IGI PUBLISHING **ITJ 4844**

701 E. Chocolate Avenue, Hershey PA 17033-1240, USA
Tel: 717/533-8845; Fax 717/533-8661; URL-http://www.igi-global.com

This paper appears in the publication, Journal of Database Management, Volume 20, Issue 2
edited by **Keng Siau © 2009, IGI Global**

Reverse Engineering from an XML Document into an Extended DTD Graph

Herbert Shiu, City University of Hong Kong, Hong Kong

Joseph Fong, City University of Hong Kong, Hong Kong

ABSTRACT

Extensible markup language (XML) has become a standard for persistent storage and data interchange via the Internet due to its openness, self-descriptiveness, and flexibility. This article proposes a systematic approach to reverse engineer arbitrary XML documents to their conceptual schema–extended DTD graphs—which is a DTD graph with data semantics. The proposed approach not only determines the structure of the XML document, but also derives candidate data semantics from the XML element instances by treating each XML element instance as a record in a table of a relational database. One application of the determined data semantics is to verify the linkages among elements. Implicit and explicit referential linkages are among XML elements modeled by the parent-children structure and `ID/IDREF(S)` *respectively. As a result, an arbitrary XML document can be reverse engineered into its conceptual schema in an extended DTD graph format.* [Article copies are available for purchase from InfoSci-on-Demand.com]

Keywords: *Data Semantics; Extended DTD Graph; Reverse Engineering; XML Document*

INTRODUCTION

As extensible markup language (XML) (Bray, Paoli, Sperbeg-McQueen, Maler, & Yergeau, 2004) has become the standard document format, the chance that users have to deal with XML documents with different structures is increasing. If the schema of the XML documents in document type definition (DTD) (Bosak, Bray, Connolly, Maler, Nicol, Sperberg-McQueen, Wood, & Clark, 1998) is given or derived from the XML documents right away (Kay, 1999; Moh, Lim, & Ng, 2000), it is easier to study the contents of the XML documents. However, the formats of these schemas are hard to read, not to mention rather poor user-friendliness.

XML has been the common format for storing and transferring data between software applications and even business parties, as most software applications can generate or handle XML documents. For example, a common scenario is that XML documents are generated and based on the data stored in a relational data-

base—and there have been various approaches for doing so (Thiran, Estiévenart, Hainaut, & Houben, 2004; Fernandez, Morishima, & Suciu, 2001). The sizes of XML documents that are generated based on the data stored in databases can be very large. Most probably, these documents are stored in a persistent storage for backup purposes, as XML is the ideal format that can be processed by any software applications in the future.

In order to handle the above scenario, it is possible to treat XML element instances in an XML document as individual entities, and the relationships from the different XML element types can be determined by reverse engineering them for their conceptual models, such as extended DTD graphs with data semantics. As such, users can have a better understanding of the contents of the XML document and further operations with the XML document become possible, such as storing and querying (Florescu & Kossman, 1999; Deutsch, Fernandez, & Suciu, 1999; Kanne, 2000).

This article proposes several algorithms that analyze XML documents for their conceptual schema. Two main categories of XML documents exist — data-centric and narrative. As the contents of narrative XML documents, such as *DocBook* (Stayton, 2008) documents, are mainly unstructured and their vocabulary is basically static, the necessity of handling them as structured contents and reverse engineering them into conceptual models is far less than that of handling data-centric ones. Therefore, this article will concentrate on data centric XML documents.

Referential Integrity in XML Documents

XML natively supports one referential integrity mechanism, which are `ID`/`IDREF`(`S`) types of attribute linkages. In every XML document, the value of an `ID` type attribute appears at most once and the value of the `IDREF`(`S`) attribute must refer to one `ID` type attribute value(s). An `IDREF`(`S`) type attribute can refer to any XML element in the same document, and each XML element can define at most one `ID` type attribute. Due to the nature of `ID`/`IDREF`(`S`) type attributes in XML documents, relationships among different XML element types can be realized and it is possible to use them to implement data semantics.

This article will discuss the various data semantics and the possible ways to implement them. The algorithms presented in the article are based on the observations of the common XML document structures.

1. Using the nested structure of an XML document (the relationship between a parent element and its child element[s]), in which the child elements implicitly refer to their parent element.
2. For an `IDREF` or `IDREFS` type attribute, the defining element is referred to the element(s) with an `ID` type attribute by the referred value. Such linkages are similar to the foreign keys in a relational database. The two associated element types are considered to be linked by an explicit linkage.
3. As an `IDREFS` type attribute can refer to more than one element, there is a one-to-many cardinality from the referring element type and the referred element type(s).

The schema of an XML document can restrict the order of the XML elements—and the order of the elements may be significant—which depends on the intentions of the original XML document designer. For example, two XML documents with their corresponding DTDs are shown in Table 1.

The two XML documents shown in Table 1 are storing the same data, which are the data of two couples. For the former one, its couple elements use the two `IDREF` type attributes to denote the corresponding `husband` and `wife` elements. However, the use of `ID`/`IDREF` cannot ensure a particular `husband` or `wife` element must be referred by one `couple` element only. For the latter XML document, the DTD restricts that the `husband` and `wife` elements must exist as a pair. Furthermore, the

Table 1. Two equivalent XML documents that can represent the same data

DTD	XML Document
<!ELEMENT couples (husband*,wife*,couple*)> <!ELEMENT husband EMPTY> <!ELEMENT wife EMPTY> <!ATTLIST husband hid ID #REQUIRED name CDATA #REQUIRED> <!ATTLIST wife wid ID #REQUIRED name CDATA #REQUIRED> <!ATTLIST couple hid IDREF #REQUIRED wid IDREF #REQUIRED>	<?xml version="1.0"?> <couples> <husband hid="A123456" name="Peter"/> <husband hid="B234567" name="John"/> <wife wid="X123456" name="Amy"/> <wife wid="Y234567" name="Bonnie"/> <couple hid="A123456" wid="X123456"/> <couple hid="B234567" wid="Y234567"/> </couples>
<!ELEMENT couples (husband,wife)*> <!ELEMENT husband EMPTY> <!ELEMENT wife EMPTY> <!ATTLIST husband hid ID #REQUIRED name CDATA #REQUIRED> <!ATTLIST wife wid ID #REQUIRED name CDATA #REQUIRED>	<?xml version="1.0"?> <couples> <husband hid="A123456" name="Peter"/> <wife wid="X123456" name="Amy"/> <husband hid="B234567" name="John"/> <wife wid="Y234567" name="Bonnie"/> </couples>

use of `ID` type attributes `hid` and `wid` ensures any husband and wife element instance must exist in the document at most once.

Extended DTD Graph

As XML element instances are treated as individual entities, the relationships from the element types are therefore related not only to the structure of the XML document but also to the linkages from the different types. As such, DTD cannot clearly indicate the relationships.

An extended DTD graph for XML is proposed to add data semantics into a DTD graph so that the data semantics can be clearly identified, which is an excellent way of presenting the structure of an XML document. As such, in order to visualize the data semantics determined based on the XML document with its optional schema, it will provide the notations to be used for presenting the various data semantics. This article uses the authors' notations of the extended DTD graph for presenting the structure and the data semantics from the elements, as follows:

1. The vertexes as squares are drawn on the graph for elements, and vertexes as circles are drawn for occurrence operators (`?`, `+` and `*`) and selection operator (`|`).
2. Attributes and simple elements are omitted from the graph, as they specify a particular attribute of their defining and parent elements respectively.
3. Data semantics, other than one-to-one and one-to-many cardinality relations, are presented in the graph as arrows pointing from the referring element to the referred element with suitable descriptions as legends.

Based on the above criteria, it is possible to consider the `ELEMENT` declarations only for constructing the extended DTD graph. Three types of `ELEMENT` declarations can be identified as follows:

1. An ELEMENT declaration defines sub-elements only.
2. An ELEMENT declaration involves sub-elements and #PCDATA as its contents.
3. An ELEMENT declaration that defines #PCDATA as its contents only.

The above three types correspond to the following three examples:

```
<!ELEMENT PARENT (CHILD1+, CHILD2*)>
<!ELEMENT MIXED_ELEMENT (#PCDATA | CHILD1 | CHILD2)*>
<!ELEMENT SIMPLE_ELEMENT (#PCDATA)>
```

For each ELEMENT declaration of the first type, the content model expression can be tokenized as individual elements and occurrence indicators and sequence separators (,), and represented as a tree structure with the element name as the root node. For example, the first example above can be visualized as the following tree diagram: in Figure 1, the sequence "," is implied in the diagram.

DTDs mostly contain more than one ELEMENT declaration but each element type can only appear once. Therefore, to construct the complete DTD graph for a DTD, the tree structures of all ELEMENT declarations in a DTD are constructed first and they are eventually merged by replacing each sub-element node in a tree by the tree structure of that element. Such merging is repeated until there is only one tree structure or all sub-elements have been replaced with their corresponding tree structures.

Cardinality / Participation

Element types are visualized as rectangles in the graph and a cardinality relationship is presented as an arrow pointing from the referring element type to the referred element type, with double-line and single line for total participation and partial participation respectively. The cardinality types, including one-to-one (1/1), one-to-many (1/m), many-to-one (m/1) and many-to-many (m/m), are shown as legends of the arrows. If the cardinality relationship is implemented as explicit ID/IDREF(S) linkages, the name of the ID type attribute of the referring element is appended to the legend, such as 1/m (parent_id). To identify explicit linkages from implicit linkages, cardinality relationships due to ID/IDREF(S) type attributes are shown as arrows with a curved line. Table 2 presents the eight possible combinations of arrows and legends.

N-ary relationship

An *n-ary* relationship is implemented as a particular element type involved in more than two binary relationships. To represent such a relationship, a diamond-shaped vertex is used

Figure 1. A sample extended DTD graph

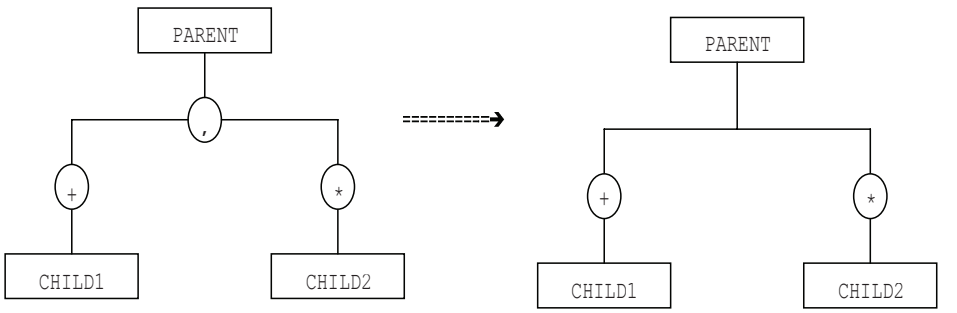


Table 2. The arrows illustrating various cardinalities with participation types

Cardinality \ Participation		
One-to-one	1/1	1/1
One-to-many	1/m	1/m
Many-to-one	m/1	m/1
Many-to-many	m/m	m/m

for such element types. Figure 2 presents a sample diagram with an *n-ary* relationship.

Aggregation Relationship

An aggregation relationship denotes that the involved element types must exist as a unity. In Figure 2, an aggregation exists as the defining characteristic of mandatory participation between parent and child elements. As such, a rectangle is to be drawn enclosing all involved element types.

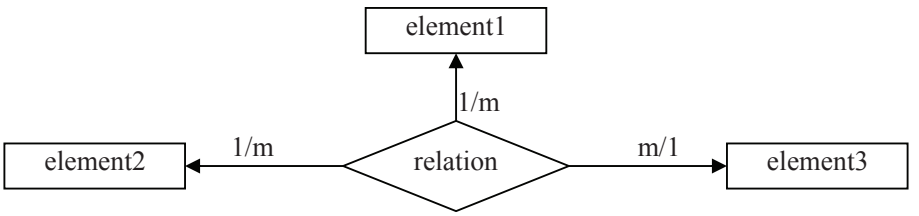
RELATED WORK

In order to have a complete picture of the reasons behind the algorithms for determining various data semantics, this article explains the existing approaches of constructing XML documents, especially those exported from relational databases.

The Determination of XML Schema

There is some existing work concerning the extraction of schema, such as DTD, from XML documents (Chidlovskii, 2001; Min, Ahn, & Chung, 2003). The outputs of these algorithms are the schemas that can validate the XML documents. However, the derived schemas provide no semantic interpretation other than the containment structures of the XML documents. The algorithms proposed in this article concern the determination of data semantics from the XML element instances rather than simply XML schema among XML elements. Compared with the approach proposed by Goldman and Widom (1997) that directly manipulates semi-structured databases, such as an

Figure 2. A sample diagram with an n-ary relationship



XML document, the algorithm proposed here provides the user with a clear picture of the data semantics from the XML element instances before further manipulating them.

The Determination of Data Semantics from XML Documents

One approach exists that can reverse engineer data semantics from XML documents (Fong & Wong, 2004), but the algorithm maps some predefined templates of document structures to data semantics, and the algorithm can only be implemented with DOM (W3C, 2003), which needs to read the entire XML document to the memory—and that is inappropriate for huge XML documents. The methodology presented in this article, however, determines basic candidate data semantics from arbitrary XML documents with SAX (Saxproject, 2004), which is applicable to XML documents of any size. Some of the determined data semantics may not be the intentions of the original writer and needs user supervision for verification.

The Implementation of Inheritance Among XML Elements

Schema for object-oriented XML (SOX)(W3C, 2005) introduced the idea of element and attribute inheritance, which enables an element to extend another element so that the derived element can have all attributes defined by the base element with its own new attributes.

Due to the limitations and low extensibility of DTD (Sahuguet, 2000), XML schema definition (XSD) (Sperberg, 2000) is becoming the popular replacement schema of DTD. Unlike DTD, XSD is an XML document itself and it can define more restrictive constraints and clear definitions of the XML documents to be validated. In other words, the set of capabilities for defining the structures and data types of XSD are the superset of that of DTD. As such, there has been research and software for converting DTD to XSD (Mello, 2001; W3C, 2000).

There are other alternative schemas, such as RELAX NG (RELAX NG, 2003) and Schematron (Schematron, 2008); and Lee and Chu () evaluated six common XML schemas, including DTD and XSD. As they are not as popular as DTD and XSD, they are not discussed in this article.

By constructing a graph by placing vertexes for elements—and the elements that are involved in a parent-child relation, which is defined by `ELEMENT` declaration in DTD, are connected with edges—it is possible to derive a graphical representation of the DTD that is commonly known as a DTD graph. Up to now, there is no formal standard for DTD graphs and various researchers are using their own conventions, as in Klettke, Schneider, and Heuer (2002), Shanmugasundaram, Shekita, Kiernan, Krishnamurthy, Viglas, Naughton, and Shematron (2001), Lu, Sun, Atay, and Fotouhi (2003), and Böttcher and Steinmetz (2003), and the graph introduced in Funderburk, Kiernan, Shanmugasundaram, Shekita, and Wei (2002) is the first one that was denoted as a DTD graph.

There is a graphical representation of XSD (Fong & Cheung, 2005), which derives an XML conceptual schema of an XML tree model from an XML schema of XSD. Its approach is different from this paper's approach by deriving an extended DTD graph from an XML document.

As the conventions of most graphs for presenting the structure of an XML document are applicable to different schema languages, the graph is also known as semantic graph (An, Borgida, & Mylopoulos, 2005). Some researchers proposed other graphical representations of XML schemas, such as the use of UML (Booch, Christerson, Fuchs, & Koistinen, 1999).

The Application of Extended DTD Graph

Data graph is a DTD in graph. Zhao and Ziau (2007) described that DTD can be a good common data model, when the majority of data sources are XML sources, for the interoperability between relational databases and XML databases. Reserve engineering XML docu-

ment into DTD graph is similar to data mining XML document into a data tree (Zhang, Lui, Ling, Bruckner, & Tija, 2006). The former is a database schema while the later is an internal data in tree structure. Trujillo and Luján-Mora (2004) demonstrated that a DTD can be used to define the correct structure and content of an XML document representing main conceptual multidimension model for data warehouses.

Compared with the approach proposed by Goldman and Widom (1997) that directly manipulates semi-structured databases such as an XML document, the algorithm proposed in this article enables the user to have a clear picture of the data semantics from the XML element instances before further manipulating them. Table 3 provides a comparison between the proposed algorithms and other existing approaches.

REVERSE ENGINEERING METHODOLOGY

There are basically two different definitions in a DTD, which are `ELEMENT` and `ATTLIST`. Each `ATTLIST` definition defines the attributes of a particular element, whereas `ELEMENT` defines its possible containments, and each `ELEMENT` definition can be represented in a tree structure with the element name as the root element with its child sub-elements as leaves, and there must be another `ELEMENT` definition for each of its child elements.

It is not mandatory to define the `ELEMENT` declaration prior to all its child elements, and it is actually uncertain which element is the root element of the corresponding XML documents. The root element of the XML document is defined by the `DOCTYPE` declaration before the root element start tag.

Implementations of Various Data Semantics in XML

The following subsections provide all possible implementations of various data semantics, some of which are consistent with those proposed by other researchers (Lee, Mani, & Chu, 2003; Lee & Chu, 2000).

Cardinalities

One-to-many cardinalities can be realized by both explicit and implicit referential linkages. By implicit referential linkages, a parent element can have child elements of the same type, such as,

```
<PURCHASE_ORDER>
  <PURCHASE_ORDER_LINE .../>
  <PURCHASE_ORDER_LINE .../>
</PURCHASE_ORDER>
```

Table 3. A comparison between the proposed and other existing approaches

	Proposed approach	Other approaches
Input	XML document with optional schema	XML document
Output	Conceptual schema with data semantics	Schema without data semantics
Completeness	All common data semantics can be determined	Schemas that can validate the XML document can be derived
User friendliness	Algorithms can be implemented with a user friendly GUI, such as the prototype	Commercial products exist that provide a user friendly GUI
Performance	Good	Not available as no mathematical proofs were provided

The parent element PURCHASE_ORDER and the child elements PURCHASE_ORDER_LINE are implicitly in a one-to-many relationship. If the occurrences of child element PURCHASE_ORDER_LINE are at most one for all PURCHASE_ORDER elements, they are in a one-to-one relationship instead.

If the schema of the XML document is given, it can specify the ID/IDREF(S) type attributes. If an XML element defines an IDREF attribute and all such elements refer to the same element type, there is a one-to-many relationship between the referred and referring XML elements. For example, sample DTD and XML documents are shown in Figure 3.

For explicit referential linkages, to determine if the cardinality is one-to-one or one-to-many, it is necessary to scan the entire XML document. An XML element type may be involved in more than one one-to-many relationship. In other words, all elements of such XML element types define more than one linkage. For example, if an XML element type defines an IDREF(S) type attribute, all elements of such XML element type actually define two linkages, one implicit linkage by the nested structure and one explicit linkage by the IDREF(S) type attribute. If the two linkages are both one-to-many relationships, the two referred element types by such a referring element type can be considered to be in a many-to-many relationship. For example, the XML document in Figure 4 illustrates a many-to-many relationship.

For an XML element type that defines two linkages and hence two one-to-many relationships, the two referred XML element types can be considered to be in a many-to-many relationship.

The linkages from the XML elements in an XML document are identified by the referring element name, linkage name and the referred element name. The algorithm shown in Figure 6 is used to determine Table 4 of the linkages.

Figure 5 illustrates the meanings of the four attributes.

There are eight XML elements in the document and there is only one implicit linkage from them. The values of the above four linkage attributes for such implicit linkage are:

Figure 3. A many-to-one cardinality implemented by an IDREF type attribute

```
<!ELEMENT PURCHASE_ORDER ...>
<!ELEMENT PURCHASE_ORDER_LINE ...>
<!ATTLIST PURCHASE_ORDER
  P   O_ID ID #REQUIRED
  .   ..
>
<!ATTLIST PURCHASE_ORDER_LINE
  P   O_ID IDREF #REQUIRED
  .   ..
>
<PURCHASE_ORDER PO_ID="PO001" ... />
...
<PURCHASE_ORDER_LINE
      PO_ID="PO001"
      ... />
<PURCHASE_ORDER_LINE
      PO_ID="PO001"
      ... />
```

Figure 4. A many-to-many cardinality implemented by an element type with two IDREF type attributes

```
<!ELEMENT KEYWORD ...>
<!ELEMENT TOPIC ...>
<!ELEMENT MESSAGE ...>
<!ATTLIST KEYWORD
KEYWORD_ID ID #REQUIRED
  . ..
>
<!ATTLIST TOPIC
TOPIC_ID ID #REQUIRED
  . ..
>
<!ATTLIST MESSAGE
MSG_ID ID #REQUIRED
TOPIC_ID IDREF #REQUIRED
KEYWORD_ID IDREF #REQUIRED
  . ..
>
<KEYWORD KEYWORD_ID="KW001" NAME="XML"/>
<KEYWORD KEYWORD_ID="KW002" NAME="DATABASE"/>
...
<TOPIC TOPIC_ID="TP001" NAME="Reverse Engineer an XML document"/>
<TOPIC TOPIC_ID="TP002" NAME="Exporting a database as an XML document"/>
...
<MESSAGE MSG_ID="MG001"
         TOPIC_ID="TP001"
         KEYWORD_ID="KW001"
.../>
<MESSAGE MSG_ID="MG002"
         TOPIC_ID="TP002"
         KEYWORD_ID="KW002"
.../>
```

Table 4. The attributes and their sources for determining data semantics

Attribute	Description	Value
MaxReferring	The maximum number of referred elements referred by a single referring element	Get from Referring Info with key *(RGE, RDE, L)*
MaxReferred	The maximum number of the referring elements that is referring to the same referred element with the same linkage type.	Get from Referred Info with key (*RGE*, *RDE*, *L*)
SumReferring	The number of referring elements that possess the linkage.	Get from ReferringInfo with key (*RGE*, *RDE*, *L*)
NumberElements	The number of referring elements in the document.	Get from ElementNameCount with key RGE

Figure 5. MaxReferring, MaxReferred, SumReferring, and NumberElements example

```
<?xml version="1.0"?>
<message id="ID1" ... >
   <message id="ID2" ... >
      <message id="ID3" ... >
      <message id="ID4" ... >
      <message id="ID5" ... >
   </message>
   <message id="ID6" ... >
      <message id="ID7" ... >
      <message id="ID8" ... >
   </message>
</message>
```

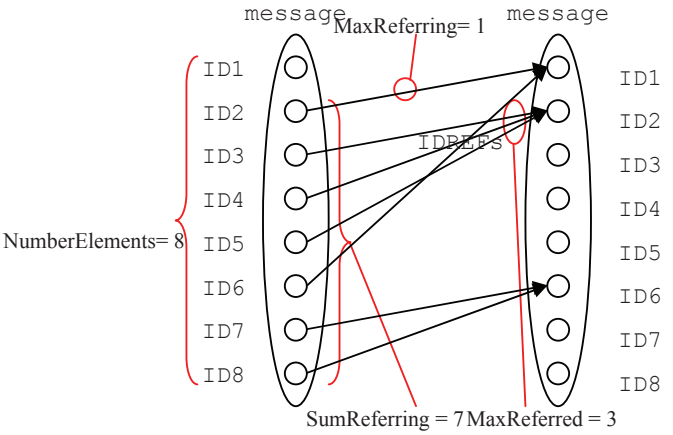


Table 5. Descriptions of variables in reverse engineering algorithms

Attribute Name	Value	Explanations
MaxReferring	1	All linkages are implicit and each child element has one implicit parent element only.
MaxReferred	3	The root message element with attribute ID value ID1 is referred by two sub elements (with attribute ID values ID2 and ID6). The message element with attribute ID value ID2 is referred by three sub elements (with attribute ID values ID3, ID4 and ID5). The message element with attribute ID value ID6 is referred by two sub elements (with attribute ID values ID7 and ID8). Therefore, the value of MND is 3.
SumReferring	7	Except the root message element with attribute id value ID1, all other message elements define such linkages. The value of NL is therefore 7.
NumberElements	8	There are eight message elements.

According to the combination of the values of the four attributes, it is possible to determine the cardinality data semantics for the involved elements. The rules are show in table 6.

The algorithm is composed of two passes of parsing of the same XML document. The first pass assigns a synthetic element identity to each XML element in the document and determines all `ID` type attribute values and their corresponding element types. For the second pass, the XML document is traversed again and the linkages of each XML element are investigated and their attributes are stored. Finally, the stored linkage attributes are consolidated to give the four linkage attributes mentioned above and in Table 4.

The algorithm shown in Figure 6 can determine whether the XML document is valid, in particular whether a non-existing ID value is referred by an IDREF(S) type attribute. If the XML document is valid, three tables can be obtained — *ReferringInfo*, *ReferredInfo*, and *ElementNameCount*. The key for the former two tables is the composite key (*RGE*, *RDE*, *L*), that is, the referring element name, the referred element name and the linkage name, whereas the key for the *ElementNameCount* is simply the element name. With three such tables, it

Table 6. Matrix for determining cardinality & participation based on the determined linkage attributes

		Participation	
		Total	Partial
Cardinality	One-to-one	MaxReferring= 1 MaxReferred = 1 SumReferring= NumberElements	MaxReferring = 1 MaxReferred= 1 SumReferring < NumberElements
	One-to-many	MaxReferring = 1 MaxReferred > 1 SumReferring = NumberElements	MaxReferring = 1 MaxReferred > 1 SumReferring < NumberElements
	Many-to-one	MaxReferring > 1 MaxReferred = 1 SumReferring = NumberElements	MaxReferring > 1 MaxReferred = 1 SumReferring < NumberElements
	Many-to-many	MaxReferring > 1 MaxReferred > 1 SumReferring = NumberElements	MaxReferring > 1 MaxReferred > 1 SumReferring < NumberElements

is possible to derive the linkage attributes as shown in Table 4.

The complete algorithm is presented in Figure 6 and the following is a list of definitions for the variables to be used:

Once the four attributes of a linkage are determined, the data semantics can be determined by using the matrix shown in Table 6. According to the determined one-to-one and one-to-many relationships, it is then possible to consolidate the related ones into many-to-many and *n-ary* relationships.

As mentioned above, if an XML element type defines two linkages that are determined to be many-to-one cardinalities, the two referred XML element types are considered to be in a many-to-many relationship. Similarly, if an XML element type defines more than two linkages that are determined to be many-to-one cardinalities, the referred XML element types are considered to be in an *n-ary* relationship. Therefore, based on the one-to-many cardinalities determined by the previous algorithm, the many-to-many and *n-ary* relationships can be determined, and the algorithm is shown in Figure 7.

The many-to-one relationship to be considered should be those implemented by explicit linkages; that is, those defined by ID/IDREF(S) linkages. Otherwise, an element type exhibits implicit a one-to-many relationship due to nested structure and defines a many-to-one relationship that will be considered to be a many-to-many relationship, but the two referred elements are actually not related at all.

PARTICIPATION

Participation concerns whether all instances of a particular element type are involved in a relationship with the corresponding element type.

For implicit referential linkage by a parent-child relation, such as the following DTD `ELEMENT` declaration,

```
<!ELEMENT PARENT (CHILD*)>
```

and there are no other `ELEMENT` declarations that define `CHILD` as their child elements, all `CHILD` element instances must appear as the child element of a `PARENT` element, and hence the participation can be considered to be total, as all instances of `CHILD` must be involved in the one-to-many cardinality relation with `PARENT`. If no schema is provided, and if all instances of an element type always appear as the child

Figure 6. The algorithm for determining linkage information by traversing the XML document

Variable name	Definition
EID	The current element ID. While processing the XML document sequentially, the EID determines the ID to be assigned to individual element encountered.
E	The current element to be handled.
A	An attribute of the current element to be handled.
AV	The attribute value of attribute *A*.
L	A linkage of the current element. It can be an implicit linkage with its parent element or an explicit linkage with an IDREF(S) type attribute. For a non-root element without IDREF(S) attribute, the element has only one implicit linkage to its parent element. Otherwise, the element can have more than one linkage, one implicit linkage and at least one explicit linkage.
L_{value}	The element ID of the linkage *L* for the current element *E*. For example, if *L* is an implicit linkage, L_{value} is the element ID of the parent element of *E*. Otherwise, L_{value} is the attribute value of IDREF value and the value should be an ID type attribute of an element in the same document.
NG	The number of referring element of the same element name is referring to the same referred element with the same link.
RGE	The referring element of a link.
RDE	The referred element by a link.

```
Pass One:
Let EID = 1;
Repeat until all XML document elements are read
    Let E be the current element to be processed
    If ∃ record in Table_ElementNameCount where ElementName = element name of E
        Get record (ElementName, NumberElement) from Table_ElementNameCount
        Increment NumberElement by 1;
        Update (ElementName, NumberElement) into Table_ElementNameCount;
    Else
        Add (ElementName, 1) into Set_ElementNameCount;
    End If
    Add (EID, ElementName) into Set_ElementIDName;
    If there exists ID type attribute A of element E with attribute value AV
        Add (AV, ElementName) into Set_ElementIDName;
    End If
    Increment EID by 1;
    Navigate to the next element E in the XML document

Pass Two:
Repeat until all XML document elements are read
    Let RGE is the current element to be handled
    For each linkage, L, of RGE
        For each linkage value, L_value of linkage L of RGE
            Get record (EID,ElementName) from Table_ElementIDName
                    where primary key value is L_value
            If no such record exist in Table_ElementIDName
                XML document is invalid
            Else
                Let RDE = ElementName of the record obtained from Table_ElementIDName
            End If

            Get record (RGE, RDE, L, L_value, ND) from Table_RawReferredInfo
                    for primary key (RGE, RDE, L, L_value);
            If record exists
```

continued on following page

Figure 6. continued

```
                    Increment ND of the record by 1;
                    Update the record to Table_RawReferredInfo;
                Else
                    Add record (RGE, RDE, L, L_value, 1) to the Table_RawReferredInfo;
                End If

                For each referred element type, RDE
                    Let NG = number of RDE referred by this linkage, L;
                    Get record (RGE, RDE, L, MaxReferring, SumReferring)
                        from the Table_ReferringInfo for primary key (RGE, RDE, L);
                    If record exists
                        If NG > MaxReferring from the record
                            Update MaxReferring of the record to be NG
                        End If
                        Increment SumReferring of the record by 1;
                        Update the record to the Table_ReferringInfo;
                    Else
                        Add record (RGE, RDE, L, NG, 1) to the Table_ReferringInfo;
                    End If
                End For
            End For
        End For
        Navigator to the next element RGE in the XML document

    Consolidate the records with same combination of (RGE, RDE, L) in table RawReferredInfo;
      let MaxReferred = maximum of the ND values of all records;
      Add record (RGE, RDE, L, MaxReferred) to the table ReferredInfo;


    The above operation can be represented by the following SQL,
    SELECT
        RGE, RDE, L,
        ReferringInfo.MaxReferring,
        ReferredInfo.MaxReferred,
        ReferringInfo.SumReferring,
        ElementNameCount.NumberElements
    FROM
        ReferringInfo
        INNER JOIN ReferredInfo
            ON ReferringInfo.RGE = ReferredInfo.RGE
            AND ReferringInfo.RDE = ReferredInfo.RDE
            AND ReferringInfo.L = ReferredInfo.L
        INNER JOIN ElementNameCount
            ON ReferringInfo.RGE = ElementNameCount.E
```

elements of the same parent element type, the participation is also considered to be total.

For explicit referential linkage by `ID/IDREF(S)` attributes, if all instances of an element type use the same attribute with values referring instances of the same element type, the relationship is considered to be total participation. Otherwise, the relation is considered to be partial. The DTD of the XML document can only identify the `ID/IDREF(S)` type attributes but it cannot restrict the referring and referred element types. As such, actually parsing the XML document is required to determine the type of participation.

Figure 7. The algorithm for determining many-to-many and n-ary relationships

```
Get referring XML element types from one-to-many cardinalities;
For each referring XML element T_referring type
        Get referred XML element types, S_referred referred by T_referring via explicit linkages;
        If the size of the set S_referred = 2
   XML element types in S_referred = many-to-many relationship with T_referring;
  Else
        If size of S_referred > 2
   XML element types in S_referred = n-ary relationship with T_referring;
```

Aggregation

An aggregation means that the creation of a whole part of an element depends on the existences of its component sub elements. An aggregation relation is signified by the scenario that elements of different types are considered to be a single entity and all constituting elements must exist altogether. An XML document by itself does not provide any facility to enforce such a constraint. At best, the schema can hint at the correlations of the existence of the elements in the corresponding XML document.

For implicit referential linkage by an aggregation relationship, such as the following DTD `ELEMENT` declaration,

```
<!ELEMENT AGGREGATION (COMPONENT1, COMPONENT2,….COMPONENTN)+>
```

For example, the following `ELEMENT` declaration can restrict the existence of the elements `enrollment`, `student`, and `course`.

```
<!ELEMENT enrollment (student, course)+>
```

Besides, no `student` or `course` elements exist in the document that are not the sub-elements of an `enrollment` element. For example, if there is another `ELEMENT` declaration in the same DTD, such as,

```
<!ELEMENT student_list (student*)>
```

`student` elements can exist in the document as the sub-elements of a `student_list` element. As such, the co-existence relationship of `enrollment`, `student` and `course` elements no longer holds.

Such a co-existence relationship specified in the schema can be extended to more than one nested level. For example, if the existence of a `course` element must be accompanied by a `lecturer` element and a `tutor` element, that is,

```
<!ELEMENT course (lecturer, tutor)+>
```

the elements `enrollment`, `student`, `course`, `lecturer`, and `tutor` must exist as a whole. Then, all these elements are considered as an aggregation relationship. From another perspective, an aggregation relationship is actually composed of two one-to-one cardinality relations (`course` – `lecturer` and `course` – `tutor`), which are both total participation.

An exceptional case is that if the sub-elements are actually the attribute of the parent element, such as in example one, it is inappropriate to consider that the involved elements are in an aggregation relationship. As a result, user supervision is needed in the process.

Based on the DTD of the XML document, it is possible to determine the aggregation relationships from the elements. As the requirements of an aggregation relationship is the co-existence of the involved elements and the order of the sub-elements for a parent

Figure 8. The algorithm for determining aggregation relationships

Let $Set_{temporary}$ = empty;
For each ELEMENT declaration for element E_{parent}
    For each child element, $element_{child}$

    If $element_{child}$ = mandatory and non-repeatable
        Add an aggregation relation (E_{parent}, E_{child}) to $Set_{temporary}$;

Let $Set_{aggregation}$ and Set_{root} = empty;
For each relation R (E_{parent}, E_{child}) in $Set_{temporary}$
    If ($\exists$ tree, T, in $Set_{aggregation}$) $\wedge$ (E_{parent} is a node in T) $\wedge$ (E_{child} is not a node in T)

Add a path E_{parent} to E_{child} to T;
    Else
        ($\exists$ tree, T, in $Set_{aggregation}$) $\wedge$ (E_{child} is a node of T) $\wedge$ (E_{parent} is not a node)

    If (E_{child} = root node) $\wedge$ (E_{child} not in Set_{root} of T)

Add the path E_{parent} to E_{child} to T;

    Else

    Add $E_{child}$to Set_{root}
        Remove the sub-tree starting with E_{child} from T;
        If $\exists$ sub-tree starting with E_{child} in multiple nodes
            Add sub-tree to $Set_{aggregation}$;
    Else
            $\exists$ tree T_i with a node for E_{parent} and T_j with E_{child} as root node;

    Merge trees T_i and T_j with a path from node for E_{parent} in T_i to root of T_j
    Else
        $\neg\exists$ subtree in $Set_{aggregation}$ with node for either E_{parent} and E_{child};

    Add a new tree with a path E_{parent} to E_{child} to $Set_{aggregation}$;

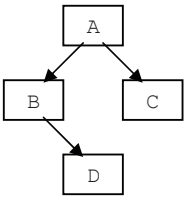
element is insignificant, the nested structure of the elements should first be simplified with the algorithm presented in Figure 8 where T is an aggregation tree.

The determination of aggregation relationships is separated into two parts. The first part first discovers the pair of parent and child elements that must co-exist. Once the pairs are determined, the second part of the algorithm treats each pair as a path from parent element to the child element in a sub-tree, and these sub-trees are merged to form a bigger tree. Eventually, the nodes in each tree must co-exist, and they are in aggregation relationship. The second part is straightforward except there is a tricky point that if a child element is found to be a non-root node of a particular sub-tree, it implies that such an element can have more than one parent element, and the aggregation relation that includes such element must start with the parent element.

For example, for a list of `ELEMENT` declaration in the DTD,

```
<!ELEMENT A (B, C)>
<!ELEMENT B (D)>
<!ELEMENT C (D)>
<!ELEMENT D (E, F)>
```

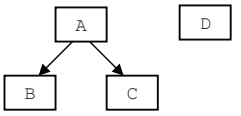
The determined pairs of raw aggregation relations are (A, B), (A, C), (B, D), (C, D), (D, E) and (D, F). While merging the raw aggregation relations,



Relations to be added

(C, D), (D, E) and (D, F)

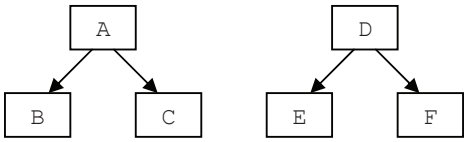
While adding the path (C, D) to the sub-tree, as D is not a root node, D should be removed from the sub-tree and it is considered to be an individual sub-tree with D as the single node.



Relations to be added

(D, E) and (D, F)

After the path (D, E) and (D, F) is added to the sub-tree with node D as the root node, two sub-trees are obtained,



As such, the elements A, B and C, and the elements D, E and F, are considered as being two individual aggregation relationships.

Case Study and Prototype

To illustrate the applicability and correctness of the algorithms mentioned in this paper, a prototype was built that implements the algorithms proposed in this paper. For actually drawing the DTD graph, the algorithm proposed by (Shiren, 2001) is used to define the layout of the vertexes on the graph. With such a prototype, a sample XML document with DTD file as shown in Figures 9 is provided to the prototype.

For this case study, both `ID/IDREF` type attributes are considered and the minimum number of common attributes is one. All elements with at least one attribute are sorted in ascending order of the lengths of their attribute lists. Therefore, the order of the elements to be processed is:

element1, element2, element3

According to the DTD of the XML document, only one `ELEMENT` declaration is used for constructing the extended DTD graph, as the contents of other element types are `EMPTY`.

```
<!ELEMENT test (element
   1*,element2*,element3*)>
```

Therefore, only those explicit one-to-many relationships are to be added to the graph, and the graph will become the one shown in Figure 10 and 11. The detailed derivation of the reverse engineering can be referred to in Shiu (2006).

Figure 9. test.xml and test.dtd

```
<?xml version="1.0"?>
<test>
  <element1 id="id1"/>
  <element1 id="id2"/>
  <element2 id="id3"/>
  <element2 id="id4"/>
  <element3 id="id5" idref1="id1" idref2="id3"/>
  <element3 id="id6" idref1="id2" idref2="id4"/>
  <element3 id="id7" idref1="id1" idref2="id4"/>
  <element3 id="id8" idref1="id2" idref2="id3"/>
</test>
```

```
<!ELEMENT test (element1*,element2*,element3*)>
<!ELEMENT element1 EMPTY>
<!ELEMENT element2 EMPTY>
<!ELEMENT element3 EMPTY>

<!ATTLIST element1
          id ID #REQUIRED>
<!ATTLIST element2
          id ID #REQUIRED>
<!ATTLIST element3
          id ID #REQUIRED
          idref1 IDREF #REQUIRED
          idref2 IDREF #REQUIRED>
```

Figure 10. The determined data semantics

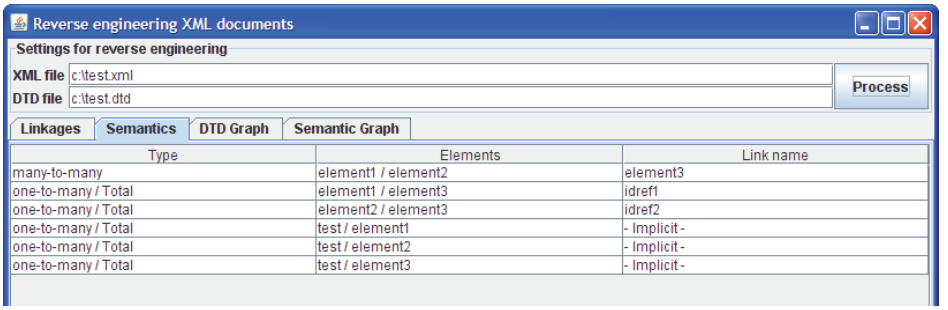
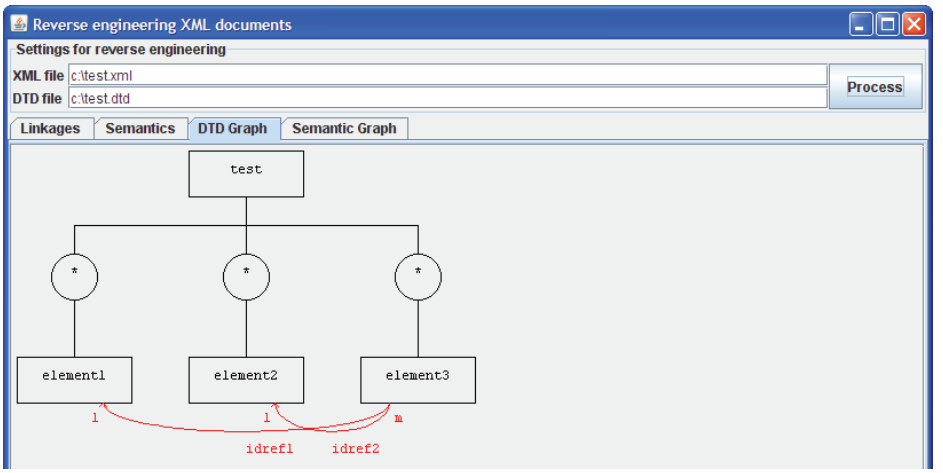


Figure 11. Extended DTD graph based on the DTD and the determined cardinality references



CONCLUSION

In order to make use of the XML document, software developers and end users must have a thorough understanding of the contents in the XML document, especially those historical and huge XML documents. Sometimes the schemas of XML documents are missing and the XML documents cannot be opened to be inspected on the screen due to their huge size. Therefore, it is necessary to determine as much information as possible regarding the relationships from the elements in the document.

By reverse engineering the XML document with DTD, all explicit linkages can be determined and the resultant DTD graph can be used to verify the correctness of `ID`/`IDREF`(`S`) linkages, as any incorrect `IDREF`(`S`) linkage will be indicated as an extra cardinality and shown in the extended DTD graph. This article provides algorithms to help the users to understand the relationships from the elements by reverse engineering data semantics from the XML document, including:

1. Cardinality relationships
2. Participation relationships
3. *n-ary* relationships
4. Aggregation relationships
5. Many-to-many relationships (a special case of cardinality relationships)

In summary, to visualize the determined data semantics, a new extended DTD graph is

proposed. XML documents natively support one-to-one, one-to-many and participation, data semantics. With a corresponding schema, such as DTD, the `ID` and `IDREFS` attributes of the elements can be identified, and many-to-many, *n-ary* and aggregation relationships can also be determined.

ACKNOWLEDGMENT

This paper is funded by Strategic Research Grant 7002325 of City University of Hong Kong.

REFERENCES

An, Y., Borgida, A., & Mylopoulos, J. (2005). Constructing complex semantic mappings between XML data and ontologies. In *Proceedings of the International Semantic Web Conference, ISWC 2005, Galway, Ireland (pp. 6-20)*.

Booch, G., Christerson, M., Fuchs, M., & Koistinen, J. (1999). UML for XML schema mapping specification. Retrieved from *http://xml.coverpages.org/fuchs-uml_xmlschema33.pdf*

Bosak, J., Bray, T., Connolly, D., Maler, E., Nicol, G., Sperberg-McQueen, C.M., Wood, L., & Clark, J. (1998). *Guide to the W3C XML specification (XMLspec) DTD* Version 2.1. Retrieved from http://www.w3.org/XML/1998/06/xmlspec-report-v21.htm

Bray, T., Paoli, J., Sperberg-McQueen, C.M., Maler, E., & Yergeau, F. (2004). *Extensible markup language (XML) 1.0* (3rd ed.). Retrieved from *http://www.w3.org/TR/2004/REC-xml-20040204*.

Böttcher, S., & Steinmetz, R. (2003). A DTD graph based XPath query subsumption test. In *Proceedings of the First International XML Database Symposium (XSym 2003), Berlin, Germany* (pp. 85-99).

Chidlovskii, B. (2001). Schema extraction from XML data: A grammatical inference approach. In *KRDB'01 Workshop (Knowledge Representation and Databases)*.

Deutsch, A., Fernandez, M., & Suciu, D. (1999). Storing semi-structured data with STORED. In *Proceedings of the 1999 ACM SIGMOD International Conference on Management of Data (SIGMOD)*, Philadelphia, Pennsylvania, USA (pp. 431-442)

Fernandez, M., Morishima, A., & Suciu, D. (2001). Publishing relational data in XML: The SilkRoute approach. *IEEE Data Engineering Bulletin, 24*(2),12-19.

Florescu, D., & Kossmann, D. (1999). Storing and querying XML data using an RDBMS. *Bulletin of the Technical Committee on Data Engineering, 22*(3), 27-34.

Fong, J., & Wong, H.K. (2004). XTOPO, An XML-based technology for information highway on the Internet. *Journal of Database Management, 15*(3), 18-44.

Fong, J., & Cheung, S.K. (2005). Translating relational schema into XML schema definition with data semantic preservation and XSD graph. *Information and Software Technology, 47*(7), 437-462.

Funderburk, J.E., Kiernan, G., Shanmugasundaram, J., Shekita, E., & Wei, C. (2002). XTABLES: Bridging relational technology and XML. *IBM Systems Journal, 41*(4).

Goldman, R., & Widom, J. (1997). DataGuides: Enabling query formulation and optimization. In VLDB'97, Proceedings of 23rd International Conference on Very Large Data Bases, Athens, Greece (pp. 436-445).

Kay, M. (1999). DTDGenerator – A tool to generate XML DTDs. Retrieved from *http://users.breathe.com/mhkay/saxon/dtdgen.html*

Klettke, M., Schneider, L., & Heuer, A. (2002). Metrics for XML document collections. In *Proceedings of the Workshops XMLDM, MDDE, and YRWS on XML-Based Data Management and Multimedia Engineering-Revised Papers* (LNCS 2490, pp. 15-28).

Koike, Y. (2001). A conversion tool from DTD to XML schema. Retrieved from *http://www.w3.org/2000/04/schema_hack/*

Lee, D.W., & Chu, W.W. (2000). Comparative analysis of six XML schema languages. *SIGMOD Records, 29*(3).

Lee, D.W., Mani, M., & Chu, W.W. (2003). Schema Conversion Methods between XML and Relational Models. *Knowledge Transformation for the*

Semantic Web. Frontiers in Artificial Intelligence and Applications, 95, 1-17.

Lee, D.W., & Chu, W.W. (2000). Constraints-preserving transformation from {XML} document type definition to relational schema. In *International Conference on Conceptual Modeling/The Entity Relationship Approach* (LNCS 1920, pp. 323-338).

Lu, S., Sun, Y., Atay, M., & Fotouhi, F. (2003). A new inlining algorithm for mapping XML DTDs to relational schemas. In *Proceedings of the First International Workshop on XML Schema and Data Management in Conjunction with the 22nd ACM International Conference on Conceptual Modeling (ER2003).*

Mello, R., & Heuser, C. (2001). A rule-based conversion of a {DTD} to a conceptual schema. In *Proceedings of the 20th International Conference on Conceptual Modeling,* Yokohama, Japan (LN CS 2224, pp. 133-148).

Min, J.K., Ahn, J.Y., & Chung, C.W. (2003). Efficient extraction of schemas for XML documents. *Information Processing Letters, 85*(1).

Moh. C., Lim, E., & Ng, W. (2000). DTD-Miner: A tool for mining DTD from XML documents. In *Proceedings of the Second International Workshop on Advanced Issues of E-Commerce and Web-Based Information Systems* (pp. 144-151).

Sahuguet, A. (2000). Everything you ever wanted to know about DTDs, but were afraid to ask. In *Selected Papers of the 3rd International Workshop WebDB-2000*, Dallas, TX, USA (LNCS 1997, pp. 171-183).

RELAX NG. (2003). *RELAX NG* Retrieved from *http://www.relaxng.org/.*

Semistructured Databases, *Very Large Data Bases, Proceedings of the 23rd International Conference on Very Large Data Bases*).

Shanmugasundaram, J., Shekita, E., Kiernan, J., Krishnamurthy, R., Viglas, E., Naughton, J., & Shematron. (2008). *Schematron*. Retrieved from *http://www.schematron.com/*

Shiren, Y., Xiujun, G., Zhongzhi, S., & Bing, W. (2001). Tree drawing algorithm and visualizing methods. In *CAD/Graphics'2001*.

Shiu, H. (2006). *Reverse engineering data semantics from arbitrary XML document*. Unpublished doctoral dissertation, Computer Science department, City University of Hong Kong.

Sperberg-MCQueen, C., & Thompson, H. (2000). W3C XML schema. Retrieved from *http://www.w3.org/XML/Schema*

Stayton, B. (2008). DocBook. Retrieved from *http://www.docbook.org/*

Tatarinov, I. (2001). A general technique for querying XML documents using a relational database system. *SIGMOD Record, 30*(3), 261--270.

Thiran, P.H., Estiévenart, F., Hainaut. J.L., & Houben, G.J. (2004). Exporting databases in XML - a conceptual and generic approach. In *Proceedings of CAiSE Workshops (WISM'04)*.

Trujillo, J., & Luján-Mora, S., (2004). Applying UML and XML for designing and interchanging information for data warehouses and OLAP applications. *Journal of Database Management, 15*(1), 41-72.

W3C. (1998). *Schema for object-oriented XML*. Retrieve3d from *http://www.w3.org/TR/1998/NOTE-SOX-19980930/*

W3C. (2003). *Document object model DOM*. Retrieved from *http://www.w3.org/DOM*

W3C. (2004). *Simple API for XML, SAX*. Retrieved from *http://www.saxproject.org/*

Zhang, J., Liu, H., Ling, T., Bruckner, R., & Tija, A. (2006). A framework for efficient association rule mining in XML data. *Journal of Database Management, 17*(3), 19-40.

Zhao, L., & Siau, K. (2007). Information mediation using metamodels: An approach using XML and common warehouse metamodel. *Journal of Database Management, 18*(3), 69-82.

Herbert Shiu was the project manager of a funded research project under the Department of Computer Science at City University of Hong Kong. He graduated with a BSc in computer science from the University of Hong Kong in 1992, a MSc, and MPhil in computer science from City University of Hong Kong in 1998 and 2006 respectively. He is now a PhD student at City University of Hong Kong. His current research interests are in database, XML and object-oriented software design and development.

Joseph Fong is currently an associate professor in the Department of Computer Science at City University of Hong Kong. He graduated at University of Sunderland in Computing in 1993. He is a fellow of Hong Kong Computer Society and an editorial board member of International Journal of Web Information Systems. *He was the founder chairman of the Hong Kong Computer Society Database Special Interest Group, the annual International Database Workshop, the Sybase Hong Kong User Group, the Hong Kong Web Society, the International Conference on Web-based Learning, and the International Conference on Hybrid Learning. His research interests are in database, data warehousing, data mining XML and hybrid learning. His above 100 publications include SCI Journals, Conferences, Patent (U.S. and Hong Kong), edited books, and text books on* Information Systems Reengineering and Integration *by Springer Verlag. He teaches data warehousing, data mining, data engineering, database systems and xml technologies. his expertise are in database reengineering and interoperability. He supervised and graduated three PhD students and eight MPhil students.*