PAPER

Efficient Graph Sequence Mining Using Reverse Search

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SUMMARY The mining of frequent subgraphs from labeled graph data has been studied extensively. Furthermore, much attention has recently been paid to frequent pattern mining from graph sequences. A method, called GTRACE, has been proposed to mine frequent patterns from graph sequences under the assumption that changes in graphs are gradual. Although GTRACE mines the frequent patterns efficiently, it still needs substantial computation time to mine the patterns from graph sequences containing large graphs and long sequences. In this paper, we propose a new version of GTRACE that permits efficient mining of frequent patterns based on the principle of a reverse search. The underlying concept of the reverse search is a general scheme for designing efficient algorithms for hard enumeration problems. Our performance study shows that the proposed method is efficient and scalable for mining both long and large graph sequence patterns and is several orders of magnitude faster than the original GTRACE.

key words: *frequent pattern, graph sequence, reverse search*

1. Introduction

Studies on data mining have established many approaches for finding characteristic patterns from a variety of structured data. Graph mining, which efficiently mines all subgraphs appearing more frequently than a given threshold from a set of graphs, focuses on the topological relations between vertices in the graphs [7]. AGM [12], gSpan [21], and Gaston [18] mine frequent subgraphs, starting with those of size 1, using the anti-monotonicity of the support values. Although the major algorithms for graph mining are quite efficient in practice, they require substantial computation time to mine complex frequent subgraphs, owing to the NP-completeness of subgraph isomorphism matching [10]. Accordingly, the conventional methods are not suitable for very complex graphs, such as graph sequences.

Graph sequences, however, are used extensively to model objects in many real-world applications. For example, a human network can be represented as a graph, where a human and the relationship between two humans correspond to a vertex and an edge, respectively. If a human joins (or leaves) the community in the human network, the numbers of vertices and edges in the graph increase (or decrease). Similarly, a gene network consisting of genes and their interactions produces a graph sequence in the course of its evolutionary history by acquiring new genes, deleting genes, and mutating genes.

Recently, much attention has been paid to relevant frequent pattern mining[*] from graph sequences [13] (dynamic graphs [5] or evolving graphs [4]). Figure 1 (a) shows an example of a graph sequence containing 4 steps and 5 vertex IDs, denoted by the numbers attached to the vertices. The problem we address in this paper is how to mine patterns, as shown in Fig. 1 (b), that appear more frequently than a given threshold from a set of graph sequences. We have proposed transformation rules (TRs) for representing graph sequences compactly under the assumption that the change in each graph in the graph sequence is gradual [13]. In other words, only a small part of the structure changes, while the other part remains unchanged between two successive graphs $g^{(j)}$ and $g^{(j+1)}$ in the graph sequence. For example, the change between successive graphs $g^{(j)}$ and $g^{(j+1)}$ in the graph sequence shown in Fig. 2 is represented as an ordered sequence of two TRs $\langle vi^{(j)}_{[1,A]}, ed^{(j)}_{[(2,3),\bullet]}\rangle$. This sequence of TRs implies that a vertex with vertex ID 1 and label A is inserted (vi), and then the edge between the vertices with vertex IDs 2 and 3 is deleted (ed). By assuming that the change in each graph is gradual, we can represent a graph sequence compactly even if the graph in the graph sequence has many vertices and edges. Based on this idea, Inokuchi and Washio proposed a method, called GTRACE (graph transformation sequence mining), for efficiently mining all frequent patterns, called relevant FTSs (frequent transformation subsequences), from ordered sequences of TRs [13]. In a similar manner to PrefixSpan [21], GTRACE first recursively mines FTSs, appending a TR to the tail of the mined FTS, and then removes irrelevant FTSs during post-processing. Since most of the FTSs mined from graph sequences by GTRACE are

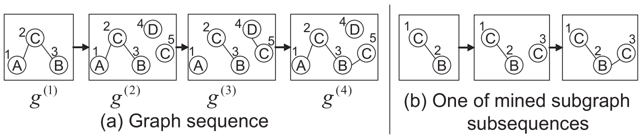

Fig. 1 Examples of a graph sequence and subgraph subsequence for mining.

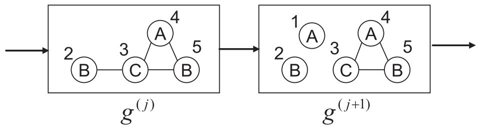

Fig. 2 Change between two successive graphs.

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[*]The relevancy of frequent patterns is defined in Sect. 2.2.

irrelevant, if we mine only relevant FTSs from the graph sequences, we can greatly reduce the computation time for this mining process, thus making it suitable for graph sequences containing large graphs and long sequences.

Our objective graph sequence is more general than both the dynamic graph and evolving graph, and GTRACE and the proposed method in this paper are applicable to both dynamic graphs and evolving graphs, although methods [4], [5] for mining relevant frequent patterns are not applicable to graph sequences. Borgwardt et al. proposed a method [5] for mining relevant frequent patterns from a graph sequence represented by a dynamic graph. They assumed that the number of edges in a dynamic graph increases and decreases, while the number of vertices remains constant. They also assumed that labels assigned to vertices in the dynamic graph do not change and that no labels are assigned to edges. On the other hand, Berlingerio et al. proposed a method to mine relevant frequent patterns from a graph sequence represented by an evolving graph [4]. They assumed that the numbers of vertices and edges in an evolving graph increase, but do not decrease, and that labels assigned to vertices and edges in the evolving graph do not change. In addition, a vertex in an evolving graph always comes with an edge connected to the vertex.

In this paper, we propose a new version of GTRACE that enables more efficient mining of only relevant FTSs based on the principle of a reverse search [3]. Our performance study shows that the proposed method is efficient and scalable for mining both long and large graph sequence patterns, and is several orders of magnitude faster than the original GTRACE.

The rest of this paper is organized as follows. The remainder of this section reviews conventional frequent graph mining. In Sect. 2, we review the problem of mining graph sequences. In Sect. 3, we propose an efficient method to mine only relevant FTSs from a set of graph sequences, and we explain how to implement our proposed method for efficient mining of relevant FTSs in Sect. 4. In Sect. 5, the fundamental performance and practicality of the proposed method are demonstrated through experiments. Finally, in Sect. 6 we present a discussion, and we conclude the paper in Sect. 7.

1.1 Frequent Graph Mining

Graph mining is the task of finding novel, useful, and "understandable" graph-theoretic patterns in a graph representation of data [6]. Frequent graph mining is a representative task in graph mining that efficiently mines all subgraphs that appear more frequently than a given threshold from a set of labeled graphs.

Let *gid* and *g* be a graph ID and a labeled graph, respectively. A graph database *DB* is a set of tuples $\langle gid, g\rangle$. A tuple $\langle gid, g\rangle$ is said to contain a graph *p*, if *p* is a subgraph of *g*, *i.e.*, $p \sqsubseteq g$. The support of graph *p* in database *DB* is the number of tuples in the database containing *p*, *i.e.*, $\sigma(p) = |\{gid \mid (\langle gid, g\rangle \in DB) \wedge (p \sqsubseteq g)\}|$. Given a positive integer σ' as the support threshold, a graph *p* is called a "frequent subgraph" pattern in the graph database *DB*, if at least σ' tuples in the database contain *p*, *i.e.*, $\sigma(p) \geq \sigma'$. Representative methods for frequent graph mining, such as AGM [12], gSpan [21], and Gaston [18], mine frequent subgraphs starting with those of size 1, using the anti-monotonicity of the support values.

We briefly review gSpan, because it is used to implement the method proposed in this paper. Here, for the sake of simplicity, we assume that edges in graphs have labels, whereas vertices in the graphs do not. Given a frequent pattern *p* with *n* vertices and *k* edges, vertices in *p* are traversed in a depth first manner to assign vertex IDs from v_1 to v_n. The starting vertex and the last visited vertex in the traversal are called the root v_1 and the rightmost vertex v_n, respectively, while the straight path from v_1 to v_n is called the rightmost path. According to the traversal, when an edge label between vertices v_u and $v_{u'}$ ($1 \leq u, u' \leq n$) is *l*, *p* is represented by DFS code consisting of triplets (u, u', l). The linear order of the DFS codes is defined as follows. For DFS codes $\alpha = (a_1, a_2, \cdots, a_k)$ and $\beta = (b_1, b_2, \cdots, b_h)$, $\alpha \leq \beta$, iff either of the following conditions is true:

- $\exists t, 1 \leq t \leq min(k, h), a_q = b_q \, for \, q < t, a_t \prec_e b_t$
- $a_q = b_q \, for \, 0 \leq q \leq k, and \, k \leq h$

where $\prec_e$ is the linear order among the triplets (u, u', l). Since there are many DFS codes for an identical *p*, the minimal DFS code of the DFS codes representing *p* is defined as the canonical code for *p*.

Example 1: Table 1 gives the DFS codes for the different traversals shown in Fig. 3 (b)–(d) of the frequent subgraph *p* depicted in Fig. 3 (a). According to the linear order of the DFS codes, $\gamma \prec \alpha \prec \beta$, and γ is the canonical code for *p*.

A frequent subgraph *p* is extended based on the

Table 1 DFS Codes for Fig. 3.

edge *k*	α (Fig. 3 (b))	β (Fig. 3 (c))	γ (Fig. 3 (d))
1	$(1, 2, a)$	$(1, 2, d)$	$(1, 2, a)$
2	$(2, 3, b)$	$(2, 3, b)$	$(2, 3, a)$
3	$(3, 1, a)$	$(3, 4, a)$	$(3, 1, b)$
4	$(3, 4, c)$	$(4, 2, a)$	$(3, 4, d)$
5	$(4, 2, b)$	$(3, 5, c)$	$(3, 5, b)$
6	$(2, 5, d)$	$(5, 2, b)$	$(5, 1, c)$

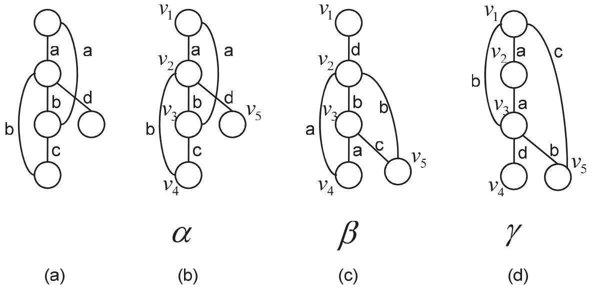


Fig. 3 Depth-first traversal for a frequent pattern.

pattern-growth principle. Given a DFS code $\alpha = (a_1, a_2, \cdots, a_k)$ for p with k edges, p is extended by adding a new edge to obtain a new pattern with $k+1$ edges, which is represented by $\alpha' = (a_1, a_2, \cdots, a_k, a_{k+1})$. The new edge can be added between the rightmost vertex and other vertices on the rightmost path (backward extension), or it can introduce a new vertex and connect to vertices on the rightmost path (forward extension). Overall, new edges are only added to the vertices along the rightmost path. With this restricted extension, gSpan reduces the generation of the same frequent subgraphs. However, it still guarantees the completeness of enumerating all frequent subgraphs.

2. Mining Graph Sequences

2.1 Representation

In this section, we briefly review the compilation used to represent graph sequences compactly in GTRACE. Figure 1 (a) shows an example of a graph sequence. Graph $g^{(j)}$ is the j-th labeled graph in the sequence. The problem we address in this paper is how to mine patterns that appear more frequently than a given threshold from a set of graph sequences. We have proposed TRs to represent graph sequences compactly under the assumption that "the change over successive graphs is gradual". In other words, only a small part of the graph changes between two successive graphs $g^{(j)}$ and $g^{(j+1)}$ in a graph sequence, while the other parts remain unchanged [13]. In the aforementioned human and gene networks, this assumption certainly holds, because most of the changes in vertices are progressive over successive steps. A direct representation of a graph sequence is not compact, because many parts of the graph remain unchanged over several steps and are therefore redundant in the representation. On the other hand, a graph sequence can be compactly represented by introducing a representation of graph transformation based on rules for insertion, deletion, and relabeling of vertices and edges under the gradual change assumption.

Let $V = \{v_1, \cdots, v_z\}$ be a set of vertices, $E \subseteq V \times V$ be a set of edges, and L be a set of labels such that $f : V \cup E \to L$. A labeled graph g is represented as $g = (V, E, L, f)$. In this paper, we assume that there are no multiple edges between vertices. A graph sequence is represented as $d = \langle g^{(1)}\ g^{(2)} \cdots g^{(n)} \rangle$. We assume that each vertex v is mutually distinct from the others in $g^{(j)}$ and has a vertex ID $id(v)$ in d. We define the set of vertex IDs to be $ID_V(d) = \{id(v) \mid v \in V(g^{(j)}), g^{(j)} \in d\}$ and the set of pairs of vertex IDs to be $ID_E(d) = \{(id(v), id(v')) \mid (v, v') \in E(g^{(j)}), g^{(j)} \in d\}$. For example, in the human network mentioned in Sect. 1, each person has a vertex ID, and his/her gender is an example of a vertex label. To represent a graph sequence compactly, we focus on the differences between two successive graphs $g^{(j)}$ and $g^{(j+1)}$ in the sequence.

Definition 1: Given a graph sequence $d = \langle g^{(1)} \cdots g^{(n)} \rangle$, the differences between $g^{(j)}$ and $g^{(j+1)}$ are interpolated by a virtual sequence $d^{(j)} = \langle g^{(j,1)} \cdots g^{(j,m_j)} \rangle$, where $g^{(j,1)} = g^{(j)}$ and $g^{(j,m_j)} = g^{(j+1)}$, such that the edit distance [20] between any two successive graphs is 1, and in which the edit distance between any two intrastates is the minimum. Therefore, d is represented by the interpolations as $d = \langle d^{(1)} \cdots d^{(n-1)} \rangle$. ■

We call $g^{(j)}$ and $g^{(j,k)}$ an interstate and intrastate, respectively. The order of interstates represents the order of graphs in a sequence. On the other hand, the order of intrastates is the order of graphs in the artificial interpolation.

The transformation is represented by the following TR.

Definition 2: A TR that transforms $g^{(j,k)}$ to $g^{(j,k+1)}$ is expressed as $tr^{(j,k)}_{[o_{jk}, l_{jk}]}$, where

- tr is a transformation type, which is either insertion, deletion, or relabeling of a vertex or an edge,
- o_{jk} is an element in $ID_V(d) \cup ID_E(d)$ to be transformed, and
- $l_{jk} \in L$ is the label to be assigned to the element by the transformation. ■

For the sake of simplicity, we denote the TR $tr^{(j,k)}_{[o_{jk}, l_{jk}]}$ as $tr^{(j,k)}_{[o,l]}$ by omitting the subscripts for o_{jk} and l_{jk}, except where this is likely to cause ambiguity. We have introduced six TRs as defined in Table 2 [13]. In summary, we give the following definition of a transformation sequence.

Definition 3: An intrastate sequence $d^{(j)} = \langle g^{(j,1)} \cdots g^{(j,m_j)} \rangle$ is represented by an "intrastate transformation sequence" $s^{(j)}_d = \langle tr^{(j,1)}_{[o,l]} \cdots tr^{(j,m_j-1)}_{[o,l]} \rangle$. Moreover, a graph sequence $d = \langle g^{(1)} \cdots g^{(n)} \rangle$ is represented by an "interstate transformation sequence" $s_d = \langle s^{(1)}_d \cdots s^{(n-1)}_d \rangle$. ■

The notion of an interstate transformation sequence is far more compact than the original graph based representation, because only the differences between two successive inter-

Table 2 Transformation rules (TRs) representing graph sequence data.

Vertex Insertion $vi^{(j,k)}_{[u,l]}$	Insert a vertex with label l and vertex ID u into $g^{(j,k)}$ to transform to $g^{(j,k+1)}$.
Vertex Deletion $vd^{(j,k)}_{[u,\bullet]}$	Delete an isolated vertex with vertex ID u in $g^{(j,k)}$ to transform to $g^{(j,k+1)}$.
Vertex Relabeling $vr^{(j,k)}_{[u,l]}$	Relabel a vertex with vertex ID u in $g^{(j,k)}$ to be l to transform to $g^{(j,k+1)}$.
Edge Insertion $ei^{(j,k)}_{[(u_1,u_2),l]}$	Insert an edge with label l between 2 vertices with vertex IDs u_1 and u_2 into $g^{(j,k)}$ to transform to $g^{(j,k+1)}$.
Edge Deletion $ed^{(j,k)}_{[(u_1,u_2),\bullet]}$	Delete an edge between 2 vertices with vertex IDs u_1 and u_2 in $g^{(j,k)}$ to transform to $g^{(j,k+1)}$.
Edge Relabeling $er^{(j,k)}_{[(u_1,u_2),l]}$	Relabel an edge between 2 vertices with vertex IDs u_1 and u_2 in $g^{(j,k)}$ to be l to transform to $g^{(j,k+1)}$.

Since the transformations of vertex deletion vd and edge deletion ed do not assign any labels to the vertex and the edge, respectively, they have dummy arguments l, represented by '$\bullet$'.

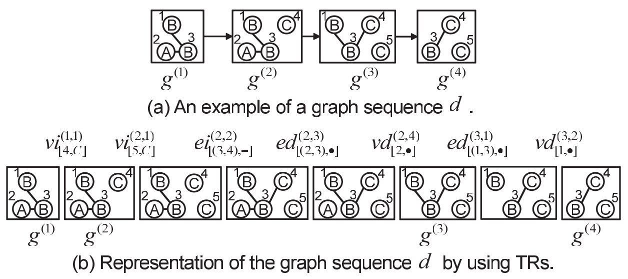

$g^{(1)}$ $g^{(2)}$ $g^{(3)}$ $g^{(4)}$
(a) An example of a graph sequence d.
$vi^{(1,1)}_{[4,C]}$ $vi^{(2,1)}_{[5,C]}$ $ei^{(2,2)}_{[(3,4),-]}$ $ed^{(2,3)}_{[(2,3),\bullet]}$ $vd^{(2,4)}_{[2,\bullet]}$ $ed^{(3,1)}_{[(1,3),\bullet]}$ $vd^{(3,2)}_{[1,\bullet]}$
(b) Representation of the graph sequence d by using TRs.

Fig. 4 A graph sequence with its transformation rules.

states appear in the sequence. In addition, in our case, computing a sequence of TRs based on differences between two graphs is solvable in linear time because all vertices have vertex IDs.

Example 2: In Fig. 4 (a), a graph sequence is expressed as a sequence of insertions and deletions of vertices and edges as shown in Fig. 4 (b). The sequence is compiled as $\langle vi^{(1,1)}_{[4,C]} vi^{(2,1)}_{[5,C]} ei^{(2,2)}_{[(3,4),-]} ed^{(2,3)}_{[(2,3),\bullet]} vd^{(2,4)}_{[2,\bullet]} ed^{(3,1)}_{[(1,3),\bullet]} vd^{(3,2)}_{[1,\bullet]} \rangle$, where "–" denotes the label of an edge.

We denote the length $n-1$ of a transformation sequence $s_d = \langle s^{(1)}_d \cdots s^{(n-1)}_d \rangle$ as $|s_d|$. The length of the transformation sequence given in Example 2 is 3.

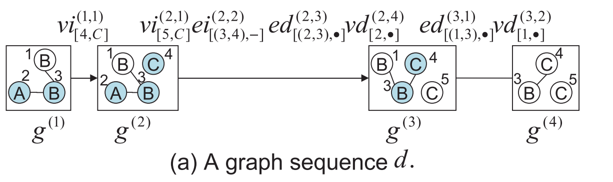
2.2 Mining Relevant Frequent Transformation Subsequences

In this section, we briefly review how GTRACE mines rFTSs (relevant frequent transformation subsequences) from a given set of graph sequences. To mine rFTSs from a set of transformation sequences, we define an inclusion relation between transformation sequences.

Definition 4: Let a transformation sequence of a pattern and a transformation sequence of a data graph sequence d be s_p and s_d, respectively. s_p is a subsequence of s_d, denoted as $s_p \sqsubseteq s_d$, iff there is a pair of injective functions (ϕ, ψ) satisfying the following conditions.

- There exist integers $1 \le \phi(1) < \phi(2) < \cdots < \phi(|s_p|) \le |s_d|$.
- There exist integers $\psi(u) \in ID_V(d)$ for vertex IDs u in s_p.
- $\forall\ tr^{(j,k)}_{[o,l]} \in s_p \Rightarrow \exists k',\ tr^{(\phi(j),k')}_{[o',l]} \in s_d$, where $o' = \psi(u)$, if the TR $tr^{(j)}_{[o,l]} \in s_p$ transforms a vertex with vertex ID u. On the other hand, $o' = (\psi(u_1), \psi(u_2))$, if the TR transforms an edge with vertex IDs u_1 and u_2. ■

The first condition in Definition 4 states that ϕ preserves the order among intrastate transformation sequences, while the second condition states an injective mapping from vertex IDs in s_p to vertex IDs in s_d. In addition, the third condition states that a TR corresponding to any TR in s_p must exist in s_d. The complexity of finding an occurrence of s_p in s_d is identical to that of subgraph isomorphism matching.


$vi^{(1,1)}_{[4,C]}$ $vi^{(2,1)}_{[5,C]} ei^{(2,2)}_{[(3,4),-]}$ $ed^{(2,3)}_{[(2,3),\bullet]} vd^{(2,4)}_{[2,\bullet]}$ $ed^{(3,1)}_{[(1,3),\bullet]} vd^{(3,2)}_{[1,\bullet]}$
$g^{(1)}$ $g^{(2)}$ $g^{(3)}$ $g^{(4)}$
(a) A graph sequence d.

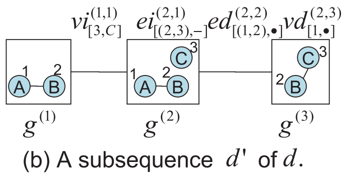

$vi^{(1,1)}_{[3,C]}$ $ei^{(2,1)}_{[(2,3),-]} ed^{(2,2)}_{[(1,2),\bullet]} vd^{(2,3)}_{[1,\bullet]}$
$g^{(1)}$ $g^{(2)}$ $g^{(3)}$
(b) A subsequence d' of d.

Fig. 5 Inclusion relation.

Example 3: Given the graph sequence d in Fig. 5 (a) represented by the transformation sequence $s_d = \langle \underline{vi^{(1,1)}_{[4,C]}} vi^{(2,1)}_{[5,C]} \underline{ei^{(2,2)}_{[(3,4),-]} ed^{(2,3)}_{[(2,3),\bullet]} vd^{(2,4)}_{[2,\bullet]}} ed^{(3,1)}_{[(1,3),\bullet]} vd^{(3,2)}_{[1,\bullet]} \rangle$, the transformation sequence $s'_d = \langle vi^{(1,1)}_{[3,C]} ei^{(2,1)}_{[(2,3),-]} ed^{(2,2)}_{[(1,2),\bullet]} vd^{(2,3)}_{[1,\bullet]} \rangle$ of the graph sequence d' in Fig. 5 (b) is a subsequence of s_d, and the TRs in s'_d match the underlined rules in s_d via $\phi(j) = j$ for $j \in \{1, 2\}$ and $\psi(i) = i + 1$ for $i \in ID_V(d') = \{1, 2, 3\}$.

To mine FTSs consisting of mutually relevant vertices only, the relevancy of vertices and edges is defined as follows[†].

Definition 5: We define the union graph of d to be $g_u(d) = (V_u, E_u)$, where $V_u = ID_V(d)$ and $E_u = ID_E(d)$. In addition, if the union graph $g_u(d)$ of d is a connected graph, vertex IDs in a graph sequence $d = \langle g^{(1)} \cdots g^{(n)} \rangle$ are relevant to one another, and d is called a "relevant graph sequence". ■

We defined the union graph of a graph sequence d. Similarly, we define the union graph of the transformation sequence s_d.

Definition 6: The union graph $g_u(s_d) = (V_u, E_u)$ of a transformation sequence s_d is defined as

$$\begin{aligned} V_u &= \{u \mid tr^{(j,k)}_{[u,l]} \in s_d, tr \in \{vi, vd, vr\}\} \\ &\quad \cup \{u, u' \mid tr^{(j,k)}_{[(u,u'),l]} \in s_d, tr \in \{ei, ed, er\}\}, \\ E_u &= \{(u, u') \mid tr^{(j,k)}_{[(u,u'),l]} \in s_d, tr \in \{ei, ed, er\}\}. \end{aligned}$$ ■

Example 4: Figure 6 (b) shows the union graph of the graph sequence depicted in Fig. 6 (a). In addition, the union graph of a transformation sequence $\langle ei^{(1,1)}_{[(1,2),-]} ei^{(2,1)}_{[(2,3),-]} \rangle$ is identical to the graph shown in Fig. 6 (b).

Given a set of data $DB = \{\langle gid, d\rangle \mid d = \langle g^{(1)} \cdots g^{(n)} \rangle\}$, the support value $\sigma(s_p)$ of a transformation subsequence s_p is given as

$$\sigma(s_p) = |\{gid \mid \langle gid, d\rangle \in DB, s_p \sqsubseteq s_d\}|,$$

where s_d is the transformation sequence of d. We call a

[†]See [13], [14] for the detail motivations for mining rFTSs.

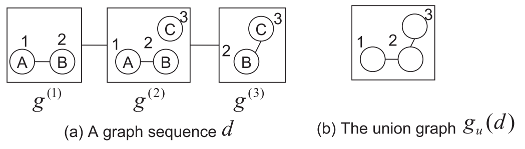


Fig. 6 Union graph.

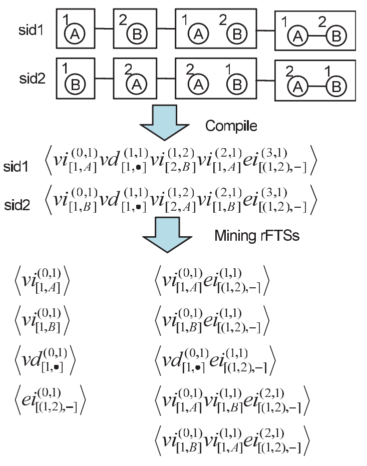

sid1
sid2
Compile
sid1 $\langle vi^{(0,1)}_{[1,A]} vd^{(1,1)}_{[1,\bullet]} vi^{(1,2)}_{[2,B]} vi^{(2,1)}_{[1,A]} ei^{(3,1)}_{[(1,2),-1]} \rangle$
sid2 $\langle vi^{(0,1)}_{[1,B]} vd^{(1,1)}_{[1,\bullet]} vi^{(1,2)}_{[2,A]} vi^{(2,1)}_{[1,B]} ei^{(3,1)}_{[(1,2),-1]} \rangle$
Mining rFTSs
$\langle vi^{(0,1)}_{[1,A]} \rangle$
$\langle vi^{(0,1)}_{[1,B]} \rangle$
$\langle vd^{(0,1)}_{[1,\bullet]} \rangle$
$\langle ei^{(0,1)}_{[(1,2),-1]} \rangle$
$\langle vi^{(0,1)}_{[1,A]} ei^{(1,1)}_{[(1,2),-1]} \rangle$
$\langle vi^{(0,1)}_{[1,B]} ei^{(1,1)}_{[(1,2),-1]} \rangle$
$\langle vd^{(0,1)}_{[1,\bullet]} ei^{(1,1)}_{[(1,2),-1]} \rangle$
$\langle vi^{(0,1)}_{[1,A]} vi^{(1,1)}_{[1,B]} ei^{(2,1)}_{[(1,2),-1]} \rangle$
$\langle vi^{(0,1)}_{[1,B]} vi^{(1,1)}_{[1,A]} ei^{(2,1)}_{[(1,2),-1]} \rangle$

Fig. 7 Mining rFTSs from DB.

transformation subsequence with support value greater than or equal to a minimum support threshold σ' a "frequent transformation subsequence" (FTS). The anti-monotonicity of this support value holds; that is, if $s_1 \sqsubset s_2$ then $\sigma(s_1) \geq \sigma(s_2)$. Using these definitions, we state our mining problem as follows.

Problem 1: Given a dataset $DB = \{\langle gid, d\rangle \mid d = \langle g^{(1)} \cdots g^{(n)}\rangle\}$ and a minimum support threshold σ' as input, enumerate all rFTSs.

Example 5: Figure 7 shows a graph sequence database DB that contains two graph sequences and nine rFTSs mined from the compiled graph sequences in DB under $\sigma' = 2$. In this example, $\langle vi^{(1,1)}_{[1,A]} vi^{(2,1)}_{[2,B]}\rangle$ and $\langle vi^{(1,1)}_{[1,B]} vi^{(2,1)}_{[2,A]}\rangle$ are common subsequences of the compiled graph sequences not mined from DB, because their union graphs are not connected.

To enumerate all rFTSs efficiently, GTRACE recursively mines FTSs by appending a TR to the tail of the current FTS, in a similar manner to PrefixSpan [19], which is a representative method for mining frequent subsequences from a set of itemset sequences. After mining all the FTSs, GTRACE removes all FTSs whose union graphs are not connected, thus outputting only rFTSs.

Example 6: Figure 8 shows the detailed procedure for mining FTSs up to s_6 using GTRACE. After mining an FTS s_i, GTRACE recursively appends a TR to s_i to mine a longer FTS s_{i+1}. After mining all FTSs, s_2, s_3, and s_4 are removed during post-processing, because their union graphs are not connected.

$$\begin{aligned}
s_1 &= \langle vi^{(1,1)}_{[1,A]} \rangle \\
s_2 &= \langle vi^{(1,1)}_{[1,A]} vi^{(2,1)}_{[2,B]} \rangle \\
s_3 &= \langle vi^{(1,1)}_{[1,A]} vi^{(2,1)}_{[2,B]} vi^{(3,1)}_{[3,C]} \rangle \\
s_4 &= \langle vi^{(1,1)}_{[1,A]} vi^{(2,1)}_{[2,B]} vi^{(3,1)}_{[3,C]} ei^{(4,1)}_{[(1,2),-]} \rangle \\
s_5 &= \langle vi^{(1,1)}_{[1,A]} vi^{(2,1)}_{[2,B]} vi^{(3,1)}_{[3,C]} ei^{(4,1)}_{[(1,2),-]} ei^{(4,2)}_{[(2,3),-]} \rangle \\
s_6 &= \langle vi^{(1,1)}_{[1,A]} vi^{(2,1)}_{[2,B]} vi^{(3,1)}_{[3,C]} ei^{(4,1)}_{[(1,2),-]} ei^{(4,2)}_{[(2,3),-]} ed^{(5,1)}_{[(2,3),-]} \rangle
\end{aligned}$$

Fig. 8 Mining procedure using GTRACE.

2.3 Drawback of GTRACE

In the previous subsection, we briefly reviewed the problem of graph sequence mining and GTRACE for mining rFTSs from graph sequences. GTRACE first mines a set of FTSs containing a complete set of rFTSs, and then removes any FTS that is not relevant from the set of mined FTSs during post-processing. Since most of the FTSs mined in the first step are not rFTSs, excessive computation time is needed to mine the vast set of FTSs, causing GTRACE to be highly inefficient.

For example, the FTS s_6 shown in Fig. 8 is relevant, because its union graph is connected. To mine this rFTS, GTRACE mines s_1, s_2, s_3, s_4, and s_5 in order appending a TR to the tail of s_i to obtain a new FTS s_{i+1} for $i = 2, \cdots, 5$. Then, s_2, s_3, and s_4 are removed during post-processing, because they are irrelevant. Therefore, to mine all rFTSs using GTRACE, a vast set of FTSs, most of which are not rFTSs, first needs to be mined, resulting in inefficient execution of GTRACE. In our experiment, 95% of FTSs mined by GTRACE are irrelevant. In addition, to mine s_2, s_3, and s_4, extra memory space is allocated in GTRACE. By designing a new algorithm that mines only rFTSs, we can reduce the computation time and memory space for mining the complete set of rFTSs. In the next section, we propose a new method for mining only rFTSs from a set of graph sequences based on the principle of a reverse search.

3. Proposed Method

3.1 Reverse Search

To mine all rFTSs efficiently, we propose a method for mining only rFTSs based on a reverse search [1], [3]. The underlying concept of the reverse search is a general scheme for designing efficient algorithms for hard enumeration problems. Let S be the set of solutions. In a reverse search, we define the parent-child relation $P : S \to S$ such that each $x \in S$ has a unique parent $P(x) \in S$. P is defined for $x \in S$ except for some solutions $S' \subseteq S$, and $x' \in S'$ is obtained by traversing the parent $P(x)$ for any x repeatedly. Using the search forest T over S defined by P, we can enumerate all solutions of S without duplicates by traversing the search forest T from the root $x' \in S'$ of each subtree of the forest

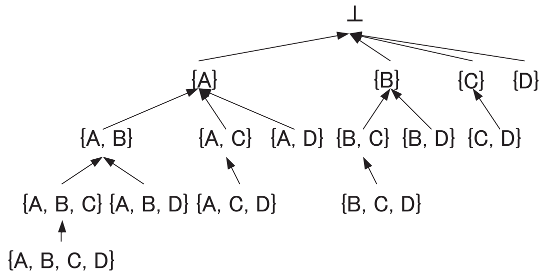


Fig. 9 Enumeration Tree for items $\{A, B, C, D\}$.

to the leaves. Therefore, if we can define the parent-child relation P such that each $x \in S$ has a "unique" parent, we can enumerate a complete set of elements in S.

For example, let a set of items be $I = \{i_1, \cdots, i_{|I|}\}$ and a set of transactions be $D = \{t \mid t \subseteq I\}$. In addition, let the support value of an itemset x be $\sigma(x) = |\{t \mid x \subseteq t, t \in D\}|$ and the minimum support threshold be σ'. The frequent itemset mining problem is to enumerate all frequent itemsets $S_I = \{x \mid x \subseteq I, \sigma(x) \geq \sigma'\}$. To enumerate the complete set of frequent itemsets efficiently, the parent-child relation P is defined as the unique itemset $x' = \{i_1, i_2, \cdots, i_{k-1}\}$ derived from $x = \{i_1, i_2, \cdots, i_{k-1}, i_k\}$ by removing the last item i_k in x, where the items in x and x' are sorted according to the linear order of the items. Starting from the root node corresponding to an empty set, traversing the search tree T over S_I defined by P enables us to enumerate a complete set of frequent itemsets without duplicates. In the traversal, $P^{-1}(x')$ is used to enumerate itemsets from itemset $x' \in S_I$ by adding an item to x'. Figure 9 shows the enumeration tree for the itemset $I = \{A, B, C, D\}$, with 2^I nodes in the tree. By traversing from the root node in a reverse direction to the arrows in the tree, all itemsets are enumerated.

However, as mentioned in Sect. 2.3, if the last TR in an rFTS s_i $(i = 2, \cdots, 6)$ is removed to derive its parent FTS s_{i-1}, s_{i-1} is not always relevant, although s_{i-1} is always frequent according to the anti-monotonicity of the support values. Therefore, the original GTRACE needs all the FTSs to enumerate all the rFTSs, which results in inefficient execution of GTRACE. In this section, to enumerate only rFTSs, we define canonical forms of rFTSs and novel parent-child relations P_1, P_2, and P_3 between the canonical rFTSs.

Definition 7: Given an rFTS s, TRs $a_k, a_{k-1}, \cdots, a_1$ in s are removed by either P_1, P_2, or P_3 in order as defined later. Vertex IDs in $g_u(s)$ are assigned in a depth-first manner similarly to gSpan. We define a code $\alpha = (a_1, \cdots, a_k)$ for s. For codes $\alpha = (a_1, \cdots, a_k)$ and $\beta = (b_1, \cdots, b_h)$, $\alpha \leq \beta$, iff either of the following conditions is true:

- $\exists t, 1 \leq t \leq min(k, h), a_q = b_q\, for\, q < t, a_t \prec_{tr} b_t$
- $a_q = b_q\, for\, 0 \leq q \leq k, and\, k \leq h,$

where $\prec_{tr}$ is the linear order among TRs $tr^{(j,k)}_{[o,l]}$. Since there are many representations for an identical transformation sequence, the representation corresponding to the minimal code among the representations of an identical transformation sequence is defined as canonical. ■

In Definition 7, P_1, P_2, and P_3 are parent-child relations among canonical rFTSs S_{rfts}, which are defined as follows.

Definition 8: Given an rFTS $s \in S_{rfts}$ containing TRs applied to vertices, we define function P_1 mapping from s to s'. The transformation sequence s' is derived from s by removing the TR located in the last position of all the TRs applied to vertices in s. ■

If the length of transformation sequence s is defined as the number of TRs in s, the following lemma is obtained.

Lemma 1: Given an rFTS $s \in S_{rfts}$ containing TRs that are applied to vertices and with length greater than 1, $g_u(P_1(s)) = g_u(s)$. ■

Proof 1: The union graph of s is a connected graph, because s is relevant. If the vertex ID, to which the TR r removed by P_1 is applied, is u, a TR to transform an edge, whose terminal vertex ID is u, must exist in s, because $g_u(s)$ is connected. Therefore, vertex u remains in $g_u(P_1(s))$ after r is removed, and the union graph of transformation sequence $P_1(s)$ is isomorphic with $g_u(s)$. On the other hand, given an rFTS $s \in S_{rfts}$ of length 1 containing a TR that is applied to a vertex, $P_1(s) = \perp$.

According to Lemma 1, $P_1(s)$ is always relevant for an rFTS s containing TRs applied to vertices. In addition, the transformation sequence $P_1(s)$ is frequent according to the anti-monotonicity of the support value and canonical according to Definition 7[†]. Therefore, $P_1(s)$ returns a "unique" rFTS in S_{rfts}.

Example 7: Given s_6 in Fig. 8, $P_1(s_6)$ and $P_1(P_1(s_6))$ are

$$\langle vi^{(1,1)}_{[1,A]} vi^{(2,1)}_{[2,B]} ei^{(3,1)}_{[(1,2),-]} ei^{(3,2)}_{[(2,3),-]} ed^{(4,1)}_{[(2,3),-]} \rangle \text{ and}$$
$$\langle vi^{(1,1)}_{[1,A]} ei^{(2,1)}_{[(1,2),-]} ei^{(2,2)}_{[(2,3),-]} ed^{(3,1)}_{[(2,3),-]} \rangle,$$

respectively. Union graphs of s_6, $P_1(s_6)$, and $P_1(P_1(s_6))$ are isomorphic to the graph shown in Fig. 6 (b).

Next, we define the second function of our parent-child relation to enumerate rFTSs.

Definition 9: Given an rFTS $s' \in S_{rfts}$ that contains only TRs applied to edges, we define function P_2 mapping from s' to s''. The transformation sequence s'' is derived from s' by removing the TR $tr^{(j,k)}_{[o,l]}$ located in the last position of all the TRs in s' if a TR $tr^{(j',k')}_{[o',l']}$ exists in s' such that $o = o'$ and $j' < j$. ■

If the rFTS s contains TRs that are applied to vertices, we can obtain an rFTS s' that does not contain TRs applied to vertices by applying P_1 to s multiple times. In addition, P_2 is applicable to s', if the length of s' is greater than the number of edges in $g_u(s')$, since at least one TR needs to be applied to each edge in $E(g_u(s'))$. According to the above definition, the following lemma is obtained.

[†]The proof is omitted due to lack of space.

$$\begin{array}{lll}
P_3(s'_1) = \perp & & \\
s'_1 = P_3(s'_2) = \langle & ei^{(1,1)}_{[(1,2),-]}\rangle & \in P_3^{-1}(\perp) \\
s'_2 = P_2(s'_3) = \langle & ei^{(1,1)}_{[(1,2),-]}ei^{(1,2)}_{[(2,3),-]}\rangle & \in P_3^{-1}(s'_1) \\
s'_3 = P_1(s'_4) = \langle & ei^{(1,1)}_{[(1,2),-]}ei^{(1,2)}_{[(2,3),-]}ed^{(2,1)}_{[(2,3),-]}\rangle & \in P_2^{-1}(s'_2) \\
s'_4 = P_1(s'_5) = \langle vi^{(1,1)}_{[1,A]} & ei^{(2,1)}_{[(1,2),-]}ei^{(2,2)}_{[(2,3),-]}ed^{(3,1)}_{[(2,3),-]}\rangle & \in P_1^{-1}(s'_3) \\
s'_5 = P_1(s_6) = \langle vi^{(1,1)}_{[1,A]}vi^{(2,1)}_{[2,B]} & ei^{(3,1)}_{[(1,2),-]}ei^{(3,2)}_{[(2,3),-]}ed^{(4,1)}_{[(2,3),-]}\rangle & \in P_1^{-1}(s'_4) \\
s_6 \quad = \langle vi^{(1,1)}_{[1,A]}vi^{(2,1)}_{[2,B]}vi^{(3,1)}_{[3,C]} & ei^{(4,1)}_{[(1,2),-]}ei^{(4,2)}_{[(2,3),-]}ed^{(5,1)}_{[(2,3),-]}\rangle & \in P_1^{-1}(s'_5)
\end{array}$$

Fig. 10 Parent-child relation between rFTSs.

Lemma 2: Given an rFTS $s' \in S_{rfts}$ containing only TRs applied to edges and whose length is greater than $|E(g_u(s'))|$, $g_u(P_2(s'))$ is identical to $g_u(s')$. ■

This lemma is proven in the same way as Lemma 1. According to Lemma 2, $P_2(s')$ is always relevant for an rFTS s' containing only TRs applied to edges. In addition, the transformation sequence $P_2(s')$ is frequent according to the anti-monotonicity of the support value and canonical according to Definition 7. Therefore, $P_2(s')$ returns a "unique" rFTS in S_{rfts}.

Example 8: Given $s'_3 = \langle ei^{(1,1)}_{[(1,2),-]}ei^{(1,2)}_{[(2,3),-]}ed^{(2,1)}_{[(2,3),-]}\rangle$, $P_2(s'_3) = \langle ei^{(1,1)}_{[(1,2),-]}ei^{(1,2)}_{[(2,3),-]}\rangle$. According to Definition 9, we cannot apply P_2 to s'_3.

Finally, we define the third function of our parent-child relation to enumerate rFTSs.

Definition 10: Given an rFTS $s'' \in S_{rfts}$ where each TR is applied to a mutually different edge in $g_u(s'')$, we define function P_3 mapping from s'' to s'''. The transformation sequence s''' is derived from s'' by removing the TR located in the last position in s'' keeping the connectivity of $g_u(s''')$. ■

If each TR in an rFTS s is not applied to a mutually different edge in $g_u(s)$, we can obtain the rFTS s'' by applying P_1 and P_2 to s multiple times. According to Definition 10, $P_3(s'')$ is always relevant for the rFTS s'', because the connectivity of $g_u(P_3(s''))$ is kept. In addition, the transformation sequence $P_3(s'')$ is frequent according to the anti-monotonicity of the support value and canonical according to Definition 7. Therefore, $P_3(s'')$ returns a "unique" rFTS in S_{rfts}.

Example 9: Since the rFTS s_6 shown in Fig. 10 contains TRs that are applied to vertices, P_1 is applied to s_6 three times until the transformation sequence does not contain TRs applied to vertices, and we obtain s'_5, s'_4, and s'_3. Next, P_2 is applied to s'_3 once, resulting in s'_2 where each TR is applied to a mutually different edge in $g_u(P_2(s'_2))$. Finally, P_3 is applied to s'_2 twice until the transformation sequence becomes $\perp$.

We have defined our parent-child relation between rFTSs in terms of three functions P_1, P_2, and P_3. Using the search tree T over S_{rfts} defined by $P = \{P_1, P_2, P_3\}$, we can enumerate a complete set of only rFTSs of S_{rfts} by traversing search tree T from its root. In the traversal, P_1^{-1}, P_2^{-1}, and P_3^{-1} are used to enumerate rFTSs from the current rFTS by adding a TR.

```
Input: an rFTS $s_p$, a dataset $DB$, $\sigma'$, and $i = 3$.
Output: the set of rFTSs $S_{rfts}$.
GTRACE-RS($s_p$, $DB$, $\sigma'$, $S_{rfts}$, $i$)
1: if $s_p \neq$ min, then
2:     return;
3: insert $s_p$ into $S_{rfts}$;
4: while $i > 0$
5:     Call Subprocedure($s_p$, $DB$, $\sigma'$, $S_{rfts}$, $i$);
6:     $i = i - 1$;
7: return;

Subprocedure($s_p$, $DB$, $\sigma'$, $S_{rfts}$, $i$)
1: set $C$ to $\emptyset$;
2: scan $DB$,
3: find all transformation rules $r$ s.t. $s_p \diamond r \in P_i^{-1}(s_p)$;
4: insert $s_p \diamond r$ in $C$ and count its frequency;
5: for each frequent $s_p \diamond r$ in $C$ do
6:     Call GTRACE-RS($s_p \diamond r$, $DB$, $\sigma'$, $S_{rfts}$, $i$);
7: return;
```

Fig. 11 Algorithm for enumerating rFTSs.

3.2 GTRACE-RS

In the previous subsection, we defined functions P_1, P_2, and P_3 for the parent-child relation between rFTSs. By traversing the tree constructed by parent-child relations in a reverse direction, we enumerate a complete set of rFTSs without enumerating any FTSs that are not also rFTSs. Figure 11 gives the pseudo code for the proposed method "GTRACE-RS" that mines all rFTSs from graph sequences DB and accumulates them in S_{rfts} with the minimum support value σ'. The method traverses the search tree T over S_{rfts} defined by $P = \{P_1, P_2, P_3\}$ in a depth-first manner. In Fig. 11, $s_p \diamond r$ means that a TR r is added to s_p such that $s_p \diamond r \in P_i^{-1}(s_p)$ for $i = 1, 2, 3$. In this process, a TR to be added is not always appended to the tail of s_p unlike the original GTRACE. "min" is the canonical form of s_p, and $s_p \neq$ min checks whether s_p has been discovered before. First, given an rFTS s_p that contains only TRs applied to edges and where each TR is applied to a mutually different edge in $g_u(s_p)$ but not any rFTS, GTRACE-RS enumerates rFTSs that are $P_3^{-1}(s_p)$. Next, given an rFTS that contains only TRs applied to edges but not any rFTS, GTRACE-RS enumerates rFTSs that are $P_2^{-1}(s_p)$. The reason why GTRACE-RS does not enumerate $P_3^{-1}(s'_p)$ and $P_2^{-1}(s'_p)$ for any rFTS s'_p is that $P_3^{-1}(s'_p)$ and $P_2^{-1}(s'_p)$ cannot be canonical according to the definitions of the canonical rFTS and the parent-child relations P_1, P_2, and P_3. Finally, given an rFTS, GTRACE-RS enumerates rFTSs that are $P_1^{-1}(s_p)$.

4. Implementation

In the previous section, we proposed a new method for mining only rFTSs from graph sequences. To mine the rFTSs efficiently, an efficient implementation of the method is also important. In this section, we explain how to implement the proposed method.

4.1 Implementation of P_3^{-1}

Given an rFTS s_p that contains only TRs applied to edges and where each TR is applied to a mutually different edge in $g_u(s_p)$, GTRACE-RS enumerates rFTSs in $P_3^{-1}(s_p)$ from s_p. During this process, the number of edges in $g_u(P_3^{-1}(s_p))$ increases one by one, similarly to gSpan [21]. So we have implemented P_3^{-1} based on gSpan[†]. Since gSpan is an algorithm for mining frequent subgraph patterns from colored graphs[††], it cannot be applied directly to graph sequences. We extend the tuple (u, u', c) of the DFS code used in gSpan to a tuple $(u, u', (l, tr, j))$ as a TR $tr^{(j,k)}_{[(u,u'),l]}$. An rFTS s_p is extended based on the pattern-growth principle. Given a code $\alpha = (a_1, \cdots, a_k)$ for s_p, α is extended by adding a tuple a_{k+1} in the form of $(u, u', (l, tr, j))$ to generate $\alpha' = (a_1, \cdots, a_k, a_{k+1})$. A TR, represented by the tuple, to transform an edge between vertices u and u' on the rightmost path in $g_u(s_p)$ can be added (backward extension), or a TR, represented by the tuple, to transform an edge between the rightmost vertex u and another vertex u' that does not exist in $g_u(s_p)$ can be added (forward extension).

4.2 Projection

After mining rFTSs using P_3^{-1}, we shrink the transformation sequences in DB for the sake of computational efficiency. We call this procedure the projection. When P_1^{-1} and P_2^{-1} grow an rFTS s_p by adding TRs one by one, the union graphs of any rFTSs generated by P_2^{-1} and P_1^{-1} are isomorphic with $g_u(s_p)$ according to Lemmas 1 and 2; that is, vertex IDs in any TRs added to s_p by P_1^{-1} and P_2^{-1} are identical with vertex IDs in s_p (A). In addition, when P_2^{-1} grows an rFTS by adding TRs $tr^{(j,k)}_{[o,l]}$ one by one, there must exist a TR $tr^{(j',k')}_{[o',l']}$ in s_p such that $o = o'$ and $j' < j$ according to Definition 9 (B). Based on the above discussion, we define the projection as follows.

Definition 11: Given a transformation sequence s_d of $\langle gid, d\rangle \in DB$ and an rFTS s_p mined by P_3^{-1} such that $s_p \sqsubseteq s_d$ via (ϕ, ψ), we define the projection of s_d onto its maximum subsequences s'_d satisfying the following conditions.

(A) $\{\psi(u), \psi(u') \mid tr^{(j,k)}_{[(u,u'),l]} \in s_p\} = \{u, u', u'' \mid tr^{(j,k)}_{[(u,u'),l]} \in s'_d, tr^{(j,k)}_{[u'',l]} \in s'_d\}$.

(B) TRs $tr^{(j',k')}_{[o',l']} \in s_d$ such that $\psi(o) = o'$ and $\phi(j) < j'$, are included in s'_d if $tr^{(j,k)}_{[o,l]} \in s_p$. ■

Projected transformation sequences are used in the implementation of P_1^{-1} and P_2^{-1}, as explained in Sect. 4.3.

4.3 Implementation of P_1^{-1} and P_2^{-1}

In the rest of this section, using a concrete example, we explain our implementation of P_1^{-1} and P_2^{-1} to enumerate rFTSs. In Sect. 3, we defined P_1 and P_2 separately for ease of explanation. However, in our implementation, P_1^{-1} and P_2^{-1} are implemented jointly for the efficiency of our GTRACE-RS. For the sake of simplicity, in this subsection, we assume that DB contains only two graph sequences $\langle gid_1, d_1\rangle$ and $\langle gid_2, d_2\rangle$ as shown in Fig. 12, and that an rFTS s_p has been mined from DB using P_3^{-1} under $\sigma' = 2$. In addition, we consider only two of the mappings from vertex IDs in s_p to vertex IDs in the transformation sequences s_{d1} and s_{d2}, although there are other mappings. The two mappings ψ_1 and ψ_2 are given as

$$\psi_1(1) = 1,\ \psi_1(2) = 2,\ \psi_1(3) = 4, \tag{1}$$

$$\psi_2(1) = 3,\ \psi_2(2) = 1,\ \psi_2(3) = 4. \tag{2}$$

In this example, vertex ID 1 in s_p corresponds to vertex ID 3 in s_{d2}, because $\psi_2(1) = 3$. Since vertex ID 3 in s_{d1} and vertex IDs 2 and 3 in s_{d2} do not correspond to any vertex IDs in s_p, the underlined TRs in s_{d1} and s_{d2} in Fig. 12 are removed in the projection, and the projected transformation sequences s'_{d1} and s'_{d2} shown in the middle of Fig. 12 are derived. Transformation sequences s'_{d1} and s'_{d2} are used in P_1^{-1} and P_2^{-1} to grow s_p. Therefore, all rFTSs mined from s'_{d1} and s'_{d2} must contain s_p as a subsequence.

Subsequently, to check efficiently whether TRs in s'_{d1} and s'_{d2} correspond to each other, we convert the projected transformation sequence s'_{d1} and s'_{d2} by reassigning all vertex IDs in the projected transformation sequences, as de-

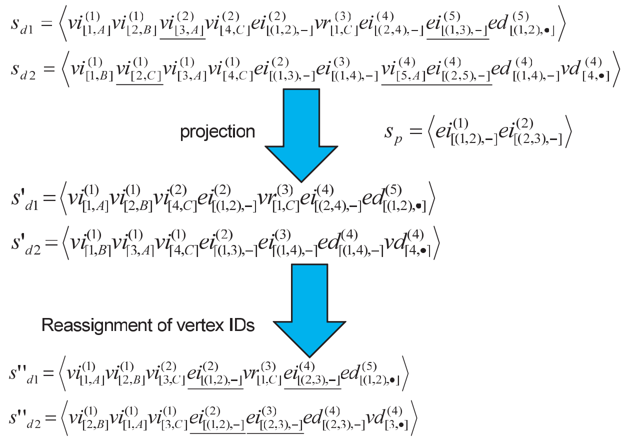

$s_{d1} = \langle vi^{(1)}_{[1,A]} vi^{(1)}_{[2,B]} \underline{vi^{(2)}_{[3,A]}} vi^{(2)}_{[4,C]} ei^{(2)}_{[(1,2),-]} vr^{(3)}_{[1,C]} ei^{(4)}_{[(2,4),-]} \underline{ei^{(5)}_{[(1,3),-]}} ed^{(5)}_{[(1,2),\bullet]} \rangle$
$s_{d2} = \langle vi^{(1)}_{[1,B]} \underline{vi^{(1)}_{[2,C]}} vi^{(1)}_{[3,A]} vi^{(1)}_{[4,C]} ei^{(2)}_{[(1,3),-]} ei^{(3)}_{[(1,4),-]} \underline{vi^{(4)}_{[5,A]} ei^{(4)}_{[(2,5),-]}} ed^{(4)}_{[(1,4),-]} vd^{(4)}_{[4,\bullet]} \rangle$
projection
$s_p = \langle ei^{(1)}_{[(1,2),-]} ei^{(2)}_{[(2,3),-]} \rangle$
$s'_{d1} = \langle vi^{(1)}_{[1,A]} vi^{(1)}_{[2,B]} vi^{(2)}_{[4,C]} ei^{(2)}_{[(1,2),-]} vr^{(3)}_{[1,C]} ei^{(4)}_{[(2,4),-]} ed^{(5)}_{[(1,2),\bullet]} \rangle$
$s'_{d2} = \langle vi^{(1)}_{[1,B]} vi^{(1)}_{[3,A]} vi^{(1)}_{[4,C]} ei^{(2)}_{[(1,3),-]} ei^{(3)}_{[(1,4),-]} ed^{(4)}_{[(1,4),-]} vd^{(4)}_{[4,\bullet]} \rangle$
Reassignment of vertex IDs
$s''_{d1} = \langle vi^{(1)}_{[1,A]} vi^{(1)}_{[2,B]} vi^{(2)}_{[3,C]} \underline{ei^{(2)}_{[(1,2),-]}} vr^{(3)}_{[1,C]} \underline{ei^{(4)}_{[(2,3),-]}} ed^{(5)}_{[(1,2),\bullet]} \rangle$
$s''_{d2} = \langle vi^{(1)}_{[2,B]} vi^{(1)}_{[1,A]} vi^{(1)}_{[3,C]} \underline{ei^{(2)}_{[(1,2),-]}} \underline{ei^{(3)}_{[(2,3),-]}} ed^{(4)}_{[(2,3),-]} vd^{(4)}_{[3,\bullet]} \rangle$

Fig. 12 Reassignment of vertex IDs (values for k are omitted in this figure).

[†]Despite having defined canonical codes of rFTSs and implemented P_3^{-1} using gSpan, we could have implemented these similarly using FSG [16] or Gaston [18], which are algorithms for solving the frequent graph mining problem.

[††]We use the term "color" instead of "label" to distinguish labels of graphs in frequent graph mining problems and labels of graph sequences in our problem.

scribed below. We are aware of all the embeddings of s_p in s'_{d1} and s'_{d2}, as well as their mappings from vertex IDs in s_p to vertex IDs in s'_{d1} and s'_{d2} as given by Eqs. (1) and (2). In this example, we reassign vertex ID 4 in s'_{d1} to vertex ID 3, because we know $\psi_1(3) = 4$. The reassigned transformation sequences s''_{d1} and s''_{d1} are shown at the bottom of Fig. 12. By reassigning the vertex IDs in s'_{d1} and s'_{d2}, corresponding TRs are written in the same representation, except for j in $tr^{(j)}_{[o,l]}$. For example, a TR $vi_{[2,B]}$ is written in the same representation in s''_{d1} and s''_{d2}, although the rule is written as $vi_{[2,B]}$ and $vi_{[1,B]}$ in s'_{d1} and s'_{d2}, respectively.

Next, because the corresponding rules are written in the same representation, we further convert the reassigned transformation sequences s''_{d1} and s''_{d2} in Fig. 12 to sequences of itemsets as follows.

$$s_1 = \langle gid_1, \langle (i_1\ i_2)\ (i_3\ \underline{i_4})\ i_5\ \underline{i_6}\ i_7 \rangle\rangle, \tag{3}$$

$$s_2 = \langle gid_2, \langle (i_1\ i_2\ i_3)\ \underline{i_4}\ \underline{i_6}\ (i_8\ i_9) \rangle\rangle, \tag{4}$$

where $vi_{[1,A]}$ in s''_{d1} and s''_{d2} is converted to i_1, $vi_{[1,B]}$ in s''_{d1} and s''_{d2} is converted to i_2, and so on. In addition, items in s_1 and s_2 are placed in the same parentheses if their corresponding TRs exist in the same intrastate transformation sequence. For brevity, parentheses are omitted if an itemset has only one item.

The objective of this subsection is to propose the implementation of P_1^{-1} and P_2^{-1} which enumerate rFTSs containing s_p. To efficiently enumerate the rFTSs containing s_p, we use PrefixSpan [19] which efficiently enumerates all frequent sequential patterns of itemsets. However, many of 17 frequent sequential patterns[†] mined from s_1 and s_2 by PrefixSpan under $\sigma' = 2$ correspond to rFTSs do not contain s_p. To mine only rFTSs containing s_p from s_{d1} and s_{d2}, we remove the underlined items from the converted sequences to obtain other converted sequences s'_1 and s'_2, mine all frequent sequential patterns from s'_1 and s'_2, and add removed items to frequent sequential patterns. In the sequences s_1 and s_2, underlined items appear in all of the converted sequences as a subsequence $s = \langle i_4\ i_6 \rangle$, because s'_{d1} and s'_{d2} are generated by the projection using the rFTS s_p and TRs in s_p correspond to the underlined items i_4 and i_6. By removing the items, we obtain the converted sequences

$$s'_1 = \langle gid_1, \langle (i_1^{(<1st)}\ i_2^{(<1st)})\ i_3^{(=1st)}\ i_5^{(<2nd)}\ i_7 \rangle\rangle,$$
$$s'_2 = \langle gid_2, \langle (i_1^{(<1st)}\ i_2^{(<1st)}\ i_3^{(<1st)})\ (i_8\ i_9) \rangle\rangle,$$

where $i_3^{(<1st)}$ denotes that i_3 appears before the 1st item in s, and $i_3^{(=1st)}$ denotes that i_3 appears at the same time as the 1st item in s. Using this representation and s, we can re-convert s'_1 and s'_2 to s_1 and s_2, respectively. Now, we have two sequences of itemsets s'_1 and s'_2. By applying PrefixSpan to the sequences of itemsets under $\sigma' = 2$, we obtain three frequent sequential patterns $\{\langle i_1^{(<1st)} \rangle, \langle i_2^{(<1st)} \rangle, \langle (i_1^{(<1st)}\ i_2^{(<1st)}) \rangle\}$. After mining the frequent sequential patterns, we reconvert each item in the frequent sequential patterns to a TR to obtain three rFTSs: $\langle vi^{(1)}_{[1,A]} ei^{(2)}_{[(1,2),-]} ei^{(3)}_{[(2,3),-]} \rangle$, $\langle vi^{(1)}_{[2,B]} ei^{(2)}_{[(1,2),-]} ei^{(3)}_{[(2,3),-]} \rangle$, and $\langle vi^{(1)}_{[1,A]} vi^{(1)}_{[2,B]} ei^{(2)}_{[(1,2),-]} ei^{(3)}_{[(2,3),-]} \rangle$.

In PrefixSpan, we can check in $O(1)$ whether TRs in s''_{d1} and s''_{d2} correspond to each other, because two corresponding TRs in the two reassigned transformation sequences have the same vertex IDs. By reassigning vertex IDs in projected transformation sequences and converting transformation sequences to sequences of itemsets, we avoid graph isomorphism matching between two transformation sequences. Since we can quickly check whether two TRs correspond by comparing two items, we can efficiently mine rFTSs from large and long graph sequences.

5. Experiments

The proposed method was implemented in C++. The experiments were executed on an HP Z600 computer with an Intel Xeon X5560 2.80 GHz processor, 4 GB of main memory and running Windows 7. The performance of the proposed method was evaluated using artificial and real-world graph sequence data.

5.1 Artificial Datasets

We compared the performance of the proposed method with the original GTRACE [13] using artificial datasets generated from the parameters listed in Table 3. First, starting from $g^{(1)}$ with $|V_{avg}|/2$ vertices generated with edge existence probability p_e, we grew each graph sequence to include $|V_{avg}|$ vertex IDs on average, by applying two ($= d_{dist}$) of (A) inserting with probability p_i, (B) deleting with probability p_d, and (C) relabeling vertices and edges with probability $1 - p_i - p_d$ at each interstate. Accordingly, if p_i is small or $|V_{avg}|$ is large, the generated transformation sequence is long. This process is continued until the sequence becomes relevant by increasing the numbers of vertices and edges. We generated $|DB|$ graph sequences. Similarly, we generated N rFTSs with $|V'_{avg}|$ vertex IDs on average. We then generated the DB in which each graph sequence was overlaid by an rFTS with probability $1/N$. Each graph sequence contained

Table 3 Parameters of the artificial datasets.

Parameters	Default values
Probability of vertex and edge insertions in transformation sequences	$p_i = 80\%$
Probability of vertex and edge deletions in transformation sequences	$p_d = 10\%$
Average number of vertex IDs in transformation sequences	$\|V_{avg}\| = 6$
Average number of vertex IDs in embedded FTSs	$\|V'_{avg}\| = 3$
Number of vertex labels	$\|L_v\| = 5$
Number of edge labels	$\|L_e\| = 5$
Number of embedded FTSs	$N = 10$
Number of transformation sequences	$\|DB\| = 1{,}000$
Edge existence probability between vertices	$p_e = 15\%$
Average edit distance between interstates	$d_{ist} = 2$
Minimum support threshold	$\sigma' = 10\%$

[†]We discuss the 17 frequent sequential patterns in detail in Sect. 6.

$|L_v|$ vertex labels and $|L_e|$ edge labels.

Table 4 lists the computation times [sec], the numbers of rFTSs mined by the proposed method, and the numbers of FTSs mined by the first step of the original GTRACE for varying values of $|DB|$, $|V_{avg}|$, p_i, L_e, and σ', with the other parameters set to their default values. In the table, "–" indicates that no results were obtained because of intractable computation times exceeding 2 hours. In addition, PM and GT denote the proposed method and GTRACE, respectively.

The first part of Table 4 shows that the computation time is proportional to the number of graph sequences $|DB|$, as is the case in conventional frequent pattern mining. The second and third parts of the table indicate that the computation times for both GTRACE-RS and GTRACE are exponential with respect to an increase in the average number of vertices $|V_{avg}|$ in the graph sequences and a decrease in the probability p_i of vertex and edge insertions in the graph sequence. The main reason that the computation time increases with the average length seems to be the increase in the numbers of rFTSs in both cases. However, the far superior efficiency of the proposed method compared to GTRACE is confirmed by the computation times. The fourth part of Table 4 shows the effect of the number of labels on the efficiency. When $|L_e|$ is small, many transformation subsequence are isomorphic with each other, and thus the computation times for GTRACE and GTRACE-RS increase. However, the computation time for GTRACE-RS remains smaller, since it mines only rFTSs. The fifth part of Table 4 shows that the proposed method is tractable even with a low minimum support threshold.

All parts of Table 4 show that the number of rFTSs mined by the proposed method is much smaller than the number of FTSs mined by GTRACE. By mining only rFTSs, the proposed method efficiently mines a complete set of rFTSs from a set of graph sequences. Therefore, the proposed method is applicable in practice to graph sequences that are both long and large.

Table 4 Results for various $|DB|$, $|V_{avg}|$, p_i, $|L_e|$, and σ'.

$\|DB\|$	1,000	3,000	7,000	10,000
avg. len.	42.9	44.0	43.5	43.4
PM comptime	2.0	6.5	15.0	21.4
# of rFTSs	6307	6872	6325	6266
GT comptime	217.3	951.2	2226.2	3465.3
# of FTSs	171787	190876	170387	170902
$\|V_{avg}\|$	6	8	15	20
avg. len.	42.9	61.2	135.5	188.7
PM comptime	2.0	6.3	228.7	4335.0
# of rFTSs	6307	20755	3653370	81012875
GT comptime	217.3	3599.3	-	-
# of FTSs	171787	936115	-	-
p_i [%]	55	70	80	100
avg. len.	116.7	65.0	42.9	18.7
PM comptime	419.0	7.5	2.0	0.7
# of rFTSs	4458046	58251	6307	585
GT comptime	-	4132.2	217.3	8.5
# of FTSs	-	2355657	171787	9765
$\|L_e\|$	1	3	7	10
avg. len.	43.5	43.7	43.8	43.0
PM comptime	54.5	5.1	1.9	0.97
# of rFTSs	70257	12972	5318	3333
GT comptime	2195.9	644.0	205.9	122.1
# of FTSs	2995499	474564	132538	62897
σ' [%]	5	7.5	10	15
avg. len.	42.9	42.9	42.9	42.9
PM comptime	377.1	30.7	2.0	1.8
# of rFTSs	90607156	5744037	6307	1630
GT comptime	2122.4	472.3	217.3	93.3
# of FTSs	176177313	11891069	171787	43100

PM: Proposed Method, GT: the original GTRACE,
comptime: computation time [sec],
avg. len.: average length of transformation sequences,
# of rFTSs (or FTSs): the number of mined rFTSs (or FTSs)

5.2 Real-World Dataset

To assess the practicality of the proposed method, it was applied to the Enron Email Dataset [8], [15]. In the dataset, we assigned a vertex ID to each person participating in an email communication, and assigned an edge to a pair communicating via email on a particular day, thereby obtaining a daily graph $g^{(j)}$. In addition, one of the labels {CEO, Employee, Director, Manager, Lawyer, President, Trader, Vice President} was assigned to each vertex and we labeled each edge according to the volume of mail. We then obtained a set of weekly graph sequence data, *i.e.*, a *DB*. The total number of weeks, *i.e.*, number of sequences, was 123. We randomly sampled $|V|$ (= 1 ∼ 182) persons to form each *DB*.

Table 5 shows the computation times (comptime [sec]) and the numbers of mined rFTSs or FTSs (# of rFTSs or # of FTSs) obtained for various numbers of vertex IDs (persons) $|V|$, minimum support σ', and numbers of interstates n in each graph sequence of the dataset. All the other parameters were set to the default values indicated at the bottom of the table. Thus, the dataset with the default values contained 123 graph sequences each consisting of 182 persons (vertex IDs) and 7 interstates. The parameter $|l_{avg}|$ = 4, 5, 6, or 7 indicates that each sequence d in DB consists of 4, 5, 6, or 7 interstates from Monday to Thursday, Friday, Saturday, or Sunday, respectively.

The upper, middle, and lower parts of the table show

Table 5 Results for the Enron dataset.

# of persons $\|V\|$	100	140	150	182
PM comptime	0.5	2.2	15.9	278.6
# of rFTSs	33227	31391	47015	1558833
GT comptime	16.8	118.3	-	-
# of FTSs	66072	154541	-	-
min. sup. σ' [%]	40	30	20	10
PM comptime	2.0	6.1	30.0	278.6
# of rFTSs	974	3548	14419	158833
GT comptime	14.4	387.3	-	-
# of FTSs	4129	29253	-	-
# of interstates n	4	5	6	7
PM comptime	5.85	34.1	95.6	278.6
# of rFTSs	5542	21214	51727	158833
GT comptime	423.8	-	-	-
# of FTSs	67997	-	-	-

PM: Proposed Method, GT: the original GTRACE.
Default: minimum support σ' = 10%, # of vertex labels $|L_v|$ = 8,
# of edge labels $|L_e|$ = 5, # of persons $|V|$ = 182, # of interstates n = 7.

the practical scalability of the proposed method with regard to the number of persons (vertex IDs), the minimum support threshold, and the number of interstates in graph sequences in the graph sequence database, respectively. The original GTRACE proved intractable for the graph sequence dataset generated from the default values, despite the change in each graph in this graph sequence database being gradual. On the other hand, execution of the proposed method is tractable with respect to the database. Good scalability of the proposed method is indicated in Table 5, because the computation times for the proposed method are smaller than those for the original GTRACE. The scalability of the proposed method comes from mining only rFTSs based on the principle of a reverse search and the efficient implementation as discussed in Sect. 4.

6. Discussion

In Sect. 4.3, we mentioned that 17 frequent sequential patterns are mined from s_1 and s_2 given by Eqs. (3) and (4), respectively. All of the mined patterns from s_1 and s_2 are given below.

$$\langle i_1 \rangle = \langle vi^{(1)}_{[1,A]} \rangle, \tag{5}$$

$$\langle i_2 \rangle = \langle vi^{(1)}_{[2,B]} \rangle, \tag{6}$$

$$\langle i_3 \rangle = \langle vi^{(1)}_{[3,C]} \rangle, \tag{7}$$

$$\langle i_4 \rangle = \langle ei^{(1)}_{[(1,2),-]} \rangle, \tag{8}$$

$$\langle i_6 \rangle = \langle ei^{(1)}_{[(2,3),-]} \rangle, \tag{9}$$

$$\langle i_1 i_4 \rangle = \langle vi^{(1)}_{[1,A]} ei^{(2)}_{[(1,2),-]} \rangle, \tag{10}$$

$$\langle i_1 i_6 \rangle = \langle vi^{(1)}_{[1,A]} ei^{(2)}_{[(2,3),-]} \rangle, \tag{11}$$

$$\langle (i_1 i_2) \rangle = \langle vi^{(1)}_{[1,A]} vi^{(1)}_{[2,B]} \rangle, \tag{12}$$

$$\langle i_2 i_4 \rangle = \langle vi^{(1)}_{[2,B]} ei^{(2)}_{[(1,2),-]} \rangle, \tag{13}$$

$$\langle i_2 i_6 \rangle = \langle vi^{(1)}_{[2,B]} ei^{(2)}_{[(2,3),-]} \rangle, \tag{14}$$

$$\langle i_3 i_6 \rangle = \langle vi^{(1)}_{[3,C]} ei^{(2)}_{[(2,3),-]} \rangle, \tag{15}$$

$$\langle (i_1 i_2) i_4 \rangle = \langle vi^{(1)}_{[1,A]} vi^{(1)}_{[2,B]} ei^{(2)}_{[(1,2),-]} \rangle, \tag{16}$$

$$\langle (i_1 i_2) i_6 \rangle = \langle vi^{(1)}_{[1,A]} vi^{(1)}_{[2,B]} ei^{(2)}_{[(2,3),-]} \rangle. \tag{17}$$

$$\langle i_4 i_6 \rangle = \langle ei^{(1)}_{[(1,2),-]} ei^{(2)}_{[(2,3),-]} \rangle, \tag{18}$$

$$\langle i_1 i_4 i_6 \rangle = \langle vi^{(1)}_{[1,A]} ei^{(2)}_{[(1,2),-]} ei^{(3)}_{[(2,3),-]} \rangle, \tag{19}$$

$$\langle i_2 i_4 i_6 \rangle = \langle vi^{(1)}_{[2,B]} ei^{(2)}_{[(1,2),-]} ei^{(3)}_{[(2,3),-]} \rangle, \text{ and} \tag{20}$$

$$\langle (i_1 i_2) i_4 i_6 \rangle = \langle vi^{(1)}_{[1,A]} vi^{(1)}_{[2,B]} ei^{(2)}_{[(1,2),-]} ei^{(3)}_{[(2,3),-]} \rangle. \tag{21}$$

Fourteen frequent sequential patterns, including Eqs. (5) to (18), of the 17 patterns should not be mined from the projected transformation sequences with respect to $s_p = \langle ei^{(1)}_{[(1,2),-]} ei^{(2)}_{[(2,3),-]} \rangle$, because the transformation sequences shown as Eqs. (5) to (18) do not contain s_p as a proper subsequence according to the principle of the reverse search. In addition, the transformation sequences shown as Eqs. (11), (12), and (17) are not rFTSs. By converting s_1 and s_2 to s'_1 and s'_2, respectively, we mine only rFTSs that should be mined from the projected transformation subsequences.

If each graph sequence in DB consists of a labeled graph, the problem, addressed in this paper, of enumerating a complete set of rFTSs from DB is equivalent to the problem of enumerating all frequent and connected subgraphs from a set of labeled graphs. In this case, only P_3^{-1} in Fig. 11 is used, and GTRACE-RS is equivalent to gSpan [21]. The problem of enumerating all frequent and connected subgraphs cannot be solved in time that is polynomial in the output, which is a class of algorithms that find all patterns in polynomial time both in the total input size and the number of patterns, unless P = NP [2], [11]. Therefore, the problem addressed in this paper cannot be solved in time that is polynomial in the output.

7. Conclusion

In this paper, we proposed an efficient method for mining all rFTSs from a given set of graph sequences. We developed a graph sequence mining program, and confirmed the efficient and practical performance of the proposed method through computational experiments using artificial and real-world datasets. The method proposed in this paper efficiently enumerates all rFTSs from a set of graph sequences, whereas the methods in [4], [5] mine all frequent patterns from a long graph sequence. In [9], [17], it is shown that the principle of growing possible patterns can be distinguished from the principle of counting support values of the patterns. Therefore, the proposed method in this paper can be extended to mine rFTSs from a long and large graph sequence based on [9], [17]. By extending our method to mine from graph sequences, we plan to compare the performance of our method with that of Berlingerio's recently proposed method.

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