Mining Closed and Maximal Frequent Subtrees from Databases of Labeled Rooted Trees

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Abstract—Tree structures are used extensively in domains such as computational biology, pattern recognition, XML databases, computer networks, and so on. One important problem in mining databases of trees is to find frequently occurring subtrees. Because of the combinatorial explosion, the number of frequent subtrees usually grows exponentially with the size of frequent subtrees and, therefore, mining *all* frequent subtrees becomes infeasible for large tree sizes. In this paper, we present *CMTreeMiner*, a computationally efficient algorithm that discovers only closed and maximal frequent subtrees in a database of labeled rooted trees, where the rooted trees can be either ordered or unordered. The algorithm mines both closed and maximal frequent subtrees by traversing an enumeration tree that systematically enumerates all frequent subtrees. Several techniques are proposed to prune the branches of the enumeration tree that do not correspond to closed or maximal frequent subtrees. Heuristic techniques are used to arrange the order of computation so that relatively expensive computation is avoided as much as possible. We study the performance of our algorithm through extensive experiments, using both synthetic data and data sets from real applications. The experimental results show that our algorithm is very efficient in reducing the search space and quickly discovers all closed and maximal frequent subtrees.

Index Terms—Trees, graph algorithms, data mining, mining methods and algorithms, frequent subtree, closed frequent subtree, maximal frequent subtree.

1 Introduction

1.1 Motivation

Graphs are widely used to represent data and relationships. Among all graphs, a particularly useful family is the family of rooted trees: In the database area, XML documents are often rooted trees where vertices represent elements or attributes and edges represent element-subelement and attribute-value relationships; in Web traffic mining, access trees are used to represent the access patterns of different users [27]; in analysis of molecular evolution, an evolutionary tree (or phylogeny) is used to describe the evolution history of certain species [11], [20]; in computer networking, multicast trees are used for packet routing [8]. From these examples, we can also see that trees in real applications are often *labeled*, with labels attached to vertices and edges where these labels are not necessarily unique.

In this paper, we study one important issue in mining databases of labeled rooted trees—finding frequently occurring subtrees. This issue has practical importance, as shown in the following examples:

1. *Gaining general information of data sources.* When a user initially studies a new data set, he or she may not yet know the characteristics of the data set. The frequent substructures of the data set will often help the user to understand the data set and guide further investigation into the details of the data set. For example, Wang and Liu [22] applied their frequent subtree mining algorithm to an Internet movie database and discovered the common structures of the movie documents.
2. *Classification and clustering.* Classification and clustering algorithms can be applied to labeled trees. By considering frequent trees as features of data points, the application of standard classification and clustering algorithms becomes possible. For example, from the Web logs of a Web site, we can obtain the access patterns (access trees) of the visitors. We can use the access trees to classify different types of users (casual versus serious customers, normal visitors versus Web crawlers, etc.). In another example, Zaki and Aggarwal [28] presented an algorithm to classify XML documents according to their subtree structures.
3. *Database indexing and access method design.* Frequent subtrees in a database of labeled trees can provide information on how to build efficient indexing structures for the databases and how to design efficient access methods for different types of queries. For example, Yang et al. [26] presented algorithms for mining frequent query patterns from the logs of historic queries on an XML document. Answers to historic frequent queries can be stored and indexed for future efficient query answering.

However, as we have observed in our previous studies [4], [6], because of the combinatorial explosion, the number of frequent subtrees usually grows exponentially with the tree size. This is the case especially when the transactions in the database are strongly correlated. Two consequences follow from this exponential growth. First, the end-users

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will be overwhelmed by the huge number of frequent subtrees presented to them and, therefore, have difficulty in gaining insights from the frequent subtrees. Second, mining algorithms may become intractable due to the exponential number of frequent subtrees. The algorithms presented by Wang and Liu [22] and Xiao et al. [23] tried to alleviate the first problem by finding and presenting to end-users only the *maximal* frequent subtrees. A *maximal* frequent subtree is a frequent subtree, none of whose proper supertrees are frequent. Usually, the number of *maximal* frequent subtrees is much smaller than the total number of *all* frequent subtrees. Nevertheless, because both of these algorithms use postprocessing techniques that prune away nonmaximal frequent subtrees after discovering all the frequent subtrees, they do not solve the second problem mentioned above. To avoid creating all the frequent subtrees in the first place, hence solving both the problems mentioned above, we propose an efficient algorithm in this paper—*CMTreeMiner*. Instead of looking for all frequent subtrees in a database of rooted trees, the algorithm directly aims at closed and maximal frequent subtrees only, where a *closed* frequent subtree is a frequent subtree t such that all of the proper supertrees of t occur in fewer transactions than t does. (We will give more rigorous definitions in the following sections.) In the proposed algorithm, we use several pruning techniques. With pruning techniques, a large part of the search space that does not contain any closed or maximal frequent subtrees is determined in the early stages of the algorithm and is pruned from the search space. Heuristic techniques are used to order the tests in such a way that the pruning takes place as early as possible and relatively expensive computation is eliminated whenever possible. As the search space is greatly reduced and the more expensive computations largely eliminated, the running time of our algorithm is much reduced in comparison to algorithms that search the entire space for all the frequent subtrees. In addition, our algorithm handles databases of rooted *ordered* trees and databases of rooted *unordered* trees equally well.

1.2 Related Work

Recently, there has been growing interest in mining databases of labeled trees. The proposed frequent subtree mining algorithms can be broadly classified into three categories. The first category are a priori-like algorithms (e.g., [19], [27]) that systematically traverse a lattice structure of all frequent subtrees through either a depth-first or a breadth-first traversal order. In [27], Zaki presented such an algorithm, *TreeMiner*, to discover all frequent embedded subtrees (i.e., those subtrees that preserve ancestor-descendant relationships) in a forest or a database of rooted *ordered* trees. The algorithm was extended in [28] to build a structural classifier for XML data. In [5], Chi et al. have studied the problem of indexing and mining free trees and developed an a priori-like algorithm, *FreeTreeMiner*, to mine all frequent free subtrees. In a priori-like algorithms, a candidate subtree is generated by joining two frequent subtrees with smaller size. The second category of algorithms is based on enumeration trees. In these algorithms, a candidate subtree is generated by extending its unique parent, which is a frequent subtree of smaller size, in the enumeration tree. In [1], Asai et al. presented such an algorithm, FREQT, to discover frequent rooted *ordered* subtrees. For mining rooted *unordered* subtrees, Asai et al. [2], Nijssen and Kok [17], and Chi et al. [4], [6], [7] proposed algorithms based on enumeration tree growing. Because there can be multiple *ordered* trees corresponding to the same *unordered* tree, similar canonical forms for rooted *unordered* trees are defined in these studies. The third category of algorithms for mining frequent subtrees (e.g., [21], [23]) adopt the idea of the FP-tree [10] in frequent itemset mining and construct a concise in-memory data structure that preserves all necessary information. This data structure is then used for mining frequent subtrees. In [23], Xiao et al. presented such an algorithm, called *PathJoin*. In addition, *PathJoin* allows the user to keep only *maximal* frequent subtrees by using a postprocessing pruning that, after obtaining all frequent subtrees, eliminates those that are not maximal.

In addition to the work we have mentioned above, closely related to mining frequent subtrees, many recent studies have focused on mining frequent subgraphs [12], [13], [15], [24]. In particular, Yan and Han [25] recently proposed an algorithm, *CloseGraph*, to mine closed frequent subgraphs. *CMTreeMiner* shares many features with *CloseGraph*, as we will discuss later. However, mining frequent subgraphs is a much more difficult problem than mining frequent subtrees (e.g., the subgraph isomorphism is an NP-complete problem, while the subtree isomorphism problem is in P).

1.3 Our Contributions

The main contributions of this paper are as follows:

1. We study *closed frequent subtrees*, their properties, and their relationship with *maximal frequent subtrees*.
2. We study the POSET (partially ordered set) structure of the set of all frequent subtrees and represent it using a special data structure—the enumeration DAG (directed acyclic graph). We introduce a novel concept, the *blanket* of a frequent subtree in the enumeration DAG.
3. We present *CMTreeMiner*, a computationally efficient algorithm that discovers all closed frequent subtrees and maximal frequent subtrees from a database of rooted *ordered* trees. In the algorithm, the blanket concept is used to determine the closedness and maximality of a frequent subtree, as well as to prune branches in the enumeration tree that will not yield closed or maximal frequent subtrees. We also propose heuristic techniques for organizing the order of tests so that the pruning occurs early and relatively expensive computation is eliminated whenever possible.
4. By using a canonical form representation for labeled rooted *unordered* trees, we extend our *CMTreeMiner* algorithm to mining frequent *unordered* subtrees. We use both synthetic data and real application data to evaluate the performance of our algorithm and compare the performance of our algorithm with those of several existing algorithms.

To the best of our knowledge, *CMTreeMiner* is the first algorithm that, instead of using postprocessing procedures, directly mines only closed and maximal frequent subtrees.

The rest of the paper is organized as follows: In Section 2, we give necessary background in graph theory, the problem definition, and various related concepts. In Section 3, we look in detail at the *CMTreeMiner* algorithm for mining closed and maximal frequent subtrees from databases of labeled rooted *ordered* trees. In Section 4, we extend the *CMTreeMiner* algorithm to handle databases of labeled rooted *unordered* trees. In Section 5, we discuss experiment results. Finally, in Section 6, we offer conclusions.

2 Background

In this section, we provide the definitions for some general concepts that will be used in the remainder of the paper. More specific concepts will be introduced in later sections.

2.1 Background in Graph Theory

A *labeled Graph* $G = [V, E, \Sigma, L]$ consists of a *vertex* set V, an *edge* set E, an *alphabet* Σ for vertex and edge labels, and a *labeling function* $L : V \cup E \rightarrow \Sigma$ that assigns labels to vertices and edges. A *rooted unordered* tree is a directed acyclic graph satisfying the following: 1) There is a distinguished vertex called the *root* that has no entering edges, 2) every other vertex has exactly one entering edge, and 3) there is a unique path from the root to any other vertex. A *rooted ordered* tree is a rooted tree that has a predefined left-to-right ordering among the children of each vertex. The *size* of a rooted tree is defined as the number of vertices. For convenience, in this paper, we call a rooted tree of size k a k-tree. We assume the reader is familiar with concepts such as *ancestor*, *descendant*, *parent*, *child*, *leaf*, etc. A rooted tree t (with vertex set V_t and edge set E_t) is called a *subtree* of another rooted tree s (with vertex set V_s and edge set E_s) if and only if 1) $V_t \subseteq V_s$, 2) $E_t \subseteq E_s$, and 3) the labeling of V_t and E_t is preserved in s. If, in addition, the size of t is strictly less than the size of s, then t is called a *proper subtree* of s. If t is a (proper) subtree of s, then s is called a (proper) *supertree* of t. Notice that the definitions of (proper) subtree and supertree apply to both rooted *ordered* trees and rooted *unordered* trees. Obviously, for a rooted *ordered* tree s and a subtree t of s, the left-to-right ordering among the children of each vertex in t is a subordering of that in s.

The subtree defined above is also called an *induced subtree*. In [27], Zaki defined a different type of subtree, called an *embedded subtree*, for rooted trees with only vertex labels: A rooted tree t (with vertex set V_t) is said to be an *embedded subtree* of s (with vertex set V_s) if and only if 1) $V_t \subseteq V_s$, 2) $(v_1, v_2) \in E_t$ (here, v_1 is the parent of v_2 in t) only if v_1 is an ancestor of v_2 in s, and 3) the labeling of V_t is preserved in s. Intuitively, as an embedded subtree, t must not break the ancestor-descendant relationship among the vertices of s. In this paper, unless otherwise specified, *subtree* means *induced subtree*.

2.2 The Frequent Subtree Mining Problem

Let D denote a database where each transaction $s \in D$ is a labeled rooted tree. (D can be either a database of labeled rooted *ordered* trees or a database of labeled rooted *unordered* trees.) For a given pattern t (where t is a rooted tree and whether t is *ordered* or *unordered* depends on D), we say t *occurs* in a transaction s if t is a subtree of s. Let $\sigma_t(s) = 1$ if t is a subtree of s, and 0 otherwise. We say s *supports* pattern t if $\sigma_t(s)$ is 1 and we define the *support* of a pattern t in the database D as $support(t) = \sum_{s \in D} \sigma_t(s)$. A pattern t is called *frequent* if its support is greater than or equal to a *minimum support* (*minsup*) specified by a user. The frequent subtree mining problem is to find all frequent subtrees in a given database.

One nice property of frequent subtrees is the a priori property, as given in the following:

Lemma 1. *Any subtree of a frequent tree is also frequent and any supertree of an infrequent tree is also infrequent.*

Proof. Directly from the definition of *subtree* and *support*. □

2.3 Closed and Maximal Frequent Subtrees

We define a frequent tree t to be *maximal* if none of the proper supertrees of t is frequent and *closed* if none of the proper supertrees of t has the same support that t has.

The set of all frequent subtrees, the set of closed frequent subtrees, and the set of maximal frequent subtrees have the following relationship:

Lemma 2. *For a database D and a given $minsup$, let $\mathcal{F}$ be the set of all frequent subtrees, $\mathcal{C}$ be the set of closed frequent subtrees, and $\mathcal{M}$ be the set of maximal frequent subtrees, then $\mathcal{M} \subseteq \mathcal{C} \subseteq \mathcal{F}$.*

Proof. $\mathcal{C} \subseteq \mathcal{F}$ is implied by the definition of $\mathcal{C}$. For $\mathcal{M} \subseteq \mathcal{C}$, we note that, for a tree $t \in \mathcal{M}$, since t is frequent and none of the proper supertrees of t are frequent, so none of the proper supertrees of t has the same support as t and, therefore, $t \in \mathcal{C}$. □

We are interested in mining closed and maximal frequent subtrees, instead of mining all frequent subtrees, because, generally, there are fewer closed or maximal frequent subtrees compared to the total number of frequent subtrees [18]. In addition, by mining only closed and maximal frequent subtrees, we do not lose much, if any, information (if we only care about the support, not the total number of occurrences of a frequent subtree). This is because the set of closed frequent subtrees maintains the same information (including support) as the set of all frequent subtrees and the set of maximal frequent subtrees subsumes all frequent subtrees.

Lemma 3. *We can obtain all frequent subtrees from the set of maximal frequent subtrees; similarly, we can obtain all frequent subtrees with their supports from the set of closed frequent subtrees with their supports.*

Proof. For the first statement, we notice that any frequent subtree is a subtree of one (or more) maximal frequent subtree(s); for the second statement, we notice that, for a frequent subtree t that is not closed, $support(t) = \max_{t'}\{support(t')\}$, where t' is a supertree of t that is closed. □

3 Mining Closed and Maximal Frequent Rooted Ordered Subtrees

In this section, we describe our *CMTreeMiner* algorithm that mines both closed and maximal frequent subtrees from a database of labeled rooted *ordered* trees. In the

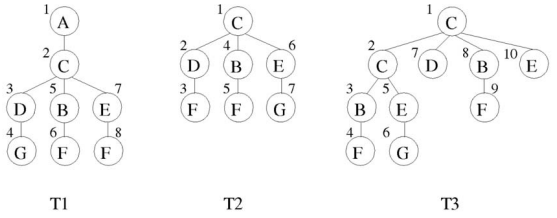


Fig. 1. A database with three transactions.

next section, we will extend the algorithm to labeled rooted *unordered* trees.

If a labeled tree is rooted, then, without loss of generality, we can assume that all edge labels are identical because each edge connects a vertex with its parent, so we can consider an edge, together with its label, as a part of the child vertex. So, for all examples in the following discussion, we assume that all edges in all trees have the same label or, equivalently, are unlabeled and we therefore ignore all edge labels.

In the following discussion, we use the database given in Fig. 1 as a running example. The database consists of three transactions and the *minsup* is set to 2. Each transaction in the database has a unique transaction id, i.e., $T1$, $T2$, and $T3$, respectively. In addition, in the database, a unique index number is assigned to each vertex in a transaction, as shown in Fig. 1.

3.1 The Enumeration DAG and Enumeration Trees

We first introduce a data structure, called the *enumeration DAG*, to represent the partially ordered set (POSET) of all frequent subtrees. As is well-known, the subtree/supertree relationship defines a partial order on the set of all frequent subtrees. We put all frequent subtrees in a lattice of multiple levels, where each level consists of frequent subtrees with size equal to the level number. In addition, directed edges are added between neighboring levels: Each edge represents a subtree/supertree relationship between two frequent subtrees in neighboring levels and points from the subtree to the supertree. The result is an enumeration DAG

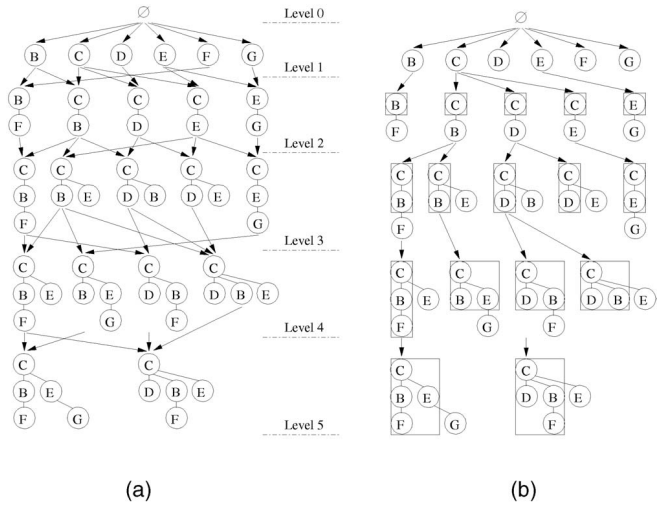


Fig. 2. (a) The enumeration DAG. (b) The enumeration tree.

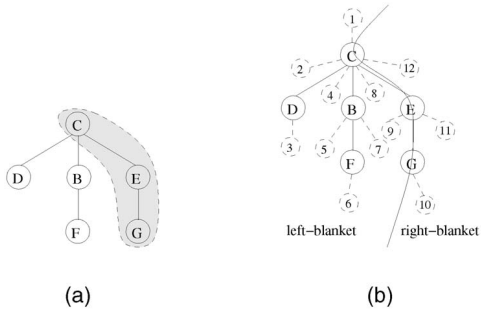


Fig. 3. (a) The rightmost path. (b) The left and right blankets.

(directed acyclic graph) whose transitive closure is the partial order defined on the POSET of all frequent subtrees. Fig. 2a gives the enumeration DAG of all frequent subtrees for the database shown in Fig. 1.

Enumeration trees, which are commonly used for frequent subtree mining, are actually spanning trees of the above enumeration DAG. Enumeration trees were first introduced by Asai et al. [1] for systematically enumerating all frequent rooted *ordered* trees. In Asai et al.'s algorithm, each candidate subtree is generated at most one time (and, therefore, redundancies are avoided) from its unique parent in the enumeration tree. The parent of a subtree is uniquely determined by removing the *rightmost* vertex of the subtree, where the *rightmost* vertex of a tree is defined as its last vertex according to the depth-first traversal order. Fig. 2b shows the enumeration tree, which is a spanning tree of the enumeration DAG in Fig. 2a. In Fig. 2b, for each frequent subtree, we use a bounding box to emphasize its parent in the enumeration tree.

As observed by Asai et al., to add a new vertex w to a frequent subtree t, in order for w to be the rightmost vertex of the new subtree, the parent of w, called v, must be a vertex on the *rightmost path* of t and w must be the rightmost child of v. The *rightmost path* of t is defined as the path from the root to the rightmost vertex of t. For example, for the root tree shown in Fig. 3a, vertex G is the rightmost vertex and the rightmost path is the path in the shaded area. A frequent subtree mining algorithm therefore systematically grows the enumeration tree by extending each frequent subtree in the enumeration tree. When extending a frequent subtree t, an additional vertex w is added as the rightmost child of one vertex on the rightmost path of t (and, therefore, w becomes the new rightmost vertex); if the resulting t' is frequent, t' becomes a child of t in the enumeration tree.

Our *CMTreeMiner* algorithm follows Asai et al.'s enumeration tree idea. However, the enumeration DAG is used to determine the closedness and the maximality of frequent subtrees. In addition, the enumeration DAG (the blanket) is also used to prune the branches of the enumeration tree that do not correspond to closed or maximal frequent subtrees.

3.2 The Blanket, the Closedness, and the Maximality

For a frequent subtree t, we define the *blanket* of t, denoted by B_t, as the set of *immediate supertrees* of t that are frequent, where an immediate supertree of t is a supertree t' of t that

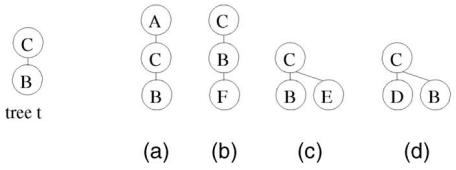


Fig. 4. A rooted ordered tree t (left) and some potential supertrees in its blanket B_t (right).

has one more vertex than t. Fig. 4 shows a rooted tree t and some supertrees that are potentially in B_t. For a node t (which represents a frequent subtree) in the enumeration DAG of all frequent subtrees, the blanket B_t of t consists of the nodes that can reach t or are reachable from t in one step. The definition of blanket applies to both rooted *ordered* trees and rooted *unordered* trees.

For a subtree t and one of its immediate supertrees $t' \in B_t$, we can add a vertex w to t to get t'. We use $t'\backslash t$ to represent the additional vertex w in t' that is not in t. Please notice that $t'\backslash t$ represents not only the vertex label of w, but also its position, i.e., which vertex is the parent of w and the order of w among its siblings. In addition, $t'\backslash t$ might be the root of t', as shown in Fig. 4a. Furthermore, there are two special cases in which $t'\backslash t$ is not uniquely defined. The first case is when t' is a chain of vertices with identical labels. In such a case, w can be either the root or the only leaf vertex of t'. The second case is when w has neighboring siblings with the same label. In such a case, w can be any of these neighboring siblings. To make $t'\backslash t$ uniquely defined, for the first case, we define $t'\backslash t$ as the leaf vertex and, for the second case, we define $t'\backslash t$ as the rightmost one among the neighboring siblings.

Using the definition of blanket, we can define maximal and closed frequent subtrees in an equivalent manner which turns out to be quite useful:

Lemma 4. *A frequent subtree t is maximal iff $B_t = \emptyset$; a frequent subtree t is closed iff, for each $t' \in B_t$, $support(t') < support(t)$.*

Proof. Directly from the definitions of the closed frequent subtree and the maximal frequent subtree. □

Therefore, instead of a postprocessing step, we can determine the closedness and the maximality of a frequent subtree t by checking the support for each of its supertrees in B_t. However, even with this check, we still have to traverse the entire enumeration tree. In the next section, we will see how the blanket helps us to prune the search of the enumeration tree.

3.3 The Pruning Techniques

The final goal of our algorithm is to find only closed and maximal frequent subtrees. Therefore, it is not necessary to grow the complete enumeration tree. In this section, we introduce techniques that prune the unwanted branches with the help of the enumeration DAG (more specifically, the blankets).

3.3.1 Occurrence-Matching and Transaction-Matching

If a subtree t occurs in a transaction s, it can occur more than once. For example, the two-tree with C as the root and

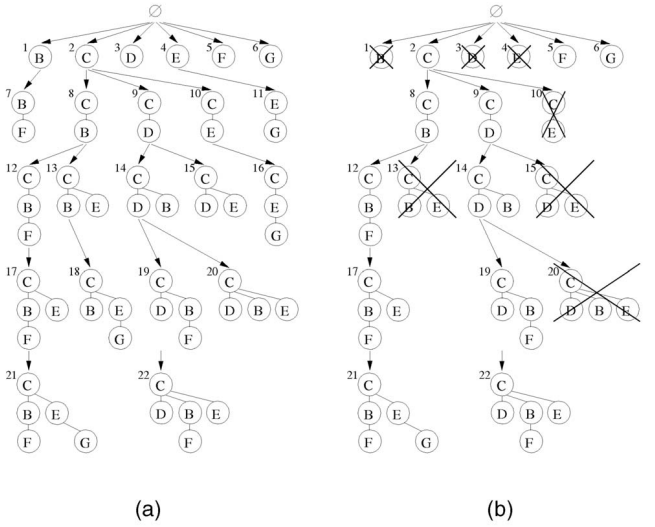


Fig. 5. The enumeration tree. (a) Before pruning. (b) After pruning.

B as the only child of C (i.e., t_8 in Fig. 5a) occurs once in $T1$, once in $T2$, and twice in $T3$. We call each of them an *occurrence* of t in the database. For $t' \in B_t$, we define t' and t as *occurrence-matched* if, for each occurrence of t in (a transaction of) the database, there is at least one (there could be more than one) corresponding occurrence of t'; we say that t' and t are *transaction-matched* if, for each transaction $s \in D$ such that $\sigma_t(s) = 1$, we have $\sigma_{t'}(s) = 1$. Occurrence-matching was first introduced by Yan and Han [25], under the name of *equivalent occurrence* for mining subgraphs.

Lemma 5. *If t' and t are occurrence-matched, then they are transaction-matched.*

Proof. Directly implied by the two definitions. □

For example, t_{13} and t_{10} in Fig. 5a are occurrence-matched. (Fig. 5a is a redrawn enumeration tree for our database with indices added for convenience of discussion.) This is because 1) $t_{13} \in B_{t_{10}}$ and 2) whenever t_{10} occurs in any position of any transaction in the database, there is a vertex B ($t_{13}\backslash t_{10}$) as the left sibling of the vertex E in t_{10}. On the other hand, t_{14} and t_8 are transaction-matched but not occurrence-matched; although t_{14} occurs in all transactions where t_8 occurs ($T1$, $T2$, and $T3$), t_{14} does not occur in *all* positions that t_8 occurs. In $T3$, t_8 occurs twice, but t_{14} only occurs once.

3.3.2 The Left-Blanket Pruning

For a frequent subtree t and one of its supertrees $t' \in B_t$, the vertex $t'\backslash t$ can be at different locations, such as position 1 through position 12 as shown in Fig. 3b. According to whether $t'\backslash t$ is the rightmost vertex of t', we divide B_t into two parts: the *left-blanket* B_{t_left} and the *right-blanket* B_{t_right}, as shown in Fig. 3b. For every $t' \in B_{t\_right}$, $t'\backslash t$ is the rightmost vertex of t'. (In Fig. 3b, this corresponds to $t'\backslash t$ being at position 10, 11, or 12.) For every $t' \in B_{t\_left}$, $t'\backslash t$ is not the rightmost vertex of t'. (In Fig. 3b, this corresponds to $t'\backslash t$ to be at position one through nine.) An equivalent definition for the left-blanket and right-blanket is that

$$B_{t\_right} = \{t' \in B_t | t' \text{ is a child of } t \text{ in the enumeration tree}\}$$

and $B_{t\_left} = B_t \backslash B_{t\_right}$. (Here $B_t \backslash B_{t\_right}$ means $B_t \cap \overline{B_{t\_right}}$.)

Now, we are ready to introduce the first pruning technique—the *left-blanket pruning*.

Lemma 6. *For a frequent subtree t in the enumeration tree, if there exists a $t' \in B_{t\_left}$ such that t' and t are occurrence-matched, then 1) t is not closed (and therefore not maximal) and 2) for each child t'' of t in the enumeration tree (i.e., for each $t'' \in B_{t\_right}$), there exists at least one supertree $t''' \in B_{t''\_left}$ so that t''' and t'' are occurrence-matched.*

Proof. The first statement is true because $support(t) = support(t')$. For the second statement, we notice that $t' \backslash t$ occurs at each occurrence of t, so it occurs at each occurrence of t''; in addition, $t' \backslash t$ is on the left of the rightmost path of t, so $t' \backslash t$ will never occur in t''. Therefore, we can obtain the t''' that satisfies the requirement by adding $t' \backslash t$ to t''. □

Theorem 1. *For a frequent subtree t in the enumeration tree, if there exists a $t' \in B_{t\_left}$ such that t' and t are occurrence-matched, then neither t nor any of the descendants of t in the enumeration tree can be closed (or maximal) and, therefore, t (together with all of the descendants of t) can be pruned from the enumeration tree.*

Proof. By inductively applying Lemma 6 to t and its children in the enumeration tree. □

In the example shown in Fig. 5b, t_1, t_3, t_4, t_{10} and t_{15} are pruned from the enumeration tree by using left-blanket pruning.

In Theorem 1, we have used *occurrence-matching* because a transaction-matching element in B_{t_left} does not allow us to prune t. For example, $t_{14} \in B_{t_8\_left}$ and t_{14} and t_8 are transaction-matched. But, if we prune t_8 and its descendants from the enumeration tree, we will miss t_{22}, which is a closed (and maximal) frequent subtree.

3.3.3 The Right-Blanket Pruning

If an occurrence-matching t' occurs in the right blanket B_{t_right} of t, we cannot prune t from the enumeration tree. However, depending on the location of $t' \backslash t$, we still can possibly prune some children of t in the enumeration tree. For example, assume that the rooted tree t in Fig. 3a is frequent and we want to extend t by finding all of the children of t in the enumeration tree. To find the children of t, we add a vertex at position 10, 11, or 12 in Fig. 3b to see if the resulting supertree t' of t is frequent. However, if there is an element $t' \in B_{t\_right}$ such that $t' \backslash t$ is at position 10 in Fig. 3b and if t' and t are occurrence-matched, then after exploring t' in the enumeration tree, we do not have to further extend t by adding a new rightmost vertex to position 11 or position 12 in Fig. 3b. In other words, we can prune some children of t in B_{t_right} by skipping the exploration of the ancestors of vertex G on the rightmost path of t.

Theorem 2. *For a frequent subtree t in the enumeration tree, if there exists $t' \in B_{t\_right}$ such that t' and t are occurrence-matched and the parent of $t' \backslash t$ is v (where v is a vertex on the rightmost path of t), then we do not have to extend t by adding new rightmost vertices to any proper ancestor of v.*

Proof. Assume the preconditions in the theorem hold and there is a child t'' of t in the enumeration tree that is obtained by adding a new rightmost vertex $t'' \backslash t$ to t, where the parent v' of $t'' \backslash t$ is a proper ancestor of v. Because v' is a proper ancestor of v, v is on the left of the rightmost path of t''; in addition, because $t' \backslash t$ is a child of v, $t' \backslash t$ is also on the left of the rightmost path of t''. As a result we can construct a $t''' \in B_{t''\_left}$ by adding $t' \backslash t$ to t'' and, obviously, t''' and t'' are occurrence-matched. Therefore, by Theorem 1, neither t'' nor its descendants in the enumeration tree can be closed (or maximal). □

In the example shown in Fig. 5b, t_{13} and t_{20} will not be generated because they are pruned from the enumeration tree by using the right-blanket pruning of t_8 and t_{14}, respectively.

3.4 The Order of Computation—A Heuristic

To extend a frequent subtree t in the enumeration tree, supertrees in B_t and their supports are needed. However, in some cases, only a subset of B_t is needed (e.g., when t can be pruned using the left-blanket pruning). In this section, we show that different subsets of B_t have different computational costs. We also organize the order of computation for these subsets to avoid, whenever possible, computing the subset with the highest computational cost.

3.4.1 The Subsets to Be Computed

To determine if a frequent subtree t is closed/maximal and whether it can be pruned from the enumeration tree, we will have to compute one or more of the following mutually exclusive subsets of B_t:

$$B_t^{OM} = \{t' \in B_t | t' \text{ and } t \text{ are occurrence-matched}\}$$
$$B_t^{TM} = \{t' \in B_t \backslash B_t^{OM} | t' \text{ and t are trans.-matched}\}$$
$$B_t^{F} = B_t \backslash (B_t^{OM} \cup B_t^{TM})$$

Each of these three subsets can be further partitioned into a left part and a right part by projecting them on B_{t_left} and B_{t_right}. (For example, $B_t^{OM} = B_{t\_left}^{OM} \cup B_{t\_right}^{OM}$.) If there exists $t' \in B_{t\_left}^{OM}$, then neither t nor any of the descendants of t can possibly be closed or maximal, so we can safely prune t and all the descendants of t from the enumeration tree. If $B_{t\_left}^{OM} = \emptyset$, but there exists $t' \in B_{t\_right}^{OM}$, then t still cannot be closed or maximal. In this case, although we cannot prune t, we can possibly apply Theorem 2 to prune some of the children of t. If $B_t^{OM} = \emptyset$, then no pruning is possible and we have to compute B_t^{TM} to determine if t is closed. If $B_t^{TM} \neq \emptyset$, then t is not closed and, therefore, not maximal; if $B_t^{TM} = \emptyset$, then t is closed. In this case, t can also be maximal and whether or not $B_t^{F} = \emptyset$ determines whether or not t is maximal.

3.4.2 How to Compute the Subsets

Now, we study in detail how to compute each of these three subsets and show that their computational costs are different.

For a frequent subtree t, each occurrence of t has some candidate supertrees for B_t^{OM}. To finally determine B_t^{OM}, we compute the *intersection* of these candidate supertrees from each occurrence of t because, for a supertree $t' \in B_t^{OM}$,

$t'\backslash t$ should occur with *each* occurrence of t. For example, assume that we want to compute $B_{t_8}^{OM}$ for t_8 in Fig. 5a. As we can see, t_8 occurs once in $T1$, once in $T2$, and twice in $T3$. We first look at the first occurrence of t_8 for candidate supertrees in $B_{t_8}^{OM}$. The first occurrence happens in $T1$ and there are three candidate supertrees of t_8 (here, we only show $t'_8\backslash t_8$): D (as the left sibling of B), E (as the right sibling of B), and F (as the child of B). (We ignore A because it is not frequent.) Next, we look at all the remaining occurrences of t_8 to see if any of these three candidate supertrees occur in all of them. It turns out that only two, E and F, are in all occurrences and, therefore, $B_{t_8}^{OM}$ consists of these two supertrees. From this example we see that computing B_t^{OM} is not an expensive operation, B_t^{OM} is just the intersection of the candidate supertrees from all occurrences of t.

Computing B_t^{TM} is similar to computing B_t^{OM}, except that each *transaction*, instead of each *occurrence*, has its candidate supertrees for B_t^{TM}. If there are multiple occurrences of t in the same transaction, then the *union* of the candidate supertrees from these occurrences is taken as the candidate supertrees for the transaction. For example, assume that we want to compute $B_{t_{17}}^{TM}$ for t_{17} in Fig. 5a. The occurrence of t_{17} in $T1$ has two candidate supertrees (here, we only show $t'_{17}\backslash t_{17}$): a D (as the left sibling of B) and an F (as the child of E); the occurrence of t_{17} in $T2$ has two candidate supertrees: a D (as the left sibling of B) and a G (as the child of E). However, t_{17} occurs twice in $T3$, so we compute the union of all the candidate supertrees from both occurrences, which results in four candidate supertrees: a C (as the left sibling of B), a D (as the left sibling of B), a G (as the child of E), and another C (as the parent of C). The intersection of these candidate supertrees in each transaction yields a single element in $B_{t_{17}}^{TM}$—a D as the left sibling of B. Again, we can see that computing B_t^{TM} is not an expensive operation, although it is slightly more expensive than computing B_t^{OM}. In addition, we can see that the computation of B_t^{OM} and B_t^{TM} does not involve storing any support and the computation may be terminated before visiting all the occurrences of t; whenever the intersection of candidate supertrees becomes empty, the rest of the occurrences can be skipped.

To compute B_t^F, however, is relatively expensive for the following reason: Again, each transaction has candidate supertrees for B_t^F and, if there are multiple occurrences of t in a transaction, the union of the candidate supertrees from each of these occurrences is the set of candidate supertrees from the transaction. This time, however, instead of a simple intersection, the *union* of all the candidate supertrees from each transaction is used. Furthermore, the support of each candidate supertree must be stored and updated in the process, although a large part of the candidate supertrees may ultimately turn out to be infrequent. For example, assume that we want to compute $B_{t_{22}}^F$ for t_{22} in Fig. 5a. t_{22} occurs once in each of $T1$, $T2$, and $T3$. For the occurrence in $T1$, two candidate supertrees need to be recorded (here, we only show $t'_{22}\backslash t_{22}$): a G (as the child of D) and an F (as the child of E); for the occurrence in $T2$, two candidate supertrees need to be recorded: an F (as the child of D) and a G (as the child of E); for the occurrence in $T3$, one candidate supertree needs to be recorded: a C (as the left sibling of D). Although ultimately none of these candidate supertrees turn out to be frequent, during the process we have to store all of them and update their support because we do not know which are frequent. This also implies that the memory usage for computing B_t^F is not bounded by the size of any transaction. Therefore, computing B_t^F can be relatively expensive.

Algorithm **CMTreeMiner**(D, $minsup$)

▷ inputs: the database D, the minimum support $minsup$.

▷ outputs: the set of all closed frequent subtrees CL, the set of all maximal frequent subtrees MX.

1: $CL \leftarrow \emptyset$, $MX \leftarrow \emptyset$;
2: $C \leftarrow$ frequent 1-trees;
3: CM-Grow(C, CL, MX, D, $minsup$);
4: **return** CL, MX;

Fig. 6. The CMTreeMiner algorithm.

3.4.3 The Order of Computation

Fortunately, the subset of B_t that has the most pruning power, i.e., B_t^{OM}, costs the least to compute. In order to avoid computing B_t^F as much as possible, we adopt the following order to compute the three subsets:

1. Compute B_t^{OM}. If $\exists t' \in B_{t\_left}^{OM}$, prune t; else if $\exists t' \in B_{t\_right}^{OM}$, apply Theorem 2. In either case, there is no need to compute B_t^{TM} or B_t^F because t is neither closed nor maximal.
2. Compute B_t^{TM} if $B_t^{OM} = \emptyset$. If $B_t^{TM} \neq \emptyset$, there is no need to compute B_t^F because t is neither closed nor maximal; else, t is closed.
3. Explore t in the enumeration tree. If any children t' of t turn out to be frequent, then there is no need to compute B_t^F because t is not maximal.
4. Compute $B_{t\_left}^F$ if $B_t^{OM} = \emptyset$, $B_t^{TM} = \emptyset$, and none of the children of t in the enumeration tree are frequent. If $B_{t\_left}^F = \emptyset$, then t is both closed and maximal; otherwise, t is closed but not maximal.

3.5 Putting It All Together—The CMTreeMiner Algorithm

Fig. 6 and Fig. 7 summarize the final *CMTreeMiner* algorithm. The inputs to the algorithm are the database and the user-defined minimum support and the outputs are the closed frequent subtrees and the maximal frequent subtrees. Applying the algorithm to the database shown in Fig. 1, the outputs will be three closed frequent subtrees (t_6, t_{21}, and t_{22} in Fig. 5b), among which two (t_{21} and t_{22}) are maximal frequent subtrees.

3.6 Possible Variations

It is worthwhile to point out some possible variations to the *CMTreeMiner* algorithm. The algorithm mines both closed frequent subtrees and maximal frequent subtrees at the same time. However, the algorithm can be easily changed to mine only closed frequent subtrees or only maximal

Subroutine **CM-Grow**(C, CL, MX, D, $minsup$)

```
1:  for each t ∈ C do
2:    E ← ∅;
3:    compute B_t^OM;
4:    if B_t^OM = ∅ then compute B_t^TM;
5:    if ∃t' ∈ B_t_left^OM then continue;
6:    else
7:      for each vertex v on the rightmost path of t do
        ▷ (in a bottom-up fashion)
8:        for each valid new rightmost vertex w of t do
9:          t' ← t plus vertex w, with v as w's parent;
10:         if support(t') ≥ minsup then E ← E ∪ t';
11:       if ∃t' ∈ B_t_right^OM s.t. v is the parent of t'\t then
12:         break;
13:   if E ≠ ∅ then CM-Grow(E, CL, MX, D, minsup);
14:   if B_t^OM = ∅ and B_t^TM = ∅ then
15:     CL ← CL ∪ t;
16:     if E = ∅ then
17:       compute B_t_left^F;
18:       if B_t_left^F = ∅ then MX ← MX ∪ t;
19: return;
```

Fig. 7. The CM-Grow subroutine.

frequent subtrees. To mine only closed frequent subtrees, the algorithm is modified to skip the step of computing $B^F_{t\_left}$ (i.e., lines 16, 17, and 18 in Subroutine *CM-Grow*). For mining only maximal frequent subtrees, the algorithm modification is to skip computing B^{TM}_t and use B^{OM}_t to prune the subtrees that are not maximal. This pruning is indirect: B^{OM}_t only prunes the subtrees that are not closed, but, if a subtree is not closed, then it cannot be maximal. If $B^{OM}_t = \emptyset$, for better pruning effects we can still compute B^{TM}_t to determine if we want to compute $B^F_{t\_left}$. In this case, although we only want the maximal frequent subtrees, the set of closed frequent subtrees is a byproduct of the algorithm.

4 Mining Closed and Maximal Frequent Rooted *Unordered* Subtrees

In this section, we extend the *CMTreeMiner* algorithm to handle databases of labeled rooted *unordered* trees. By defining a canonical form for labeled rooted *unordered* trees, we extend the concepts that are introduced in the previous section, such as the enumeration DAG, the enumeration tree, and the blanket. In addition, all the pruning and heuristic techniques in the *CMTreeMiner* algorithm are applicable to mining labeled rooted *unordered* trees.

4.1 The Canonical Form for Rooted Labeled *Unordered* Trees

From a rooted *unordered* tree we can derive many rooted *ordered* trees, as shown in Fig. 8. From these rooted *ordered* trees, we want to uniquely select one as the canonical form to represent the corresponding rooted *unordered* tree.

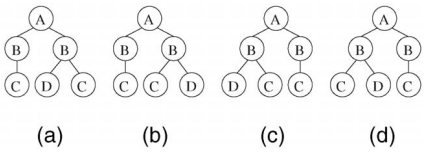


Fig. 8. Four rooted *ordered* trees obtained from the same rooted *unordered* tree.

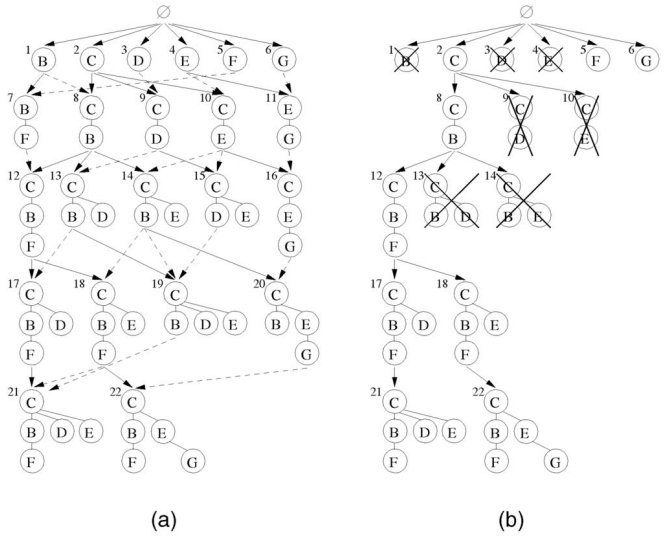
Without loss of generality, we assume that there are two special symbols, "$" and "#", which are not in the alphabet of edge labels and vertex labels. In addition, we assume that 1) there exists a total ordering among edge and vertex labels and 2) "#" sorts greater than "$" and both sort greater than any other symbol in the alphabet of vertex and edge labels. We first define the *depth-first string encoding* for a rooted *ordered* tree as the string of labels obtained through a *depth-first* traversal of the tree, where a "$" represents a backtrack and a "#" represents the end of the string encoding. The depth-first string encodings for each of the four trees in Fig. 8 are, for 1), $ABC\$\$BD\$C\#$, for 2), $ABC\$\$BC\$D\#$, for 3), $ABD\$C\$\$BC\#$, and, for 4), $ABC\$D\$\$BC\#$. With the string encoding, we define the *depth-first canonical form (DFCF)* for a labeled rooted *unordered* tree using the following recursive definition:

1. A labeled rooted *unordered* tree with a single vertex is trivial in DFCF;
2. For a labeled rooted *unordered* tree t with more than one vertex, its DFCF is obtained by the following recursive procedure: Assuming that the root r of t has K children denoted by $r_1, \ldots, r_K$, we first determine the DFCFs for the subtrees $t_{r_1}, \ldots, t_{r_K}$ rooted at $r_1, \ldots, r_K$, then reorder these DFCFs (which are labeled rooted *ordered* trees) from left to right in increasing lexicographical order of their depth-first string encodings.

In Fig. 8, tree (d) is the DFCF for the corresponding labeled rooted *unordered* tree. Note that the *depth-first string encoding* we use here is equivalent to the string encoding that was first proposed by Zaki [27] to represent labeled rooted *ordered* trees. Independent of our work [5], Asai et al. [2] and Nijssen and Kok [17] proposed similar canonical forms, which are equivalent to our DFCF, for labeled rooted *unordered* trees.

4.2 Extending the Enumeration DAG and the Enumeration Tree

Similar to the case of rooted *ordered* trees, we can also build an enumeration DAG to represent the POSET of all frequent rooted *unordered* trees. In the enumeration DAG, each node represents a frequent rooted *unordered* tree in its canonical form (DFCF). Fig. 9a shows the enumeration DAG of all the frequent rooted *unordered* trees in the database given in Fig. 1. An enumeration tree, which is a spanning tree of the enumeration DAG, can be obtained by uniquely determining the parent of each frequent subtree in the enumeration DAG. In our algorithm, we again adopt the enumeration tree defined by Asai et al. [2], in which the parent of a



(a) (b)

Fig. 9. (a) The enumeration DAG and enumeration tree. (b) The enumeration tree after pruning.

frequent subtree t is determined by removing the rightmost vertex from the DFCF of t. Fig. 9a shows such an enumeration tree (ignore the dashed arrows). In the figure, t_6, t_{21}, and t_{22} are closed and, among them, t_{21} and t_{22} are maximal.

4.3 Extending the Blanket and Other Concepts

The concepts of the blanket, occurrence-matching, and transaction-matching all apply to rooted *unordered* trees as well. The enumeration tree growing method is similar as well: For a frequent *unordered* subtree t in the enumeration tree (without loss of generality, when we talk about a subtree t in the enumeration tree, we assume that t is in its DFCF), to create a candidate child for t, a new vertex w is added as a child of some vertex v on the rightmost path of t. However, even if the resulting t' is frequent, in order for t' (which is in DFCF) to be the child of t in the enumeration tree, w must be the rightmost vertex of t'. This requirement restricts the range of labels w can take, as will become evident from the following discussion.

Again, we define the left and the right blankets for a frequent subtree t in the enumeration tree as

$$B_{t\_right} = \{t' \in B_t | t' \text{ is a child of } t \text{ in the enumeration tree}\}$$

and $B_{t\_left} = B_t \backslash B_{t\_right}$. However, for a $t' \in B_t$, whether t' is in B_{t_left} or in B_{t_right} not only depends on the location of $t'\backslash t$, it may also depend on the vertex label of $t'\backslash t$. For example, in Fig. 10, if the parent of $t'\backslash t$ is not a vertex on the rightmost path of t (as shown in case I and case II), then $t' \in B_{t\_left}$; if the parent of $t'\backslash t$ is a vertex on the rightmost path of t, then, depending on the vertex label, $t'\backslash t$ may (as shown in case IV) or may not (as shown in case III) be the rightmost vertex of the DFCF for t'. In the former case, $t' \in B_{t\_right}$ because t' is a child of t in the enumeration tree (i.e., removing the rightmost vertex from t' will result in t); in the latter case, $t' \in B_{t\_left}$.

To distinguish case III and case IV in Fig. 10 for each vertex v on the rightmost path of t, we compute the range of labels that the new vertex w can take in each case. For

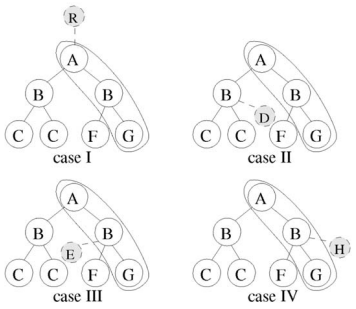


Fig. 10. Locations for an additional vertex to be added to a subtree.

case IV, the label for w should be in such a range that adding w as the child of v will give us a supertree $t' \in B_{t\_right}$ with w as the rightmost vertex; w with other labels it will give us case III. Techniques have been developed in [2] and [6] for this computation. It is worth mentioning that this information is also important when we extend t because it tells us which are valid children of t in the enumeration tree.

4.4 Extending the Pruning and the Heuristic Techniques

With the left-blanket and right-blanket defined, the pruning techniques developed in the previous section for labeled rooted *ordered* trees can be applied to labeled rooted *unordered* trees as well. This is because Lemma 6, Theorem 1, and Theorem 2 are still valid for the enumeration tree of *unordered* frequent subtrees. For example, in Fig. 9b, t_1, t_3, and t_4 are pruned by the left-blanket pruning; t_{13} and t_{14} are pruned by the right-blanket pruning.

Moreover, the right-blanket pruning for *unordered* trees can be more powerful than that for *ordered* trees:

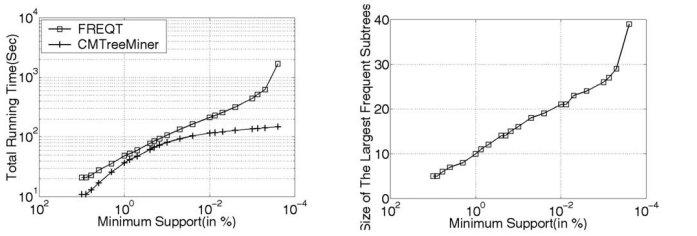
Theorem 3. *For a frequent subtree t in the enumeration tree of frequent rooted unordered trees, if there exists $t' \in B_{t\_right}$ such that t' and t are occurrence-matched and the parent of $t'\backslash t$ is v (where v is a vertex on the rightmost path of t), then 1) we do not have to extend t by adding new rightmost vertices to any proper ancestors of v and 2) we do not have to extend t by adding to v a new rightmost vertex with vertex label lexicographically greater than $t'\backslash t$.*

Proof. The first statement can be proven in the same way as Theorem 2. For the second statement, we notice that for any $t'' \in B_{t\_right}$ such that the parent of $t''\backslash t$ is v and $t''\backslash t$ is lexicographically greater than $t'\backslash t$, we have that $t'\backslash t$ is the left sibling of $t''\backslash t$ in *all* occurrences of t'' and, therefore, neither t'' nor any of its descendants can be closed or maximal. □

For example, in Fig. 9b, t_9 and t_{10} are pruned by the right-blanket pruning because t_8 and t_2 are occurrence-matched. Here, although $t_9\backslash t_2$ and $t_{10}\backslash t_2$ share the same parent (vertex C) with $t_8\backslash t_2$, they are still pruned because $t_8\backslash t_2 < t_9\backslash t_2$ ($B < D$) and $t_8\backslash t_2 < t_{10}\backslash t_2$ ($B < E$).

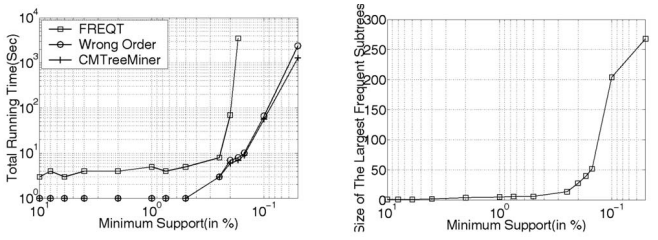
Finally, the heuristic order of computation for reducing relatively expensive computation can be used for extending the enumeration tree of *unordered* frequent subtrees as well.

To summarize, with the definition of the canonical form (DFCF) and with only minor changes (e.g., the procedure to



(a) (b)

Fig. 11. Support thresholds versus running time and the maximum size of frequent subtrees for T1M.



(a) (b)

Fig. 12. Support thresholds versus running time and the maximum size of frequent subtrees for CSLOGS.

determine left and right blankets), the *CMTreeMiner* algorithm developed in the previous section can be used for mining frequent subtrees from databases of labeled rooted *unordered* trees.

4.5 Comparing with CloseGraph

CMTreeMiner shares many common techniques with *CloseGraph* [25], a recent algorithm proposed by Yan and Han for mining closed frequent graphs, and both algorithms borrowed techniques from the field of mining closed frequent itemsets [18]. The main difference between *CMTreeMiner* and *CloseGraph* is that, because *CMTreeMiner* is developed for mining tree structures, it takes advantage of special properties of trees. For example, when extending a tree, *CMTreeMiner* can determine a priori if a given extension will result in a canonical form (which takes amortized constant time [2], [17]); in contrast, in *CloseGraph*, a postprocessing step is needed after an extension to check if the extension is valid (and this step needs to solve a subgraph isomorphism problem, which is not known to be in P or $NP\text{-}complete$ [9]). Furthermore, because the canonical form for tree structures can be obtained in linear time [16], the *left-blanket* and *right-blanket* can be determined efficiently beforehand; in contrast, *CloseGraph* again uses a postprocessing step for pruning after a graph is extended.

5 Experiments

We performed extensive experiments to evaluate the performance of the *CMTreeMiner* algorithm using both synthetic data sets and data sets from real applications. All experiments were done on a 2GHz Intel Pentium IV PC with 1GB main memory, running the RedHat Linux 7.3 operating system. All algorithms were implemented in C++ and compiled using the g++ 2.96 compiler.

5.1 Experiments on Rooted *Ordered* Trees

Since, to our knowledge, there is no existing work on mining closed or maximal frequent *ordered* subtrees, we compare *CMTreeMiner* with the class of algorithms that use postprocessing techniques to get closed or maximal frequent *ordered* trees and use the cost of *FREQT*, which was developed by Asai et al. [1] and implemented by Kudo [14], as a lower bound for this class of algorithms. In the following experiments, we only consider the cost of *FREQT* for discovering all frequent *ordered* subtrees and assume zero cost in the postprocessing stage to obtain the closed or maximal *ordered* subtrees.

5.1.1 The Synthetic Data Set versus the Real Data Set

The synthetic data set T1M is generated by the tree generation program provided by Zaki [27]. In brief, a mother tree is generated first with the following parameters: the number of distinct node labels $N = 100$, the total number of nodes in the tree $M = 10,000$, the maximal depth of the tree $D = 10$, and the maximum fanout $F = 10$. The data set is then generated by creating subtrees of the mother tree. In our experiments, we set the total number of trees in the data set to be $T = 1,000,000$. The average number of nodes in each tree is 6.94.

The real data set CSLOGS is provided by Zaki [27] and is composed of users' access trees to the CS department Website at RPI. An access tree not only records the sequence of Web pages that have been visited in a user session, but also integrates the Website's topological information. It is possible that the labels in an access tree are not unique. That means the same page is visited multiple times in a user's access sequence. CSLOGS contains 59,691 trees that cover a total of 13,361 unique Web pages. The average size of each tree is 12.

5.1.2 Performance Comparison

Fig. 11a shows the time spent by *CMTreeMiner* and *FREQT* under different support thresholds for the synthetic data set T1M. The rate of increase in running time for *CMTreeMiner* is much slower than that for *FREQT* as the support threshold decreases. Also, when the support threshold is low, the trends in the running time of *CMTreeMiner* and *FREQT* become more distinct. The significant increase in the running time of *FREQT* at low support thresholds can be explained by the jump in the maximum frequent subtree size in Fig. 11b. The increase in the maximum frequent subtree size leads to an exponential increase in the number of frequent subtrees and, finally, the exponential increase in running time. Since *CMTreeMiner* does not directly mine frequent subtrees but the closed and maximal frequent subtrees, it is less affected than *FREQT*.

The above trends for *CMTreeMiner* and *FREQT* can also be observed in the real data set CSLOGS (see Fig. 12a and Fig. 12b), only they are more pronounced. The maximum frequent subtree size increases dramatically from 28 to 204 when the support threshold drops from 0.2 percent to 0.1 percent and it becomes difficult for *FREQT* to find all frequent subtrees at support threshold 0.17 percent or lower. On the other hand, *CMTreeMiner* can still handle these lower support thresholds.

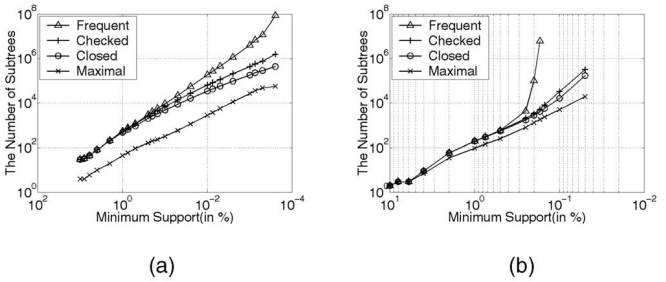


Fig. 13. Support thresholds versus the number of frequent subtrees for T1M and CSLOGS, respectively.

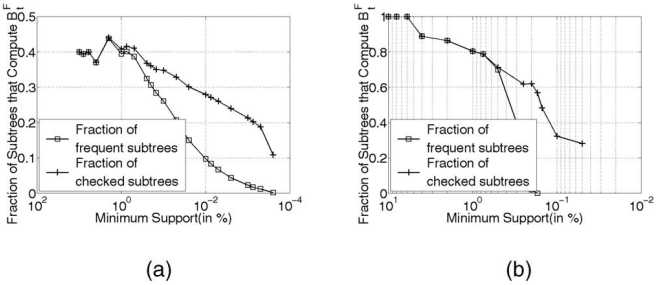


Fig. 14. Support thresholds versus the fraction of subtrees that compute B_t^F for T1M and CSLOGS, respectively.

In addition, to check the effect of the heuristic order of computation that is introduced in Section 3.4.3, we reversed the order of computation such that B_t^F is always computed first. The running time of this version of *CMTreeMiner* is given in Fig. 12a under the name "Wrong Order." As can be seen, this version always performs worse than the original version. For example, when the minimum support is 0.05 percent, the running time of the original version of *CMTreeMiner* is 1,284 seconds, while that for the version with wrong order is 2,396. In other words, in this case, the heuristic of computation order reduces the running time by a half.

The time savings achieved by *CMTreeMiner* comes from the difference between the number of frequent subtrees and closed frequent subtrees. The larger this difference is, the more significant are the savings. In fact, the savings are a function of the correlations among the frequent subtrees. Strong correlations imply that the same set of frequent subtrees can be represented by a relatively small number of closed frequent subtrees. In real applications, strong correlations do exist and it is a motivation of frequent subtree mining algorithms to discover these strong correlations. Fig. 13a and Fig. 13b show the number of frequent subtrees, the number of trees that have been checked by *CMTreeMiner*, the number of closed frequent subtrees, and the number of maximal frequent subtrees in data set T1M and CSLOGS, respectively, under different support thresholds. It is easily seen that, in both data sets, the number of closed frequent subtrees is significantly less than the total number of frequent subtrees, especially when the support threshold is low. The number of subtrees that have been checked by *CMTreeMiner* is also significantly less than the number of frequent subtrees at low support thresholds.

In *CMTreeMiner*, the most expensive operation is to compute the subset B_t^F of the blanket B_t for a frequent subtree t. Fig. 14a shows the fraction of frequent subtrees for which this operation is actually performed and the fraction of closed subtrees in *CMTreeMiner* for which B_t^F is computed. As we can see, as the support threshold decreases, these fractions decrease also. Our understanding of this phenomenon is that the pruning of nonclosed subtrees occurs at places near the root of the enumeration tree. A similar trend can be observed in the data set CSLOGS (see Fig. 14b).

We also studied the memory usage of both *CMTreeMiner* and *FREQT* and found that they are comparable. At the lowest support threshold 0.00025 percent for data set T1M, the memory used by *CMTreeMiner* is 256M, while that by *FREQT* is around 254M. As for CSLOGS, at the support threshold 0.17 percent, the memory usage of *CMTreeMiner* and *FREQT* are 159M and 176M, respectively.

However, as described in [1], *FREQT* uses a special technique to reduce its memory requirement and decreases its computation time: It only stores the occurrences of the rightmost vertex in a frequent subtree; in contrast, *CMTreeMiner* has to store all the occurrences for all the vertices of the frequent subtrees in order to compute the blanket. Therefore, if the number of distinct labels decrease dramatically (so different occurrences for the same pattern increase dramatically), the memory usage of *CMTreeMiner* is expected to increase and its performance is expected to deteriorate. To study the performance under this special case and to modify *CMTreeMiner* to handle it is a topic for future work.

5.2 Experiments on Rooted *Unordered* Trees

In this section, we study the performance of *CMTreeMiner* on mining frequent *unordered* subtrees. We compare the performance of *CMTreeMiner* with that of *PathJoin* [23], a recently proposed algorithm that mines maximal frequent *unordered* subtrees. For this comparison, we use both a synthetic data set and a real application data set—the MBONE multicast data.

5.2.1 Synthetic Data Set

PathJoin [23] mines maximal frequent subtrees from a database of labeled rooted *unordered* trees. However, because *PathJoin* uses the paths from roots to leaves to help subtree mining, it does not allow any siblings in a tree to have the same labels. We use the data generator described in [6] to generate the data set. The detailed procedure for generating the data set is described in [6] and here we give a very brief description. A set of $|N|$ (= 90) subtrees with size $|I|$ are sampled from a large base (labeled) graph. We call this set of $|N|$ subtrees the *seed trees*. Each seed tree is the starting point for $|D| \cdot |S|$ transactions where $|D|$ (= 100,000) is the number of transactions in the database and $|S|$ (= 1 percent) is the minimum support. Each of these $|D| \cdot |S|$ transactions is obtained by first randomly permuting the seed tree, then adding more random vertices to increase the size of the transaction to $|T|$ (= 50). After this step, more random transactions with size $|T|$ are added to the database to increase the cardinality of the database to $|D|$. The number of distinct edge and vertex labels is controlled by

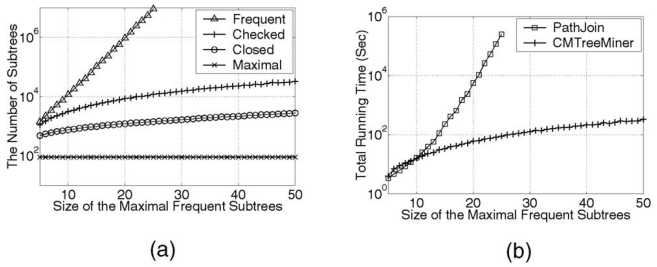


Fig. 15. CMTreeMiner versus PathJoin on synthetic data sets.

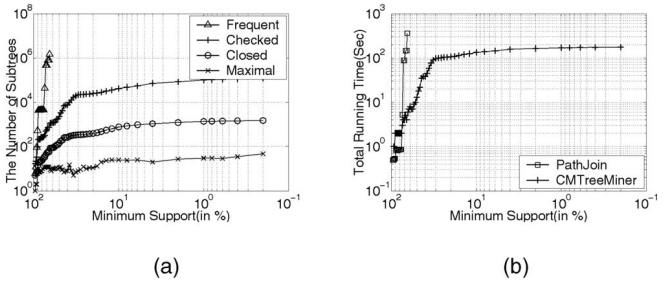


Fig. 16. CMTreeMiner versus PathJoin on the multicast data set.

the parameter $|L|$ (= 1,000), which is both the number of distinct edge labels and the number of distinct vertex labels. The size of the seed trees $|I|$ increases from 5 to 50. (For $|I| > 25$, *PathJoin* exhausts all available memory.)

Fig. 15 compares the performance of *PathJoin* with that of *CMTreeMiner* on this data set. Fig. 15a gives the total number of frequent subtrees obtained by *PathJoin*, the number of subtrees checked by *CMTreeMiner*, the number of closed frequent subtrees, and the number of maximal frequent subtrees. The number of subtrees that are checked by *CMTreeMiner* and the number of closed subtrees grow in polynomial fashion. In contrast, the total number of all frequent subtrees (which is a lower bound of the number of subtrees checked by *PathJoin*) grows exponentially. As a result, as demonstrated in Fig. 15b, although *PathJoin* is very efficient for data sets with small tree sizes, as tree sizes increase beyond some value (say 10), it becomes obvious that *PathJoin* suffers from the exponential growth of computation time while *CMTreeMiner* does not. Note that the Y-axis is drawn on a logarithmic scale and, therefore, orders of magnitude of improvement are achieved by *CMTreeMiner*. For example, with the size of maximal frequent subtrees to be 25 in the data set, it took *PathJoin* nearly three days to find all maximal frequent subtrees, while it took *CMTreeMiner* only 90 seconds! The memory usage of *CMTreeMiner* is also smaller than that of *PathJoin*. When *PathJoin* exhausts the 1GB available memory at $|I| = 26$, *CMTreeMiner* uses about 302 MB memory; when $|I| = 50$, *CMTreeMiner* uses about 567 MB memory.

5.2.2 Real Application Data Set

We also compared the performance of *CMTreeMiner* with that of *PathJoin* using a data set of IP multicast trees. IP multicast is an efficient way to send messages to a group of users. In our experiment, we have used the MBONE multicast data provided in [3]. The data was measured during the NASA shuttle launch between 14th and 21st of February, 1999. It has 333 vertices where each vertex takes an IP address as its label. We sampled the data from this NASA data set in 10 minute sampling intervals and got a data set with 1,000 transactions. Therefore, the transactions are the multicast trees for the same NASA event at different times.

Fig. 16 compares the performance of *PathJoin* with that of *CMTreeMiner* on the multicast data set. As shown in Fig. 16a, this data set is extremely dense: As the support decreases, the total number of frequent subtrees dramatically increases. However, the number of subtrees checked by *CMTreeMiner*, the number of closed frequent subtrees, and the number of maximal frequent subtrees grow relatively slowly. Therefore, as we can see from Fig. 16b, even before *PathJoin* exhausts available memory, its running time becomes impractical. In contrast, *CMTreeMiner* can handle very low support values (e.g., 0.2 percent, which corresponds to a subtree occurring in only two transactions) within 180 seconds.

6 Conclusion

In this paper, we have introduced the problem of mining closed and maximal frequent subtrees from databases of rooted labeled trees. We presented a novel algorithm, *CMTreeMiner*, that efficiently mines closed and maximal frequent subtrees without first generating *all* frequent subtrees. Various pruning and heuristic techniques are used in the algorithm to reduce the search space and to improve the computational efficiency. Our algorithm can be used for mining both labeled rooted *ordered* trees and labeled rooted *unordered* trees. Extensive experiments showed that our algorithm outperformed other state-of-the-art frequent subtree mining algorithms.

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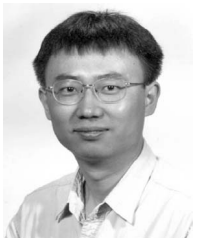

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