A Progressive Clustering Algorithm to Group the XML Data by Structural and Semantic Similarity

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Abstract. *Since the emergence in the popularity of XML for data representation and exchange over the Web, the distribution of XML documents has rapidly increased. Therefore it is a new challenge for the field of data mining to turn these documents into a more useful information utility. We present a novel clustering algorithm PCXSS that keeps the heterogeneous XML documents into various groups according to the similar structural and semantic representations. We introduce a global criterion function CPSim that progressively measures the similarity between a XML document and existing clusters, ignoring the need to compute the similarity between two individual documents. The experimental analysis shows the method to be fast and accurate.*

1. Introduction

As the World Wide Web (WWW) becomes more prevalent for exchanging and discovering information, there is an increasing wealth of knowledge with the potential for finding information about anything. Moreover XML (eXtensible Markup Language) [35] has gained popularity for the representation and exchange of data over the Web. The explosive growth in XML sources presents an enormous opportunity and challenge for grouping XML data based on their context and structure for efficient data management and retrieval.

Clustering of XML documents facilitates a number of applications such as improved information retrieval, data and schema integration, document classification analysis, structure summary and indexing, data warehousing, and improved query processing [3, 25]. For example, the computation of structural similarity is a great value to the management of Web data. Many techniques for the extraction and integration of relevant information from Web data sources require grouping Web data sources according to their structural similarity [9, 11]. Efficient data management techniques such as indexing based on structural similarity can support an effective document storage and retrieval [25].

The clustering process is an unsupervised data mining technique that categories a large amount of data source without prior knowledge on the taxonomy [11]. Clustering has frequently been used on database objects, flat file data such as text files, and semi-structured documents like HTML. However, clustering of XML documents is more challenging. XML allows the representation of semi-structured and hierarchal data, containing not only the values of individual items but also the relationships between data items by tagging the pertinent information. Due to the inherent flexibility of XML, in both structure and semantics, clustering XML data is

faced with new challenges as well as benefits. Mining of structure along with content provides new insights and means into the process of clustering.

Consider parts of two documents: <*craft*>*boat building*</*craft*> and <*craft*> *boat* </*craft*>. The intended interpretation of the former is 'occupation', and of the latter 'vessel'. The similarity of the content does not distinguish the semantic intention of the tags. Use of structural similarity in this case provides probabilities of a tag having a particular meaning. For example, the paths \occupation\design\craft and \vessel\type\craft assist to determine the appropriate interpretation for such homographic tags. Hence, consideration of structure and content of documents in mining assist to clarify in case when two documents appearing similar are actually completely different.

A variety of clustering algorithms has recently emerged for XML document clustering, majority of them are built on pair-wise similarity between documents or schemas [4, 5, 8, 10, 15, 17, 21, 24]. The pair-wise similarity is measured using the *local* criterion function between each pair of documents to maximize the intra-cluster similarity and to minimize the inter-cluster similarity. Since each document is composed of many elements, the similarity between each pair of elements of two documents is measured and aggregated to form a similarity measure (distance) between two documents. A similarity matrix is generated that contains the similarity value for each pair of documents. This matrix is the input for the clustering process using either the hierarchical agglomerative clustering algorithm or k-means algorithms [13]. Pair-wise similarity can be computationally expensive when dealing with large data sources due to the need of measuring similarity between each pair of data.

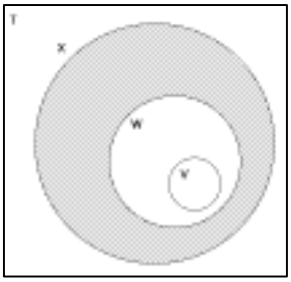
To reduce the computational efforts while maintaining the accuracy, we develop a *global* criterion function *CPSim* (common path coefficient) that measures the similarity between a XML data and existing clusters of XML data, instead of computing pair-wise similarity between each pair of data. The *CPSim* function includes the semantic as well as hierarchical structure similarity of elements. We then incorporate *CPSim* into progressively grouping the XML data.

This paper presents the novel ***P****rogressively* ***C****lustering* ***X****ML by* ***S****emantic and* ***S****tructural similarity (*PCXSS) algorithm that quantitatively determines the similarity between heterogeneous XML documents by considering the semantic as well as hierarchical structure similarity of elements. We show the effectiveness of PCXSS with several experiments. The results indicate that PCXSS is much faster than the pair-wise similarity based method and provides a good quality clustering solution as well. It is also not heavily influenced by thresholds such as the clustering and path similarity.

The next two sections briefly introduce the XML data and the PCXSS method. Sections 4 and 5 explain the pre-processing and clustering phases included in this method respectively. Section 6 details the empirical evaluation. Related work is covered in section 7. We finally conclude the paper in section 8.

2. XML Documents and schemas

XML is a flexible representation language. There are many varieties of XML material on the Web. Figure 1 illustrates the relationship between all XML materials. Let all textual objects be the set T. Let web pages containing XML - to be called XML material for the remainder of this discussion - be X, such that $X \subseteq T$. If D denotes the set of XML documents, then $D \subset X$, that is, XML material is not automatically classed as XML documents. Strictly, web pages are classed as XML documents only if they are well formed, D = W, where W is the set of well-formed XML documents. Additionally, $V \subseteq W$, where V is the set of valid XML documents. Finally, this allows the definition of ill-formed XML material, given as $X \cap \overline{W}$.



T: textual web objects,
X: XML material,
: ill-formed XML material,

W: well-formed XML documents,
V: valid XML documents

Figure 1: Venn diagram of XML

An XML document has a schema that defines the data definition and structure of the XML document [1]. A XML schema provides a definitive description of the document, while document instances give a snapshot of what the document may contain. The schema includes what elements are (and are not) allowed; what attributes for any elements may be and the number of occurrences of elements; etc.

To be well-formed, a page's XML must have properly nested tags, unique attributes (per element), one or more elements, exactly one root element, plus a number of schema-related constraints. Well-formed documents may have a schema, but they do not conform to it. Valid XML documents are a subset of well-formed XML documents. To be valid, an XML document must additionally conform (at least) to an explicitly associated schema. A schema for a document may be included as both internally and externally (located within the same file or a different file, respectively).

There are several XML schema languages, but only two are commonly used. They are DTD (Document Type Definition) and XML Schema or XML Schema Definition (XSD), both of which allow the structure of XML documents to be described and their contents to be constrained. DTD is considered limited as it only supports limited set of data types, loose structure constraints, limitation of content to textual, etc. To overcome the above limitations of DTD, XSD provides novel important features, such as simple and complex types, rich datatype sets, occurrence constraints and inheritance. Figure 2 illustrates a simple example of XML document and its corresponding DTD. Figure 3 shows a respective XML Schema.

```
<?xml version="1.0" encoding="UTF-8"?>
<Companies>
   <Company>
         <Symbol> Eagle.img </Title>
         <Name> EagleFarm </Name>
         <Industry> Dairy </Industry>
         <Profile>
              <MarketCap> 1000 </ MarketCap >
            <EmployeeNo> 20 </ EmployeeNo >
            <Address>
                  <State> QLD </State>
            </Address>
            <Description> gdsfkls </Description>
         </Profile>
   </Company>
         <!-- Some more instances -->
         ….
</Companies>
```

```
<!DOCTYPE Companies [
<!ELEMENT Companies (Company+)>
<!ELEMENT Company (Symbol, Name,
         Sector?, Industry, (Profile))>
<!ELEMENT Profile (MarketCap,
         EmployeeNo, (Address),
         Description)>
<!ELEMENT Address (State,City?)>
<!ELEMENT Symbol(#PCDATA)>
<!ELEMENT Name (#PCDATA)>
<!ELEMENT Sector (#PCDATA)>
<!ELEMENT Industry (#PCDATA)>
<!ELEMENT MarketCap (#PCDATA)>
<!ELEMENT EmployeeNo (#PCDATA)>
<!ELEMENT State (#PCDATA)>
<!ELEMENT City (#PCDATA)>
]>
```

Figure 2: Example of a XML document and its respective DTD

```
<xsd:schema xmlns:xsd=http://www.w3.org/2001/XMLSchema>
 <xsd:element name="Companies"  >
   <xsd:complexType>
     <xsd:sequence>
       <xsd:element name=”Company" maxOccurs=”unbounded”>
         <xsd:complexType>
           <xsd:sequence>
             <xsd:element name="Symbol" type="xsd:string"/>
             <xsd:element name="Name" type="xsd:string"/>
             <xsd:element name="Sector" type="xsd:string"/>
             <xsd:element name="Industry" type="xsd:string"/>
              <xsd:element name="Profile" >
                <xsd:complexType>
                    <xsd:sequence>
                      <xsd:element name="MarketCap" type="xsd:string"/>
                      <xsd:element name="EmployeeNumber" type="xsd:unsignedInt"/>
                      <xsd:element name="Address" >
                       <xsd:complexType>
                      <xsd:sequence>
                          <xsd:element name="State" type="xsd:string"/>
                          <xsd:element name=”City" type="xsd:string"/>
                        </xsd:sequence>
                      </xsd:complexType>
                      </xsd:element>
                      <xsd:element name="Description" type="xsd:string"/>
                    </xsd:sequence>
                  </xsd:complexType>
                </xsd:element>
              </xsd:sequence>
            </xsd:complexType>
          </xsd:element>
        </xsd:sequence>
      </xsd:complexType>
  </element>
</xsd:schema>
```

Figure 3: Example of the respective XSD or the above document

Throughout this paper, we use the term ‘schema’ to express both XML-DTD and XML-Schema (XSD) unless clearly specified. Additionally, XML data is used to express both XML documents and schemas.

3. The PCXSS methodology: overview

Since the documents may be provided without schema, a method of clustering XML data should deal both documents and schema. It should work in both ways: when a document is standalone; and when a document comes with a schema.

Considering this, PCXSS has two phases: Pre-processing phase and Clustering phase. The pre-processing phase first converts every XML document or XML schema (if provided) into a tree representation. This representation captures the hierarchical structure of XML data defined by its element and sub-element relationship. Every XML tree is then decomposed into structured path information called node paths (each path contains the node properties from the root node to the leaf node).

Figure 4 illustrates a high level view of the PCXSS methodology. The clustering phase groups each XML document into an existing cluster with which it has the maximum *CPSim* or assigns it to a new cluster. This phase consists of two stages: structure matching and clustering. Structure matching is to measure the structure similarity as well as semantic similarity of elements between a XML tree and existing clusters using their node paths. The output of the structure matching stage is common

path coefficient (*CPSim*) between a tree and a cluster. The CPSim is used in the clustering stage to select the best cluster for assigning the new tree to.

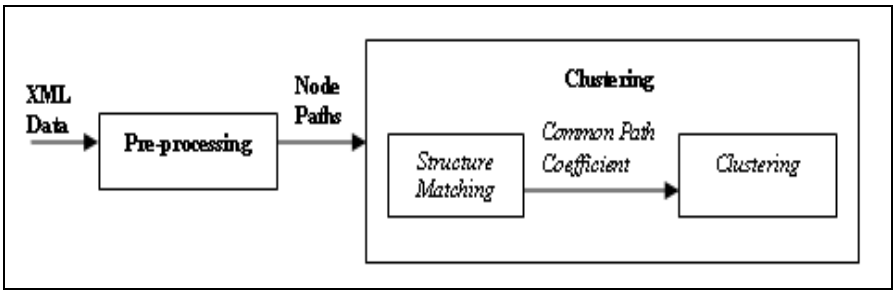


Figure 4. PCXSS methodology

4. PCXSS Phase 1: pre-processing

This phase sets the way for the clustering process. The representation and pre-processing of XML data in this phase is important in determining the structural similarity between a XML data and existing clusters. There are two types of pre-processing in the PCXSS method: pre-processing of element names and pre-processing of XML data.

4.1. Pre-processing of element names

With such a heterogeneous and flexible environment like the web, XML tags often can be a combination of lexemes (e.g. SigmodRecord, Act_Number), a single letter word (e.g. P for person), a preposition or a verb (e.g. related, from, to) that makes them syntactically different. Therefore, to improve the matching between node paths, pre-processing of element names is necessary. Element names in PCXSS are pre-processed in two steps:

1. Tokenization – the element name is parsed into a set of tokens using delimiters such as punctuation, uppercase or special symbols. E.g. PONumber → {P, O, Number}
2. Elimination – tokens that are not letters or digits will be eliminated, as well as any extraneous punctuation. E.g. Act_Number → {Act, Number}

The tokens form a *token set* for each element. A *synset* for each token is generated by retrieving the synonyms from WordNet [6]. WordNet is a thesaurus in which each word token is associated with corresponding alternative meanings, known as synonym set or *synset*. The retrieval of the synonym set (e.g. movie → film) is done in the pre-processing phase because the cost of accessing the WordNet [6] in the clustering phase is too expensive. The *synset* includes all the synonyms of each token by only going down the first synset level of WordNet, thus reducing the time of accessing WordNet.

Invoking WordNet to measure the semantic similarity in PCXSS can make the clustering process slow. To improve the efficiency while using WordNet we imply two strategies to invoke WordNet as less as possible. Firstly, we only create the WordNet dictionary once in the pre-processing phase and leave the dictionary open until the clustering is finished. Secondly, we use a hash table to store the element names that PCXSS has already searched in previous runs. Every time, when a new word is searched, the word is first checked in hash table before it starts invoking WordNet. The Principle is obvious; search a key in Hash table is much less expensive than search a word in WordNet.

4.2. Pre-processing of XML data

The next step is to transform the XML data sources into XML tree representations. Each XML is parsed and modelled as labelled tree. The parsing of a XML document to a tree is straightforward. While parsing, the multiple instances of values are ignored for an element. This is redundant information for the presentation of a structure and, moreover, the occurrence of elements is not important for clustering in most cases. The parsing of a XML Schema Definition (XSD) document requires some extra processing. XSD consists of three compositor elements: XML:sequence, XML:choice, and XML:all. The functions of the XML:sequence and XML:choice are equivalent to an AND, and OR operator, respectively. These compositor elements are ignored in the matching process as they do not facilitate much in measuring the similarity between node paths [18]. The attribute of an element is modelled exactly the same way as its child elements with the minimum occurrence and maximum occurrence assigned to 1. Each node in the tree contains its properties such as name, data type, minimum occurrence and maximum occurrence (cardinality). It also includes the synset of the node's name which is obtained in the previous step.

Figure 5 illustrates the respective XML tree representation of the schema shown in Figure 3.

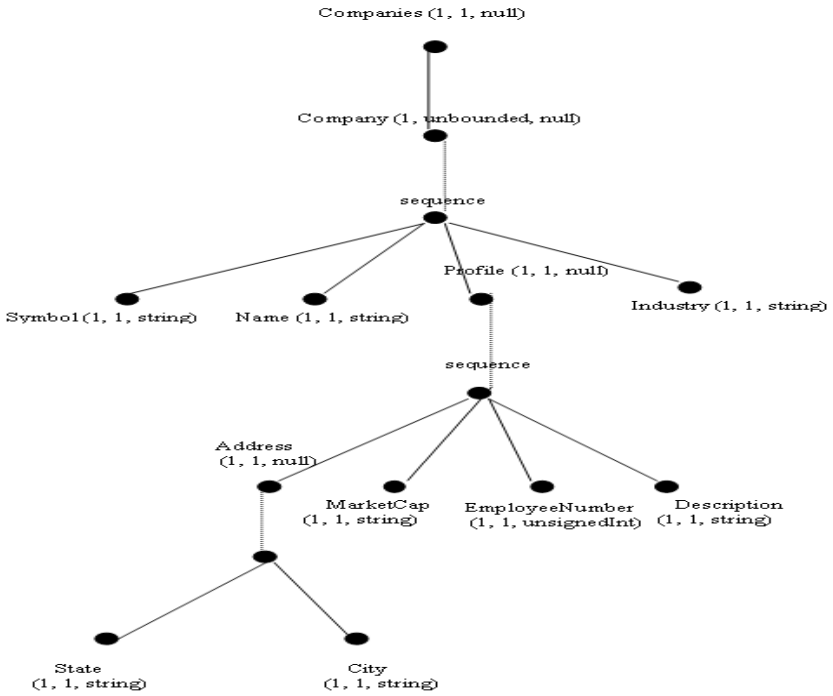


Figure 5. XML tree representation

4.3. Node paths representation

The XML tree is now decomposed into path information called node paths. A node path is an ordered set of nodes from the root node to a leaf node. For example, the node path for the node "Symbol" in Figure 5 equals the set {Companies, Company, Symbol}. Textually, a node path can be expressed with x_path syntax (e.g. Companies/ Company/ Symbol) that is shown in Figure 6.

Companies/Company/Symbol
Com Companies/Company/Name
Companies/Company/Industry
Companies/Company/Profile
Companies/Company/Profile/MarketCap
Companies/Company/Profile/EmployeeNumber
Companies/Company/Profile/Description
Companies/Company/Address/State
Companies/Company/Address/City

Figure 6. Node paths

5. PCXSS Phase 2: clustering

The node paths, obtained in the pre-processing phase, are used in the clustering phase to measure the degree of structural and semantic similarity between XML data. The proposed clustering algorithm does not require to measuring the similarity between each pair of trees (a set of node paths). It rather progressively measures the similarities between a new XML data and existing clusters by using common path coefficient (*CPSim*).

CPSim is determined in the first stage of clustering, i.e., structure matching. The structure matching stage measures the structural similarity between XML data and existing clusters by measuring the degree of similarity of nodes between node paths. The node similarity is determined by measuring its properties such as its name, data type and cardinality constraints. The output of the structure matching stage is a common path coefficient (*CPSim*) ranging from 0 to 1, 0 indicates that they have nothing in common and 1 indicates that the XML tree and the cluster are logically identical. The common path coefficient *CPSim* is used in the clustering stage to group XML documents progressively. Each XML document is grouped into an existing cluster that have the maximum *CPSim* or to a new cluster.

5.1. Structure matching stage

Figure 7 shows a high level view of the node paths matching stage. To measure the degree of structural similarity between a tree and existing clusters, node paths are used. Each node in a node path of a tree is matched with the node in a node path of existing clusters, and then aggregated to form the node path (or structure) similarity. The node similarity is determined by the similarity of its element name, data type and constraint.

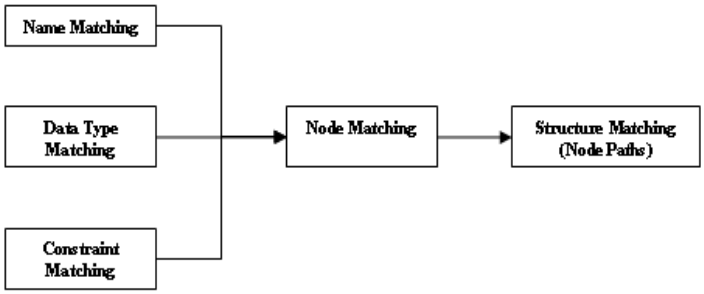


Figure 7. Structure matching

5.1.1. Name matching. Due to the flexibility in the design of XML documents, similar but unidentical elements can represent the same notion. Element names can be

semantically similar (if they are in a semantic tag similarity relationship, e.g., person or people) or syntactically similar (if they are in a syntactic tag similarity relationship, e.g., edit or xedit).

Accordingly, PCXSS uses semantic and syntactic measures to calculate the degree of similarity between a pair of names. Semantic measure considers the meaning of the nodes' name to determine the degree of similarity. For this measure to be possible, WordNet [7] is used in the pre-processing phase to form a linguistic set (*synset*). In this phase, we find a common element in the *synsets* of two names.

Syntactic measure considers the names syntax to determine the degree of similarity. It is good for identifying abbreviation and acronym words that are most commonly used in XML data. Sometime, however, it can lead to mismatches of element names, e.g, 'hot' and 'hotel'. To reduce the mismatches of element names, we use string edit distance and n-gram methods to measure the syntactic relationship between names. The average of both methods is used to measure the degree of syntactic similarity.

String edit distance is based on the cost of transforming one label into another label by using the editing operations (insertion, deletion, or substitution) [29]. It is defined as:

$$sim(t_1, t_2) = 1 - \left[\frac{edit\_distance(t_1, t_2)}{\max\{length(t_1), length(t_2)\}} \right]$$

where edit_distance (t_1 , t_2) denotes the string edit distance function between two strings t_1 and t_2. The *n*-gram method counts the same sequences of *n* characters appearing between two words [10]. PCXSS uses 2-grams (di-grams). An example of 2-grams for the word 'customer' is *cu, us, st, to, om, me, er*. It is defined as:

$$sim(t_1, t_2) = \frac{2C}{(A + B)}$$

where *A* is the number of unique n-grams in the first word, *B* the number of unique n-gram in the second word, and *C* is the number of unique n-grams common between two words. For example, let the two tokens be *customer* and *customer1*, then the syntactic similarity between two tokens is 0.933:

$$sim(t_1, t_2) = \frac{2(7)}{(7 + 8)} = 0.933$$

By using both string edit distance and n-gram methods, PCXSS is effective in matching acronyms and words with syntactic differences (e.g. *PO* and *PO1*).

```
1.  Function sim (t1, t2)
2.      if either t1 or t2 synset is empty /*Syntactic
    Relationship*/
3.          sim = (edit_distance(t1, t2)  + n-gram(t1, t2) )/2;
4.      else  /* Semantic Relationship*/
5.          sim= SemanticSim(t1, t2)
6.      end
7.      if sim ≥ threshold return sim;
8.      else return 0; /* No match */
9.  end
```

Figure 8. Measuring similarity between two name tokens

Figure 8 shows the pseudo code to combine the semantic and syntactic similarity values. The semantic relationship is first applied to exploit the degree of similarity between two tokens. If a pair of tokens is semantically matched then *the*

semantic similarity is returned *0.8*. If there exists a case where semantic relationship between two tokens can not be measured, syntactic relationship is then applied.

In the pre-processing phase, each element name is decomposed into a set of tokens. Thus, each element name is defined as a set of element name tokens *T*. The name similarity between two element names, name similarity coefficient (*Nsim*) is defined by the average of the best similarity of each token with a token in the other set:

$$Nsim(N_1, N_2) = \frac{\sum_{t_1 \in T_1}\left[\max_{t_2 \in T_2} sim(t_1, t_2)\right] + \sum_{t_2 \in T_2}\left[\max_{t_1 \in T_1} sim(t_1, t_2)\right]}{|T_1| + |T_2|}$$

where $|T_1|$ and $|T_2|$ are the length of the token sets for words N_1 and N_2, respectively. The output of *Nsim* is in the range [0, 1]. High values correspond to similar strings (i.e. 1 indicates identical strings), whereas low values correspond to different strings.

Example 1: Consider two elements names N_1*: author_fname* and N_2*: writerName* of two schemas. Tokens are derived T_1*: {author, fname}* and T_2*: {writer, name}*. *sim* (t_1, t_2) is measured between each pair of tokens. (the calculation below does not show the pair of tokens where the *sim* is equalled to 0):

sim (author, writer) = 0.8 (using the semantic similarity measure)
sim (writer, author) = 0.8 (using the semantic similarity measure)
sim (fname, name) = 0.83 (using the average of string edit and n-gram functions because fname does not have synset)
sim (name, fname) = 0.83 (using the syntactic similarity measure)

Name Similarity Coefficient: (*Nsim*): $\frac{(0.8 + 0.83) + (0.8 + 0.83)}{2 + 2} = 0.815$

5.1.2. Data type matching. Data type similarity can make a small contribution in determining node similarity while comparing XSDs. In XSD only the leaf node has data type. XSD supports 44 primitive and derived built-in data types such as string, Boolean, token, language etc. Data type similarity coefficient (*Tsim*) is ranged between [0, 1]. *Tsim* is derived from a type similarity table defined by the system user [26]. Table 1 shows a portion of the type similarity table.

Table 1. Type similarity table

Type1	Type2	Tsim
String	String	1
String	Date	0.2
Date	String	0.5
Decimal	Float	0.8
Float	Decimal	0.6

Table 2. Cardinality constraint compatible table

	*	+	?	None
*	1	0.9	0.7	0.7
+	0.9	1	0.7	0.7
?	0.7	0.7	1	0.8
None	0.7	0.7	0.8	1

5.1.3. Constraint matching. Another property of the node that also makes a small contribution in determining node similarity in XSDs is its cardinality constraints. The minOccurs and maxOccurs are used to define the minimum and maximum occurrence of an element node that may appear in the XML schema in XSDs. Authors of XClust

[18] have defined a cardinality table (Table 2) for DTD constraints. We show the mapping between DTD and XSD cardinality operators in Table 3 and adapt the cardinality constraint compatibility. The constraint similarity between two nodes is defined by constraint similarity coefficient (*Csim*), ranged between [0, 1].

Table 3. Cardinality mapping between XML and DTD

Cardinality Operator	minOccurs	maxOccurs	No. of child element(s)
[none]	1	1	One and only one
?	0	1	Zero or one
*	0	Unbounded	Zero or more
+	1	Unbounded	One or more

5.1.4. Node Matching. Node matching measures the similarity between the nodes in node paths by considering Name similarity (*Nsim*) of each node. It also includes data type similairty (*Tsim*) and constraints similarity (*Csim*) between two nodes in the case of XSDs. Node similarity is defined as follows:

$$NodeSim = w_1 * Nsim(name_1, name_2) + w_2 * Tsim(type_1, type_2) + w_3 * Csim(\min Occur, \max Occur)$$

where weights $w_1 + w_2 + w_3 = 1$.

The weight determines the importance of the measure in determining the node similarity. The default value is set as 1 for w_1 (and 0 for other weights) in case of XML documents. Default values are 0.8, 0.1 and 0.1 for w_1, w_2 *and* w_3, respectively in case of XSDs. The element name is the crucial information in determining the node similarity, so it has been assigned with the highest weight.

The degree of similarity between nodes is monitored by node similarity threshold. This threshold determines whether the two nodes are similar. If the NodeSim of two nodes exceeds the node similarity threshold then it is used to determine the path similarity between two node paths.

Example 2: Let us continue the same two elements names N_1*: author_fname* and N_2*: writerName* as in Example 1. We have already derived the *Nsim* between them as 0.815. The other constraints showing the min occurrence, max occurrence, data type and synset for these names are as follows:

1. author_fname (1, 1, string, synset)
2. writerName (1, 1, string, synset)

Considering the weights for *Nsim, Tsim* and *Csim* as 0.8, 0.1 and 0.1 respectively, the accumulated similarity of these two nodes (or tags or element names) is derived at:

NodeSim = 0.8 * 0.815 + 0.1 * 1 + 0.1 * 1 = 0.852

5.1.5. Structure Similarity: Putting it all together. The frequency of common nodes appearing in two XML structures is not sufficient to measure the similarity of XML data. XML is different from other web documents such as HTML because it contains the hierarchical structure and relationship between elements. The order of where the element resides in the structure is important in determining the structural similarity between XML trees and existing clusters.

The structural similarity between two XML data is measured by first finding the common nodes between two paths and then finding the common paths between two trees. The structure matching process can be advanced by starting at root node or starting at leaf node between two paths. The top-down approach starting the mapping at the root node misses the matching of lower-level descendants, if the higher level elements are not matched [23]. On the other hand, the bottom-up approach [5, 18, 22] starting the mapping at the leaf node is able to detect more similar elements within structures, however, it is more computation expensive than top down approach.

PCXSS uses bottom-up approach because the main focus of PCXSS methodology is to cluster a collection of heterogeneous XMLs with varied structures. Structure matching in PCXSS is a process of determining the degree of structural similarity between XML trees and existing clusters using node paths.

Common nodes finding. The degree of similarity between two node paths, defined as path similarity coefficient (*Psim)*, is measured by considering the common nodes coefficient (*CNC*) between two paths. The *CNC* is the sum of *NodeSim* of the nodes between two paths P_1 and P_2. The pseudo code for computing the *CNC* is shown in Figure 9. *Psim* of paths, P_1 and P_2 is the maximum similarity of the two *CNC* functions (P_1 to P_2 and P_2 to P_1) with respect to the maximum number of node in both paths, P_1 and P_2, defined as:

$$Psim(P_1, P_2) = \frac{Max(CNC(P_1, P_2), CNC(P_2, P_1)}{Max(|P_1|, |P_2|)}$$

Function: $CNC \quad (P_1, P_2)$
Sim:= 0; **for** each $n_i \in P_1$
  while j not end of P_2 length
    if(NodeSim(n_i, n_j)) > threshold (defined by user)
      Sim += NodeSim(n_i, n_j)
      j--
      break from 'While' loop
    else
      j--
    end if
  end while
end for
return Sim

Figure 9. The CNC algorithm

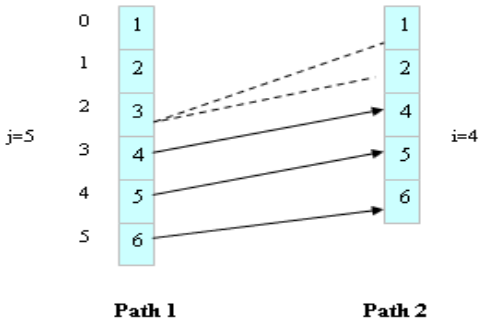


Figure 10. Example of CNC matching

Figure 10 shows an example of traversing through this *CNC* function. The Path1 1/2/3/4/5/6 contains 6 element names showed as numbers for convenience. Path 2 1/2/4/5/6 contains 5 elements. The following steps are iterated when calculating the *CNC* function:

1. Start at the leaf element of both paths (j=5, i=4). If the NodeSim coefficient of the leaf elements exceeds a threshold (a match) then increase Sim (Figure 9) with the NodeSim value and go to step 2 else go to step 3.
2. Move both paths to the next level (j--, i--) and start element matching at this level. If the NodeSim coefficient of these elements exceeds a threshold (a match) then increase Sim with the NodeSim value and repeat step 2 else go to step 3.
3. Move only path 1 to the next level (j--) then start element matching in the original level of path 2 (i) to the new element of path 1.

It is important to note that $CNC(P_1, P_2)$ is not equal to $CNC(P_2,P_1)$. If the leaf element from P_1 can not be found in P_2 then no further matching requires. In some case, one path may be a sub path of the other. If $P2$ is a sub path of P_1, and if the leaf element can not be found in P_2 then the $CNC(P_1, P_2)$ returns 0 (Figure 11(a)) however $CNC(P_2, P_1)$ returns 0.83 (Figure 11(b)).

Thus, both $CNC(P_1, P_2)$ and $CNC(P_2,P_1)$ are computed and the maximum of the two is used to measure the degree of similarity between the two paths.

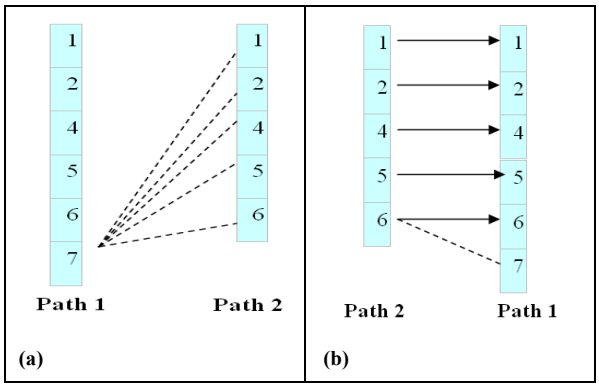


Figure 11. Example of path matching

Psim is monitored by a path similarity threshold. This threshold determines whether the two node paths are similar. If the *Psim* of two node paths exceeds the path similarity threshold then it is used to determine the structural similarity between the trees and existing clusters. The cost of computing two *CNC* functions can be expensive. To reduce the processing time, the result of the *NodeSim* for each pair of nodes is saved and is reused during the process of calculating the *CNC* between two XML trees.

Common paths finding. PCXSS measures common paths (1) between two trees and (2) between a tree and a cluster.

Tree to Tree Matching: Tree to tree matching is the matching between a new tree and a cluster that contains only one tree. Tree to tree matching is defined as:

$$CPSim(Tree_1, Tree_2) = \frac{\sum_{i=1}^{|TPath_1|} Max(\sum_{j=1}^{|TPath_2|}(Psim(P_i, P_j))}{Max(|TPath_1|, |TPath_2|)}$$

where *CPSim* is the common path similarity between two XML trees. The *CPSim* of trees, $Tree_1$ and $Tree_2$ is the sum of the best (maximum) path similar coefficient (*Psim*) of paths, P_i and P_j with respect to the maximum number of paths, $|TPath_1|$ and

$|TPath_2|$ of trees, $Tree_1$ and $Tree_2$, respectively. The clustering process in PCXSS works on the assumption that only one path from $Tree_1$ matches with one path in $Tree_2$. Thus, it only selects the maximum path similarity coefficient (*Psim*) between each pair of paths of $Tree_1$ and $Tree_2$.

Tree to Cluster Matching: Tree to cluster matching is the matching between a new tree and the common paths in a cluster. The common paths are the similar paths that are shared among the trees within the cluster (normally a cluster must contain at least 2 or more trees in the cluster to have the common paths or else tree to tree matching is required). Initially, the common paths are derived in tree to tree matching. Then every time a new tree is assigned to the cluster, the similar paths are added to the cluster if paths are not already in the cluster. Tree to cluster matching is defined as:

$$CPSim(Tree, Cluster) = \frac{\sum_{i=1}^{|TPath|} Max(\sum_{j=1}^{|CPath|}(Psim(P_i, P_j))}{|TPath|}$$

Similar to tree to tree matching, *CPSim* between a tree and a cluster is the sum of the best (maximum) path similar coefficient (*Psim*) of paths, P_i and P_j with respect to the number of paths, $|TPath|$ in *Tree*.

Example: Let us consider an example to compute *CPSim* using tree to tree matching.

$Tree_1$

P_{11}:Companies(1,1,null,synset)/Company(1,1,null,synset)/Symbol(1,1,string,synset)
P_{12}:Companies(1,1,null,synset)/Company(1,1,null,synset)/Name(1,1,string,synset)
P_{13}:Companies(1,1,null,synset)/Company(1,1,null,synset)/Profile(1,1,null,synset)/
EmployeeNumber (1, unbound,string,synset)
P_{14}:Companies(1,1,null,synset)/Company(1,1,null,synset)/Profile(1,1,null,synset)/
Description(1,1,string,synset)
P_{15}:Companies(1,1,null,synset)/Company(1,1,null,synset)/Address1(1,3,string,synset)

$Tree_2$

P_{21}:Companies(1,1,null,synset)/Company(1,1,null,synset)/Symbol(1,1,string,synset)
P_{22}:Companies(1,1,null,synset)/Company(1,1,null,synset)/Name(1,1,string,synset)
P_{23}:Companies(1,1,null,synset)/Company(1,1,null,synset)/Profile(1,1,null,synset)/
EmployeeNo(1,unbound,string,synset)
P_{24}:Companies(1,1,null,synset)/Company(1,1,null,synset)/Profile(1,1,null,synset)/
Description(1,1,string,synset)
P_{25}:Companies(1,1,null,synset)/Company(1,1,null,synset)/Address(1,1,string,synset)

After applying the *CNC* algorithm, the following shows the best *PSim* for each pair of node paths:

$PSim(P_{11},P_{21})$ = Max(CNC(1+1+1),CNC(1+1+1))/ Max(3,3) = 1
$PSim(P_{12},P_{22})$ =Max(CNC(1+1+1),CNC(1+1+1))/Max(3,3) = 1
$PSim(P_{13},P_{23})$ = Max(CNC(0.6+1+1+1),CNC(0.6+1+1))/Max(4,4)= 0.9
$PSim(P_{14},P_{24})$ = Max(CNC(1+1+1+1),CNC(1+1+1+1))/Max(4,4) = 1
$PSim(P_{15},P_{25})$ =Max(CNC(0.764+1+1),CNC(0.764+1+1))/Max(3,3) = 0.92

These *PSim* are then used to compute *CPSim* using tree to tree matching.

$CPSim(Tree_1,Tree_2)$:
(PSim(P_{11},P_{21}) + PSim(P_{12},P_{22}) + PSim(P_{13},P_{23}) + PSim(P_{14},P_{24}) + PSim(P_{15},P_{25}))/
Max(5,5) = 0.964

5.2. Clustering stage

PCXSS is motivated by incremental hierarchical clustering methods. It first starts off with no cluster. When a new tree comes in, it is assigned to a new cluster. When the next tree comes in, it matches with the existing cluster. If they match then the tree is assigned to that cluster else it is assigned to a new cluster. The number of cluster is generated progressively at run-time according to the data set.

Figure 12 shows the algorithm for the clustering process. Initially, there is no cluster. The first tree, T_1 is assigned to a new cluster, C_1 (step 1). When the next tree, T_i comes in; *CPSim* is computed between T_i and the existing cluster, C_j (steps 5 to 7). T_i is assigned to C_j if C_j has the largest *CPSim* with T_i and *CPSim* exceeds the clustering threshold (steps 9 and 10). Otherwise assign T_i to new cluster (step 12). The node paths of T_i (and T_j if tree to tree matching occurs) that are used to compute the *CPSim* are then added to C_j if T_i is assigned to C_j (step 11). The node paths in C_j are referred to as common paths. The common paths in C_j are then used to measure the *CPSim* between C_j and new trees. Since the common paths (instead of all the node paths of the trees held within a cluster) are used to compute *CPSim* with new trees, the computation time reduces significantly. In addition, the cluster contains only the distinct common paths (duplicate paths are removed from the cluster).

```
1.  assign the first tree T1 to a new cluster C1
2.  while tree file has more
3.     read the next tree (i.e. a set of node paths,
    denoted by Ti);
4.     while cluster C has more
5.        if Cj contains only one tree, Tj
6.           compute sim =CPSim(Ti, Tj);
7.        else compute sim=CPSim(Ti, Cj) end if
8.     end while
9.     if Max(sim) >= clustering threshold
10.       assign Ti to Cj ;
11.       add node paths to Cj ;
12.    else assign Ti to new cluster end if
13. end while
```

Figure 12. PCXSS clustering process

6. Empirical evaluation and discussion

Experiments are conducted on both XML documents and XML schema definition documents. The test data is carefully selected to ensure that the XMLs and XSDs are derived from the same and different domains and that each has distinct structure. To show the efficacy of PCXSS, the generated clustering solutions are evaluated against wCluto clustering solution [30]. wCluto is a pair-wise hierarchical clustering algorithm. In order to use wCluto, PCXSS first generated a matrix containing the *CPSim* (common path similarity) coefficient between each pair of trees in the data source using path similarity threshold of 0.7. The pair-wise similarity matrix is then fed into wCluto to perform the clustering process.

6.1 Scalability Evaluation

The computation time for a pair-wise similarity between XML trees is at least $O(m^2)$, where m is the number of elements in XML data that are used for the clustering.

This is infeasible for a large amount of data set. PCXSS measures the structural similarity between a XML tree with existing clusters, therefore the time complexity of PCXSS method is *O(m*c*n),* where m is the number of elements in XML data; c is the number of cluster; and *n* is number of distinct elements in clusters.

The documents grouped into a cluster should have similar structures and elements. So the number of distinct elements in clusters should always be less than the distinct elements in documents. Therefore, if the number of clusters is less than the number of documents (that is usually the case) the time cost is **linear** to the number of documents. The good scalability of this method is confirmed by the graph in Figure 13. The process time taken to complete the clustering by the PCXSS and by the wCluto pair-wise similarity method is compared in Figure 13 using the XSD dataset (Table 4). The result shows that the increment in time with the increase of the size of the data set is significant less with PCXSS in comparison to wCluto.

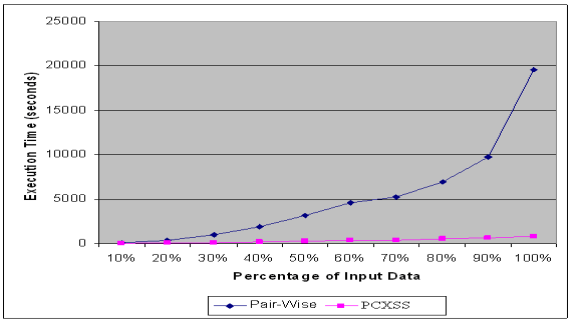


Figure 13. Clustering processing time for the wCluto pair wise method vs. PCXSS

Table 4. Datasets

Domain	No. of XSDs	No. of node	Nesting level
Car	67	76-89	2-4
Play (Shakespeare)	31	19-34	2-6
HITIS Message	17	17-304	3-17
Enrolment	29	33-102	2-11
Tei Site	50	29-103	2-10
Auction	4	32	3-5
NASA Record	93	85-129	2-10
SIGMOD Record	35	17-28	2-8
Time Card	4	13-54	3-7
Stock Plan Participant	2	36	2-5
Application Acknowledgement	5	35-46	2-9
Payroll Instruction	3	24-32	2-7
Profile	5	13	3-5
Linux Document	25	21-121	3-13

6.2 Quality Evaluation with XSD Dataset

The validity and quality of the PCXSS clustering solutions are verified using two common evaluation methods: (1) the intra-cluster and inter-cluster quality and (2)

FScore (combination of recall and precision) measure. The major characteristics of the XSD data set are shown in Table 4. Majority of them are derived from the Wisconsim's XML data bank [27]. Figure 14 shows the average XSD similarity of 14 XSD domains categories. It shows that XSDs are much different even though they come from the same domain, and the data is a good example set for clustering.

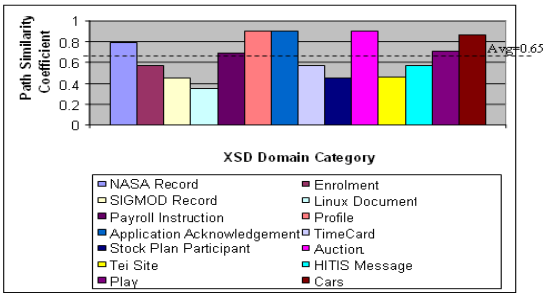


Figure 14. Average schema similarity coefficient

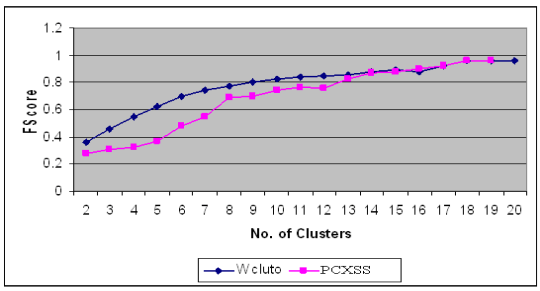


Figure 15. FScore measure

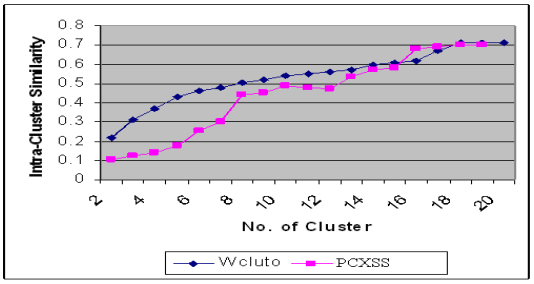


Figure 16. Intra-cluster Similarity

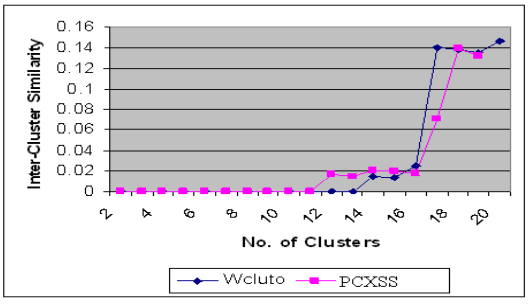
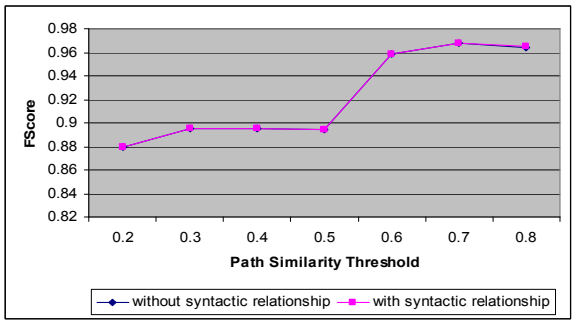


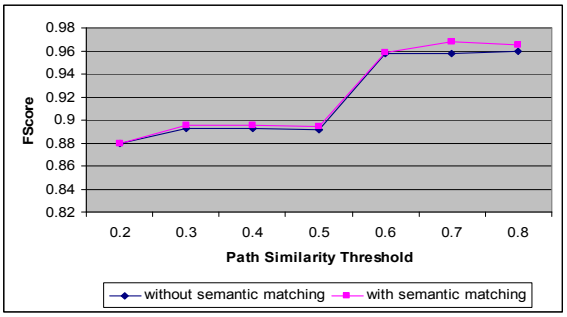
Figure 17. Inter-cluster similarity

Figures 15, 16 and 17 show the *FScore,* intra-cluster and inter-cluster similarity of the dataset respectively over the 20 different clustering solutions of PCXSS and wCluto. These results show that the performance of PCXSS is equivalent to wCluto, when the cluster number research to its optimal (in this case cluster number 19). PCXSS determines the optimal number of clusters during its processing, that is why, its performance is not as good as wCluto for the solutions before the optimal number of clusters. The results indicate that the incremental clustering algorithm PCXSS is able to achieve the similar quality results as the pair-wise clustering algorithms in much less time.

***Sensitivity testing*:** PCXSS also examines the sensitivity in computing the common path similarity coefficient (*CPSim*). During the experiment on the sensitive of PCXSS using the syntactic relationship, it has been discovered that some results can produce a worse clustering solution if we involve only one syntactic relationship, i.e. string edit distance or n-gram. This shows that element name matching using syntactic relationship may lead to mismatches of element name that may cause a poorer clustering solution. However, the effective use of these measures can improve the quality of clustering solution. It can be seen from Figures 18 and 19 that the semantic relationship plays a more important role than syntactic relationship.



Figures 18. Effect of syntactic relationships on clustering



Figures 19. Effect of semantic relationships on clustering

A number of experiments have also been carried out to evaluate the performance of PCXSS's clustering solution using different clustering and path similarity thresholds. The clustering threshold determines which clusters should the new XML be put into or a new cluster is needed. On the other hand, path similarity threshold determines the degree of similarity between two paths. It has been ascertained from the experiments (Figure 20) that the clustering and path similarity thresholds have an inverse relationship, meaning the higher the cluster thresholds, the

better the clustering solution if the path similarity threshold is set to a low value and vice versa. In Figure 20, each line represents the value of the clustering threshold on which the clustering solution was found with various path threshold values.

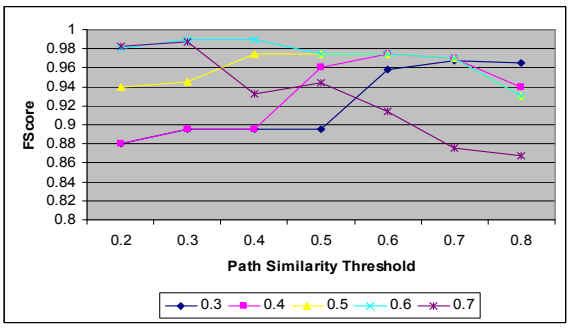


Figure 20. The effect of clustering and path similarity thresholds

6.3 Evaluation with XML Dataset

Four movie data sets and XMLFile data set have been used to conduct the clustering of XML documents. The movie data sets are from INEX 2006 document mining challenge (http://inex.is.informatik.uni-duisburg.de/2006/). Each movie set contains 4818 XML files. The four versions (m-db-s-0, m-db-s-1, m-db-s-2 and m-db-s-3) are the result of a series of transformation for adding the complexity in clustering process as we move up. The original movie data set has 190-200 distinct labels (tags).

The XMLFile data set contains 460 XML documents taken from the Wisconisn's XML data bank and the XML repository [31, 32]. The documents are from various domains such as (Movie (#Documents: 74), University (22), Automobile (208), Bibliography (16), Company (38), Hospitality message (24), Travel (10), Order (10), Auction data (4), Appointment (2), Document page (15), Bookstore (2), Play (20), Club (12), Medical (2), and Nutrition (1). The number of tags varies form 10 to 100 in these sources. The nesting level varies from 2 to 15. Majority of these domains consists of a number of different documents that have structural and semantic differences.

Table 5. PCXSS performance over various XML documents

Data set	Entropy	Purity	Fscore	Time
XMLFiles	0.021	0.977	0.965	45 mins
m-db-s-0-(1)	0.318	0.575	0.623	67 mins
m-db-s-0-(2)	0.334	0.589	0.637	66 mins
m-db-s-0-(3)	0.325	0.575	0.623	70 mins
m-db-s-0-(4)	0.328	0.579	0.629	68 mins
m-db-s-0-(5)	0.337	0.577	0.628	67 mins
m-db-s-1	0.328	0.589	0.625	72 mins
m-db-s-2	0.322	0.576	0.624	74 mins
m-db-s-3	0.319	0.575	0.624	79 mins

Incremental clustering algorithms are criticised for their sensitivity towards the order of inputs. To test the sensitivity of the PCXSS method towards the input order, we represented movie data set (m-db-s-0) in many ways such as SortByName, ReversedByName, SortByMiddleName, FirstQuarterByName and LastQuarterByName.

A good clustering solution has low entropy, high purity and high Fscore values. Results in Table 5 show a good performance of PCXSS on XMLFiles. The various representations of m-db-s-0 do not significantly alter the quality of clustering results. This shows that PCXSS is not sensitive towards the order of input data.

It is interesting to see that PCXSS performed almost evenly for all movie data sets, even though; the transformations have been done so that each series should be more difficult to cluster than the preceding. E.g., the second movie data set classes have a higher overlap than for the first one to make the clustering more difficult. The insignificant impact on the clustering solutions shows the strength of the clustering criteria and the approach that PCXSS adapts for clustering.

The contingency matrix for all the movie data sets shows that PCXSS can group most documents belonging to the same class into one cluster; it seldom puts them into separate clusters. However, it sometimes groups documents from several classes into one cluster because of their higher level similarity, reflecting the somewhat lower values obtained for Purity and Fscore and higher value obtained for Entropy. There may be many reasons behind this. Firstly the element labels of the movie data sets do not have semantic meanings. They are strings of characters to represent the overlapping complexity such as AB, ACB etc. Also, due to the nature of PCXSS, documents are not compared against each other, but, each document is compared against the existing clusters. Additionally, PCXSS does not only consider the parent-child relationship to measure the structural similarity, but also include the ancestor relationships of the data. This makes it more appropriate for clustering the heterogeneous data. Therefore, PCXSS performs excellent in heterogeneous environment like XMLFiles, but not as good as in the homogenous environment data such as movie data sets.

7. Related work

Measuring the structural similarity and clustering can be approached at two levels: structure level and element level.

Structure level: Many approaches exploit the clustering of XML data at the structure level by taking into account the structure of the XML data. [4, 28] measure the structural similarity among XML document using tree edit distance. [28] suggests that although XML documents are derived from the same XML schema (DTD) having different size due to optional and repeatable elements will not be recognized to be the same by using normal edit distance. Thus, they develop an edit distance metric that is more indicative of this notion of structural similarity. Whereas, [4] suggests the usage of tree structural summaries to improve the performance of the distance calculation. This approach extracts the structural summaries from a tree by eliminating the nested-repeated node (where the name of the non-leaf node is the same as its ancestor) and repeated node (node whose path starting from the root down to the node itself).

Tree edit distance is not adopted in PCXSS, even though PCXSS methodology also represents XML data as tree representations. Tree edit distance method is to measure the structural similarity between two trees; however, PCXSS computes the structural similarity between intentional representations of a set of trees. The matching criterion in PCXSS is it computes the structural similarity between trees by taking into account the importance of semantic of the node's name and other

properties such as cardinality constraint and data type in the case of XSDs. Element name plays an important role in exploiting the semantic of a node; as the result, relabelling from one node to another semantic unrelated node will cause an undesirable result.

[8] takes a different approach, they do not rely on tree or graph matching algorithms. They represent the XML documents as a time series in which each occurrence of a tag corresponds to a given impulse. They also take into account the order in which the tags appear in the document. They analyse the frequencies of corresponding Fourier transform to measure the degree of similarity between document structures. This approach only considers the structure of the document for clustering. It does not involve the semantic meaning of different elements from different DTDs. In some cases, documents containing the same information may not be considered the same because of their difference in structure.

Furthermore, S-GRACE [21] does not compute the distance between two trees but compute the distance between s-graphs by measuring the common set of nodes and edges appearing in either XML documents. It then applies ROCK method to exploit the links between the s-graphs in selecting the best of clusters to be merged. This approach is based on local criterion functions, meaning it needs to compute the distance between all pair initial s-graphs that requires $O(m^2)$ time, where m is the number of distinct s-graphs.

To avoid the lost of structure information from the XML documents, many techniques such as the one proposed in [17, 19, 20] have utilized the idea of sequential pattern mining to extract common paths from a collection of XML trees to measure the structural similarity. These approaches only extract the common or maximal paths to measure the structural similarity but they do not address how these can be used for the clustering process. [24] goes a bit further than the above approaches, it use sequential pattern mining to extract the frequent paths between XML schemas. It then uses the frequent paths to calculate the similarity between XML schemas; a similarity matrix is generated. It uses wCluto to cluster the XML schemas based on the similarity matrix. The main purpose of [24] approach is to generate a similarity matrix that can be used in the clustering process. However, the generation of the similarity matrix may take a bit of time since it is based on pair-wise similarity approaches.

Developing further, [15] uses sequential pattern mining to also extract the frequent paths from the XML documents, assuming that an XML document as a transaction and frequent structure of documents as the items of the transaction. It then uses CLOPE [34] and Large Items [12] clustering methods for transaction data to cluster a collection of XML documents. Using sequential pattern mining to extract the common paths of the XML documents can be computational expensive. In PCXSS, the XML is decomposed into structures path information called node path. A node path is an ordered set of nodes from the root node to a leaf node. Each node contains its properties such as name, constraint, and min and max occurrences.

The major difference between PCXSS approach and other approaches is the utilization of the common paths. PCXSS methodology does not only mine the common paths to determine the structural similarity between schemas but it also uses the common paths to measure the structural similarity between a new tree and existing clusters, making a significant saving in computational efforts.

Element Level: element level similarity matching approaches is also known as schema matching. Schema matching is the process of finding correspondence elements of two schemas or documents. Some approaches exploit schema matching at the instance level [2, 16], schema level [5, 14, 18, 22] or using both instance and schema [6, 33] to determine the semantic correspondence elements. PCXSS utilizes ideas from a number of schema matching approaches [5, 18, 22, 24, 26] on XML data to analyse the properties of the element node. It forms an important part in finding

common paths between a tree and existing clusters by analysing the linguistic of the node label and its properties such as data type and constraints.

8. Conclusions and future work

XML has become quite popular in the exchange of a variety of data on the Web and in the distribution of information related to various topics as well. With the number of XML sources growing rapidly, it becomes necessary to cluster the collection of the XML sources for effectively finding important information from them. Due to its semi-structured and flexible feature compared to the data in traditional databases, it poses challenge to develop an efficient and scalable clustering method.

We present a novel clustering method called PCXSS that progressively clusters XML data by taking into account the structural and semantic information of elements. PCXSS measures the structural similarity between XML data by finding the common paths among them. To be applicable to any XML data, the PCXSS approach employs a complex method for element matching that not only considers the element name but also other properties such as data type and cardinality to ensure the accuracy of element matching. It considers both the semantic and syntactic relationship of the element name. Furthermore, the PCXSS clustering do not require the similarity computation between each pair of data. It compares each new tree with existing clusters where each cluster contains the common paths of the trees held within.

The empirical analysis shows that PCXSS significantly reduces the computational time as compared to pair-wise computation as well as yields good accuracy of the results. The several experiments also ascertain that PCXSS clustering solution is not heavily influenced by thresholds such as the clustering and path similarity. Furthermore, the syntactic and semantic relationship measurements have also been tested. The semantic relationship has shown to be more important to determine similarity.

The clustering solution produced by PCXSS can help in reducing the complexity of integrating schemas from heterogeneous domains and in improving the speed of the integration process. The structure matching (path matching) in PCXSS can be used for finding correspondence element between two schemas that facilitate in area such as schema integration. In addition, it can be used to improve the speed and accuracy in structure indexing and information retrieval.

PCXSS needs some future work to improve its effectiveness. Both path and element matching in this approach is still very complex. Therefore, it takes longer to do the clustering process. To overcome this problem, path matching can be reduced by grouping node paths that have the same ancestors into one path.

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