whether or not a mapping is a valid embedding can also be done in PTIME.

For the NP-hardness, it suffices to show that the problem is NP-hard for nonrecursive DTDs, by reduction from 3SAT, which is NP-complete [Garey and Johnson 1979]. An instance of 3SAT is a well-formed Boolean formula $\phi = C_1 \wedge \cdots \wedge C_n$ of which we want to decide satisfiability.

Given an instance $\phi$ of 3SAT, we define two nonrecursive DTDs $S_1, S_2$ such that $\phi$ is satisfiable iff there is a valid schema embedding from $S_1$ to $S_2$. We define a similarity matrix $\text{att}$ such that for all element types $A$ in $S_1$ and $B$ in $S_2$, $\text{att}(A, B) = 1$, that is, there is no restriction on the mapping. Assume that all the propositional variables in $\phi$ are $x_1, \ldots, x_m$. We define $S_1, S_2$ as follows.

$S_1 = (E_1, P_1, r_1)$, where

$E_1 = \{ r_1, Z, W \} \cup \{ C_i \mid i \in [1, n] \} \cup \{ Y_s \mid s \in [1, m] \};$

$P_1$ is defined as:

$r \rightarrow C_1, \ldots, C_n, Y_1, \ldots, Y_m,$

$C_i \rightarrow Z, \ldots, Z; \quad /* n + i occurrences of Z */$

$Y_s \rightarrow W, \ldots, W; \quad /* 2n + s occurrences of W */$

$A \rightarrow \epsilon \quad /* for A ranging over W, Z */$
without violating the prefix-free property. We now formalize this intuition.

Consider that clauses are disjunctive, and thus clause \( \mu \) assignment below can only map to \( Y \) or \( s \) (or some ancestor thereof) in \( S \). In both \( Y \) and \( s \) can only map to \( T \) or \( F \) (or some ancestor thereof) in \( S \) due to the number of \( W \) children below \( Y \) and \( T \), \( F \) (technically, \( Y \) could map to some \( T \), \( s' > s \), but it is easy to see that for every \( Y \) to map successfully, it is necessary that \( Y \) maps to \( T \) or \( F \).

The mappings of the \( Y \) elements are to code the “negation” of a truth assignment \( \mu \) to variables in \( \phi \): \( Y \) is mapped to \( F \) if \( \mu(x) \) is true for some \( j \in [1, m] \), and \( Y \) is mapped to \( T \) if \( \mu(x) \) is false. To understand how this coding works, consider that clauses are disjunctive, and thus clause \( C \) can be satisfied by the correct assignment to any \( x \) appearing in \( C \) (i.e., to true if \( x \) appears in \( C \), and to false if \( \overline{x} \) appears in \( C \)). The paths into \( C \) thus correspond to the failure by a particular variable’s assignment to satisfy \( C \). If every variable fails to satisfy \( C \), then some \( Y \) will be mapped to every ancestor of \( C \) in \( S \), leaving no paths by which the \( C \) in \( S \) can be mapped to \( C \) in \( S \) without violating the prefix-free property. We now formalize this intuition.

We next show that \( S_1 \), \( S_2 \) are indeed a reduction from 3SAT, that is, there is a valid embedding from \( S_1 \) to \( S_2 \) if \( \phi \) is satisfiable. First, suppose that \( \phi \) is
satisfiable. Then there exists a truth assignment $\mu$ to $x_1, \ldots, x_m$ that satisfies $\phi$. We define an embedding $\sigma = (\lambda, \text{path})$ such that $\lambda(C_1) = C_i$, $\lambda(Z) = Z$, $\lambda(W) = W$, $\lambda(Y_j) = F_j$ and $\text{path}(r_1, Y_i) = X_i/F_i$ if $\mu(x_i)$ is true, $\lambda(Y_i) = T_i$ and $\text{path}(r_1, Y_i) = X_i/T_i$ if $\mu(x_i)$ is false. Furthermore, $\text{path}(r_1, C_i)$ is a path $\rho_i$ from $r_2$ to $C_i$ in $S_2$ such that there exists $j \in [1, m]$ and $X_j/T_j$ is on $\rho_i$ if clause $C_i$ is satisfied by $\mu(x_j) = \text{true}$, and $X_j/F_j$ is on $\rho_i$ if clause $C_i$ is satisfied by $\mu(x_j) = \text{false}$; since $\phi$ is satisfied by $\mu$, there must exist such a variable $x_j$ for every $C_i$.

It is easy to verify that it is easy to verify that $\sigma$ is indeed an embedding from $S_1$ to $S_2$.

Conversely, suppose that there exists a valid embedding $\sigma = (\lambda, \text{path})$ from $S_1$ to $S_2$. Observe that $\sigma$ must have the following properties. (1) for each $x_j$ there exists $Y_j$ such that $\lambda(Y_j) = V_j$, where $V_j$ is either $T_j$ or $F_j$; and (2) for $i \in [1, n]$, $\lambda(C_i)$ is either $C_i$ or $V_j$, where $V_j$ is either $T_j$ or $F_j$, such that $\lambda(Y_j) \neq \lambda(Y_k)$ and $\lambda(Y_j)$ is not an ancestor or self of $\lambda(C_i)$ for $k \neq j, i \neq j$. This is because, by the definitions of $S_1, S_2$, (1) $\lambda(C_i)$ must have $n + i$ descendants of type $Z$, like $C_i$ in $S_1$; and (2) $\lambda(Y_j)$ must have $2n + j$ descendants of type $W$, and it may not be an ancestor of $\lambda(Y_k)$ or $\lambda(C_i)$, and vice versa. We define a truth assignment $\mu$ such that $\mu(x_i) = \text{true}$ if $\lambda(Y_i) = F_i$ and $\mu(x_i)$ is false if $\lambda(Y_i) = T_i$. As a result, for each clause $C_i$, $\lambda(C_i)$ is either $Z_j$ or a child of $Z_j$, where $Z_j$ is a truth value $T_j$ or $F_j$; furthermore, if $Z_j$ is true then $\lambda(Y_j) = F_j$, and if $Z_j$ is false then $\lambda(Y_j) = T_j$. That is, $C_i$ is satisfied by the truth assignment $\mu$. Thus it is easy to verify that $\mu$ satisfies $\phi$. □

In light of the intractability result we develop efficient and accurate heuristic algorithms for computing schema embedding candidates. Below we give an outline of these algorithms. The reader is encouraged to consult Bohannon et al. [2005] for the details of the algorithms and related experimental study.

5.1 Local Mappings

A local mapping is a schema mapping in which the domain is restricted to the schema elements appearing in a single production of the source schema $S_1$. We say that two local mappings conflict if they assign some source element $A$ to different target elements in $S_2$. Based on this observation, we decompose the problem of computing schema embeddings to a) finding alternative local mappings (the Local-Embedding problem) and b) assembling non-conflicting local mappings into a valid schema embedding (the Assemble-Embedding problem). Unfortunately, each of these problems is independently NP-complete:

**Theorem 5.2.** The Local-Embedding problem is NP-complete for nonrecursive DTDs.

**Proof.** The NP-hardness can be verified by reduction from 3SAT. We omit the full proof for brevity, but note that it differs from the proof of Theorem 5.1 in that source elements are restricted to map to exactly two target elements, rather than allowing them to map to any target element as in Theorem 5.1. □

**Theorem 5.3.** The Assemble-Embedding problem is NP-complete for nonrecursive DTDs.
**Proof.** This proof is omitted for brevity. The lower bound is again verified by reduction from 3SAT. This proof is similar in spirit to the proof of 5.1, but shows that the more restrictive problem where local embeddings are fixed remains NP-hard.

5.2 Computing Embeddings

In contrast to the previous results, it turns out that if $\lambda$ is fixed (equivalently, att is unambiguous), then a schema embedding, if it exists, can be computed in low polynomial time. In other words, when the semantic correspondences between tags in the source schema and tags in the target are unique, it is easy to identify local embeddings, that is, embeddings in which the a single production in the source schema is considered; furthermore, from the local embeddings a global embedding can easily assembled. The central idea is that an unambiguous local embedding can be found by solving the prefix-free path problem, which we define as follows: Given a source node $s$ and $n$ target nodes $t_1 \ldots t_n$, find $n$ paths $p_1 \ldots p_n$ such that a) each path originates at $s$, b) path $p_i$ terminates at $t_i$, and c) no path $p_i$ is a prefix of another path $p_j$. This problem can be solved in polynomial time on a DAG by a variant of depth-first search that, upon finding a path from $s$ to some target $t_i$, returns from that search without marking $t_i$ as done. The algorithm can be extended to handle cycles by first solving the problem on a DAG of the connected components in $S_2$. See Bohannon et al. [2005] for details.

This algorithm to find local embeddings given a fixed $\lambda$ immediately yields an algorithm to find global embeddings given a fixed $\lambda$. Furthermore, the ability to find local embeddings can be generalized slightly to serve as part of a family of heuristic approaches to solving the more general Schema-Embedding problem. The idea is to randomly order the possible target matches for a source element in order to generate a candidate local mapping, and then heuristically attempt to assemble a global mapping. If the attempt fails, new random orderings can be used in an attempt to find additional local mappings.

**Assembling Schema Embeddings.** Given the ability to find valid local embeddings, a complete schema embedding can be computed if a consistent assembly of these local embeddings can be found, that is one in which all assembled local embeddings agree on the mapping of $S_1$ schema elements. We consider three heuristic approaches to Assemble-Embeddings. The first two attempt to incrementally assemble a full embedding by finding local embeddings for elements in $S_1$ in some order, either Random, or Quality-Ordered. In Random, as the name implies, the elements of $S_1$ are visited in random order. In Quality-Ordered, a quality metric based on att is used to assign a quality to local embeddings, and the elements of $S_1$ are re-ordered according to decreasing quality. The idea is to start with “better” mappings in an effort to find a good solution. The final approach reduces the Assemble-Embeddings problem to that of finding high-weight independent sets in a graph, and uses an existing heuristic solution to the latter problem [Busygın et al. 2002] to produce partial or complete embeddings.

**Experimental Results.** Experimental results of running the above heuristics on a variety of real-world schemas are reported in Bohannon et al. [2005].
The results show that the Random approach finds a high percentage of correct solutions over a wide range of att accuracies, and that running times are in the range of seconds or minutes. From this it seems reasonable that practical tools for computing schema embeddings can be included in the data integration process, and further, that it is practical to search for information-preserving embeddings without asking humans to hand-check the results of the schema-matching step first—that is, when there is ambiguity in the target element to which some of the source elements should be mapped.

6. RELATED WORK

Other than Bohannon et al. [2005] and Barbosa et al. [2005], we are aware of no previous work that has considered information preservation for XML DTD schema mappings. Schema embedding was introduced in a preliminary version of this article [Bohannon et al. 2005]. The recent work [Barbosa et al. 2005] studies invertible XML-to-relation mappings that guarantee the source XML document to remain valid in the presence of updates to the mapped relations. More specifically, it considers lossless and valid XML shredding into relations such that the original XML documents can be recovered from their relational storage (invertibility). Similar to Theorem 3.4, an undecidability result is given in Barbosa et al. [2005] for deciding whether XML shredding into relations are invertible.

It characterizes DTDs in terms of datalog constraints and proposes a systematic approach to designing invertible XML shredding. The approach is based on a recursive rewriting system by means of (atomic) equivalence-preserving transformations, along the same lines as Abiteboul and Hull [1988] (see further on). This work differs from ours in the following. (a) It focuses on XML-to-relation mappings instead of XML-to-XML mappings. (b) It considers invertibility, but not XML query preservation. (c) Its rewriting system is quite different from the notion of schema embedding. Our notion of schema embedding extends graph similarity and allows multiple source DTD schemas to be mapped to a single structurally different target DTD. Furthermore, from a schema embedding an instance mapping can be automatically derived and it guarantees both invertibility and query preserving w.r.t. regular XPath queries. The ability of finding information-preserving XML-to-XML mappings is important for data integration, migration [Lenzerini 2002] and P2P systems [Fuxman et al. 2005; Kementsietsidis et al. 2003; Halevy et al. 2004], among other things.

Information preservation has been studied for nested relational and complex data models [Abiteboul and Hull 1988; Hull 1986; Miller et al. 1993, 1994]. Hull [1986] proposed several notions of dominance and studied their relationships in the relational model. In particular, it established the equivalence between query dominance (invertibility) and calculus dominance (the existence of an injective mapping defined in relational calculus). This is consistent with Theorem 3.2, which says that for any query language $\mathcal{L}$, if $\mathcal{L}$ is composable and can express the identity mapping, then the invertibility and query preservation w.r.t. $\mathcal{L}$ coincide; indeed, relational calculus is composable and can express the identity mapping. The notions of relative information capacity were revisited in [Miller et al. 1993, 1994], which showed, among other things, the invertibility in a
complex data model is undecidable, similar to Theorem 3.4. The focus of [Abiteboul and Hull 1988; Miller et al. 1994] has mainly been on the information capacity of type constructs in complex data models that unlike DTDs, do not have recursive constructs. Information preserving schema transformations have also been studied there, based on local structural transformation rules that preserve or augment information capacity. Our study of information preservation is inspired by the prior work: our notions of invertibility and query preservation are mild extensions of calculus dominance and query dominance [Hull 1986]. We revise these notions and study their basic properties for XML DTD schemas and XML queries. Our focus is to develop the notion of DTD schema embedding that preserves information by ensuring both effective invertible mapping and efficient XML query translation, without employing a recursive rewrite system that repeatedly applies local type construct transformation rules.

A wide variety of techniques have been developed to solve different forms of schema matching or mapping for relational, ER and object-oriented models [Athitsos et al. 2005; Castano et al. 2001; Lakshmanan et al. 1996; Li and Clifton 2000; Palopoli et al. 1998]; see Rahm and Bernstein [2001] for a recent survey). While these are not focused on XML DTD schema mapping, some techniques, such as linguistic analyses and machine learning, are useful for finding name/label similarity, which our algorithms take as input.

Closer to XML schema mapping are [Doan et al. 2001; Madhavan et al. 2001; Melnik et al. 2002; Melnik et al. 2003; Miller et al. 2001; Milo and Zohar 1998]. LSD [Doan et al. 2001] proposes machine-learning techniques that make use of instance-level information to determine XML DTD tag matching, which can be used to compute similarity matrix $\mathbf{att}$. Systems of [Madhavan et al. 2001; Melnik et al. 2002; Melnik et al. 2003] target a wide class of schemas and can be tailored to a variety of data models. The similarity flooding algorithm of [Melnik et al. 2002] provides a novel schema matching tool based on graph-similarity. Cupid [Madhavan et al. 2001] is a generic system that encompasses a variety of techniques such as linguistic analyses and context dependencies. Rondo [Melnik et al. 2003] proposes a powerful set of model mapping operators. For structure-level schema matching, these systems adopt graph similarity to map a single source schema to a target. TransScm [Milo and Zohar 1998] considers instance-level mappings based on schema matching, and uses a semi-automatic mechanism to match highly similar schemas. Clio [Miller et al. 2001] also focuses on deriving instance translation from schema matching. It specifies schema matches by inclusion dependencies from source to target, from which a schema mapping can be derived by means of chase techniques for reasoning about the dependencies. None of these considers information preservation.

Query preservation is related to query rewriting and query answering using views, which have been extensively studied for conjunctive and datalog queries in the relational model and for regular path queries on semistructured data ([Abiteboul and Duschka 1998; Calvanese et al. 2002; Levy et al. 1995]; see Halevy [2000] and Lenzerini [2002] for surveys). View-based query rewriting (resp. answering) mainly studies whether a given query on the source
can be answered using materialized data from a set of views (lossless), by translating the query to an equivalent query (resp. in a particular language) on the views. In contrast, query preservation deals with the issue whether all queries in an (infinite) query language on an XML source can be rewritten to equivalent queries over XML target (view). Moreover, the focus of this work is to generate XML "views" that automatically preserves all the queries in an XML query language, rather than to determine the losslessness of views. Note that Theorem 3.2 establishes a connection between invertibility and query rewriting; e.g., if the query language $L$ includes the identity query $id$, then a view $\sigma_d$ is invertible and $\sigma_d^{-1}$ is in $L$ if and only if $id$ has a rewriting in $L$ using $\sigma_d$.

There has also been recent work on data exchange based on schema mapping specified in terms of tuple generating dependencies (TGDs; see Kolaitis [2005] for a survey). This line of research considers mostly schema mapping between relational schemas, rather than XML schemas (except Arenas and Libkin [2005]). The focus is to decide, given a schema mapping specified by TGDs from source to target and TGDs on the target, as well as an instance of the source schema, whether or not there exists a solution, that is, an instance of the target schema that satisfies the TGDs? Furthermore, it investigates, in the presence of multiple solutions, the existence of a universal solution (the most general one) and the complexity to compute the universal solution. It aims to provide a guideline for materializing target instances in the data exchange context. The connection between universal solutions and certain query answers has also been explored. While certain query answers concern all possible instantiations of the target schema, our work focuses on the ability to restore the original source data and to answer all queries in a language on source data by queries in the same language on the target data. While Arenas and Libkin [2005] considers XML-to-XML mappings, its focus is on the consistency and certain query answers in connection with a given schema mapping defined via TGDs. This line of research differs from our work in that we aim at providing a systematic method for developing schema mappings that guarantee type safety, invertibility and query preservation. A schema embedding, even a local one, is defined in terms of edge-to-path mappings that are not expressible as TGDs. Invertible mappings and their practical need are studied in Fagin [2006]. It differs from this work in that it considers relation-to-relation mapping defined via TGDs; in contrast to XML mappings of schema embedding, a mapping defined via TGDs may map a source instance to multiple target instances; the focus of Fagin [2006] thus aims to find an appropriate notion of inverse for such mappings.

7. CONCLUSIONS
We have revised information-preservation criteria for XML mappings, and have established related separation, equivalence and complexity results. To cope with the difficulties of determining information preservation, we have introduced a novel notion of schema embedding for XML DTD schemas, from which an instance-level XML mapping is automatically derived and is guaranteed to be information preserving, type safe, and able to accommodate multiple source schemas. While we show that finding a schema embedding is NP-complete, we
have provided heuristic algorithms to compute embeddings, which are efficient
and accurate as verified by our experimental results [Bohannon et al. 2005].

This is a first step toward developing a practical tool for lossless XML data
migration and integration. There is naturally much to be done. One open prob-
lem concerns how to extend the notion of schema embedding to accommodate
XML Schema [Fallside (W3C) 2000], as commonly found in practice. XML Schema
is more involved than DTDs: it supports not only a richer type system (e.g., with
inheritance) but also integrity constraints. Indeed, it is already undecidable to
determine whether or not a schema in XML Schema is consistent, i.e., whether
there exists an instance conforming to the schema [Fan and Libkin 2002]. As a
consequence, all the negative results of Section 3 remain intact for XML Schema,
and it is nontrivial to develop a simple yet clean notion of schema embedding
for XML Schema to capture both types and constraints. On the other hand, it is
natural and not very difficult to extend schema embedding to specialized DTDs
proposed in Papakonstantinou and Vianu [2000], an extension of DTDs.

Another extension is by allowing certain queries in XQuery in the path() func-
tion. The need for this is evident in practice. In data integration, for example,
one often wants to group certain source data elements together and map the
grouped data to a target element. Referring to schema $S$ of Figure 1(c), for
example, one may want to group courses under taking of students in order to
map instances of $S$ to a student document. This calls for a nontrivial extension
of the path() function to support upward traversal and also group-by. We are
currently investigating this extension.

A third open problem concerns query preservation w.r.t. practical XQuery
fragments. While the results of Section 3 carry over to any XQuery fragments
that subsume regular XPath expressions, the notion of schema embedding has
to be extended in order to ensure query preservation w.r.t. these richer query
languages. In this context it is not clear whether the lower bound of Theorem 5.1
is tight; in other words, it remains unknown whether or not the problem of
finding (extended) schema embedding is still in NP.

Finally, it is important to develop a notion of partial information preserva-
tion. In some applications one may find the notion of information preservation
studied in this work too strong: one often wants to select part of the source data
and require this part of data to be transformed to a target document without
loss of information, instead of insisting on lossless mapping of the entire source
data. We are currently revising the notions of invertibility and query preser-
vation in response to this need, and are developing specification languages for
users to identify the part of source data for which the information should be
preserved.

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