# 國立交通大學

資訊科學與工程研究所

**碩 士 論 文**

# 在未標號圖形資料中高效率的圖形探勘演算法

# An Efficient Algorithm for Mining Frequent Unlabeled Graphs

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**中 華 民 國　九 十 九 年 六 月**

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## 摘要

近年來頻繁樣式探勘由頻繁項目集探勘及循序樣式探勘逐漸發展至探勘更具結構性之資料，例如樹、絡及圖形等資料。圖形可用於表示許多複雜的資料及資料間的關係，因此被廣泛應用於許多領域，如化學資訊學、生物資訊學及網路探索等等。由於圖形資料的高複雜度，其子圖的個數呈指數成長，如何有效率的探勘大型圖形樣式是一項重大的挑戰。在過去十年間，發展出了許多圖形探勘演算法，我們研究目前已知最好的演算法 gSpan ，希望能更進一步改善其效率。gSpan 採用 right-most 延伸法來產生候選圖形，與傳統方法比較，其產生之重覆的候選圖形數目顯著減少。但由於 right-most 延伸法原本是用於有根樹的探勘演算法，以此為基礎用於圖形探勘，仍會產生許多重覆的候選圖形。此情況造成 gSpan 的效能降低，尤其在針對標記種類較少、或甚至未標號的圖形做處理時，效能的降低更為顯著。因此我們修正此延伸法以進一步減少候選圖形個數，並將之用於未標號圖形資料中。我們對合成資料以及實際之化學化合資料進行實驗，驗證了所提演算法之正確性，並且有效的減少了候選圖形的個數。

# An Efficient Algorithm for Mining Frequent Unlabeled Graphs

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## Abstract

In recent years, academic research on pattern discovery progressed from mining frequent itemsets and sequences to mining structured patterns including trees, lattices, and graphs. Among them, graphs serve as a general model to represent data and have consequently been widely and extensively used in many domains like cheminformatics, bioinformatics, web exploration, etc. However, mining large graph patterns effectively and efficiently is challenging due to the presence of an exponential number of frequent subgraphs and the complexity of graph data. In response to the dilemma, several graph miners, such as gSpan, have been published in the last decade and all of these newly developed graph miners work on undirected labeled simple graph. By examining the state-of-the-art pattern growth algorithm gSpan, which uses a right-most extension method, we learn that it dramatically reduces the number of candidate graphs, compared with traditional join method. Nevertheless, right-most extension was designed originally for rooted trees. It still generates many duplicate graphs when being applied to a free graph. This problem causes remarkable performance degradation when the graphs are denser and with fewer labels available, especially when the graphs are unlabeled. We propose a modified extension method to further decrease the number of duplicate graphs, and apply it to unlabeled graph datasets, hoping to make gSpan an even better miner than it already is. We present the results on mining both synthetic datasets and a chemical compound dataset.

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# Chapter 1

# Introduction

Over the past few decades, frequent pattern mining has been an active and prevalent research topic in data mining with many techniques. These techniques were developed for the purpose of mining association rules [1], frequent itemsets [6, 7, 13, 27], sequential patterns [2, 17, 19], trees [3, 26], as well as graphs [10, 14, 15, 16, 28, 30].

Among all these data types, graphs, as a general data structure, can be used to model more complicated relations among data. For instance, the chemical structure of a given chemical compound can be modeled by an undirected labeled graph in which each vertex corresponds to an atom and each edge corresponds to a chemical bond between atoms. In electronic transactions, the vertices of graphs represent the account owners and the edges of graphs indicate the occurrence of payments. Fig.1-1 shows a sample set of chemical structures and their related graphs. Graphs have been used in chemical informatics [4, 5, 22, 23], computer vision [25], video indexing [20], machine learning [14], and text retrieval [12], etc.

The frequent subgraph mining problem is to find frequent subgraphs over a collection of graphs. It is to discover all the subgraphs whose occurrence frequency is no less than a user-specified threshold.

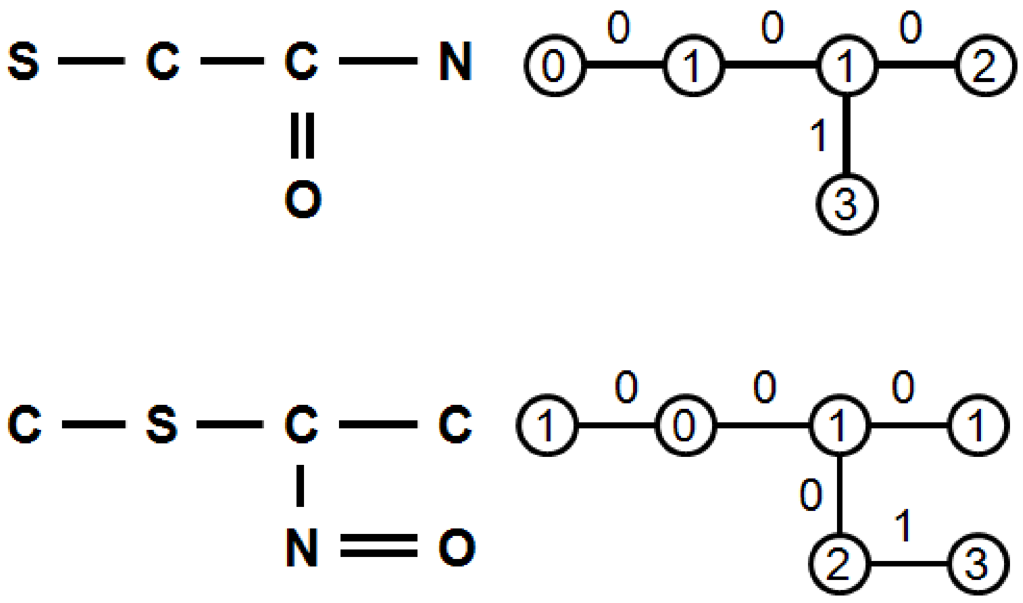


**Fig. 1-1:** A sample graph data set of chemical structures.

The kernel of frequent subgraph mining lies in the subgraph isomorphism test. A number of isomorphism test algorithms were developed in the past three decades, such as Backtracking proposed by J. R. Ullmann[24] and Nauty proposed by B. D. McKay [18]. They solve the graph isomorphism problem by calculating the canonical labels [35] of graphs. The canonical label is one of the most generic and important graph invariants. The Nauty algorithm is known to be one of the fastest algorithm for graph isomorphism. We adopted this algorithm for the isomorphism test. However, the isomorphism problem of a general graph has been proved to be NP-complete [31]. Therefore, no polynomial algorithm is able to solve it. The time-consuming process of the isomorphism test leads to the fact that the candidate test cannot be done with ease. Early implementations of graph miner generate huge candidate set which contains a large number of duplicate graphs. For each candidate graph, lots of isomorphism tests need to be performed to determine whether it is a duplicate graph. As a result, testing of false candidates degrades the performance to a certain degree.

Recently, Yan and Han [28] proposed a pattern growth based graph pattern mining algorithm, gSpan, which was inspired by PrefixSpan [19], TreeMinerV [26], and FREQT [3]. gSpan adopts a canonical labeling system, i.e. DFS (depth-first search) lexicographic order. Each graph is assigned a unique minimum DFS code. In the mining process, a graph is a duplicate if and only if its DFS code is not minimum. gSpan detects duplicate graphs by calculating their minimum DFS codes. gSpan also adopts a right-most extension strategy, which generates fewer candidate graphs. The right-most extension grows a graph pattern by adding a new edge to the vertices on the right-most path, but not to an arbitrary vertex. A right-most path of a graph is the path from the first vertex to the latest added vertex. Fig. 1-2 shows a result of extending *g* which adds new edges to arbitrary positions. Fig. 1-3 shows all the potential right-most extensions of a given graph g. The darkened edges indicate the right-most path of *g*. The dotted line show the new edges added to *g*. In this example, the number of candidate graphs is decreased from eleven to four. Consequently, a huge number of isomorphism tests are avoided. As a result, the storage cost is reduced and the performance is improved significantly. However, gSpan generates some duplicate graphs since the right-most extension method is originally used for rooted tree mining. For example, Fig.1-4 shows three isomorphic graphs. In the mining process of gSpan, all of these three graphs will be generated, but two of them will be discarded after the candidate tests. These two discarded graphs turn out to be a waste of computing time and storage space. This problem causes remarkable performance degradation when gSpan deals with large and complex graphs (denser graphs with fewer labels available), especially when deals with unlabeled graphs.

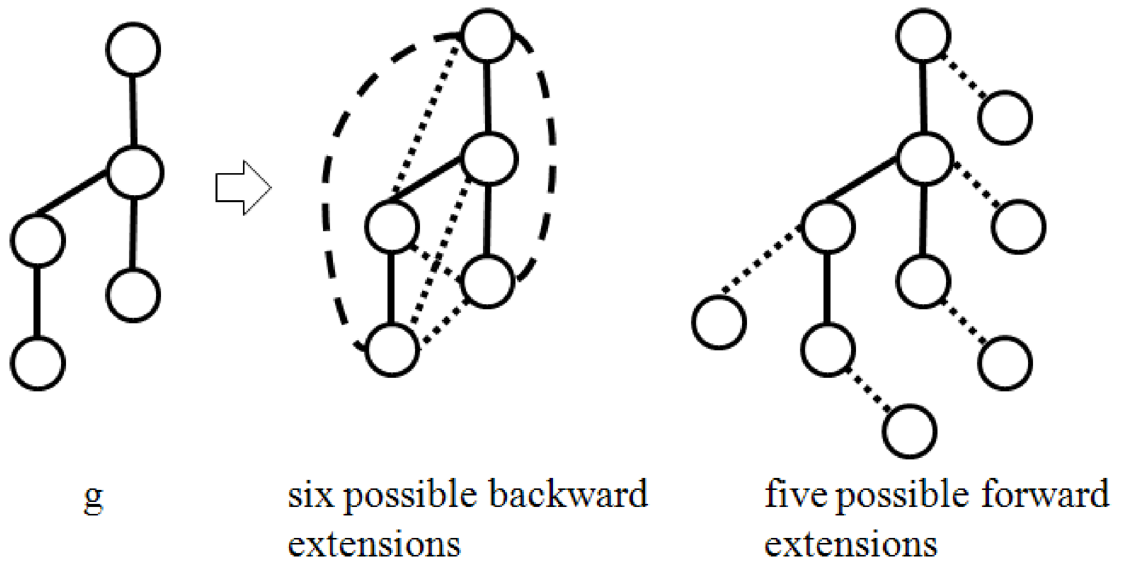

g
six possible backward extensions
five possible forward extensions

**Fig. 1-2:** Free extension.

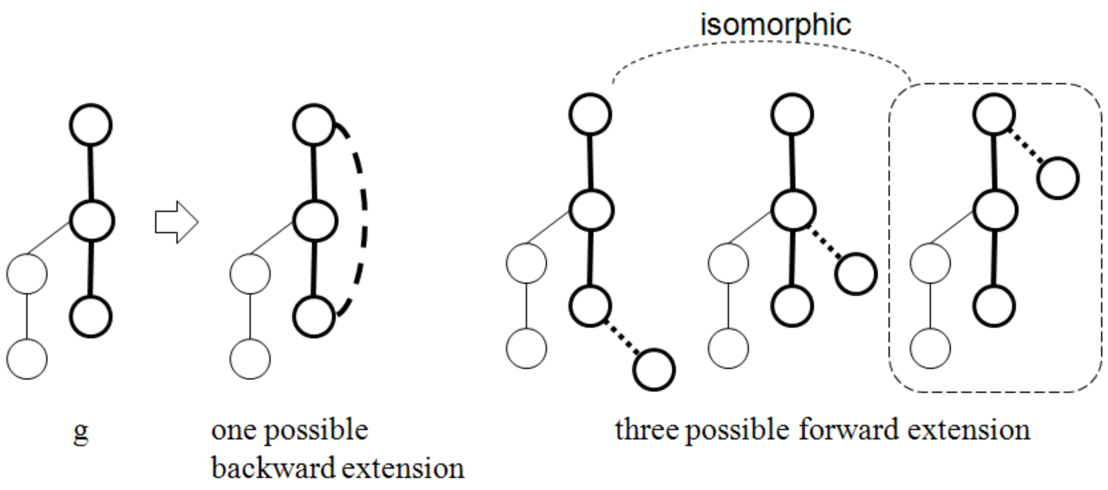

isomorphic
g
one possible backward extension
three possible forward extension

**Fig. 1-3** Right-most extension

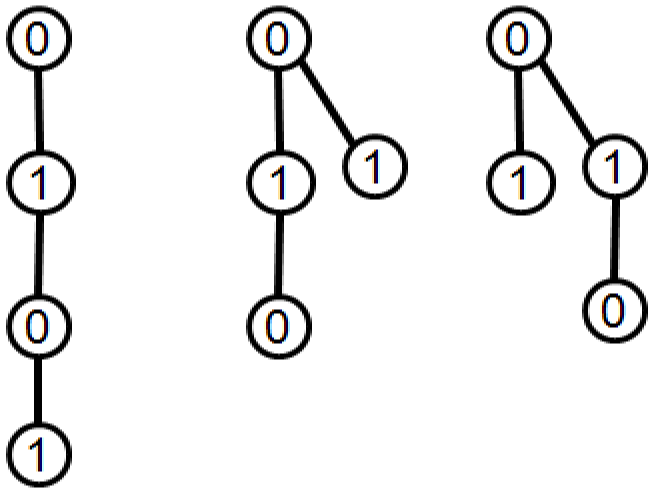


**Fig. 1-4:** Three isomorphic graphs.

In mining the rooted tree, the right-most extension method does not generate any duplicate while in mining the free graph, it *does*. Therefore, in Fig. 1-3, we can see one isomorphic duplicate, the result of mining the free graph. We modify the right-most extension method to make it more suitable for general graphs, which prevents some duplicate graphs from generating. We apply this method to unlabeled graph datasets to evaluate the percentage of decreased duplicate graphs.

The rest of this thesis is organized as follows. Chapter 2 focuses on related works. Chapter 3 provides the details of problem definitions. Chapter 4 introduces the algorithm of gSpan and formulates our graph mining algorithm. Chapter 5 gives the experimental results. Chapter 6 summarizes the entire work and proposes the future prospect.

# Chapter 2

# Related Works

Recent studies have developed several graph-based data mining methods. The pioneering work appeared in around 1994, when Holder et al. [14] proposed SUBDUE to carry out approximate subgraph pattern discovery based on minimum description length and background knowledge. Since SUBDUE uses a computationally-constrained beam search, it cannot discover the complete set of frequent patterns. The first system to try complete search for the wider class of frequent subgraph named WARMR was later proposed by Dehaspe et al. [32] in 1998. It applied inductive logic programming to the prediction of chemical carcinogenicity by mining subgraphs. Besides these studies, recent approaches of graph-based data mining can be categorized into two groups, an Apriori-based approach and a pattern-growth approach. In the following a brief recount of these approaches will be introduced.

## 2.1 The Apriori-based Approach

Algorithms in this category use a level-wise search scheme like Apriori. The search starts with graphs of small size, and proceeds in a bottom-up manner. At each iteration, the size of subgraphs is increased by one. These new subgraphs are first generated by joining two similar frequent subgraphs that were discovered already. Afterwards, the occurrence of the new graphs is checked. Typical Apriori-based frequent subgraph mining algorithms include AGM by Inokuchi et al. [15], and FSG by Kuramochi and Karypis [16].

**AGM** (Apriori-based Graph Mining) adopts a vertex-based candidate generation strategy that increases the subgraph size by one vertex at each iteration. Two size-k frequent graphs are joined only when the two graphs have the same size-(k-1) subgraph. Fig. 2-1 shows the two subgraphs joined by two paths. AGM actually forms two candidates because it is impossible to determine whether there is an edge connecting the additional two vertices before the generation.

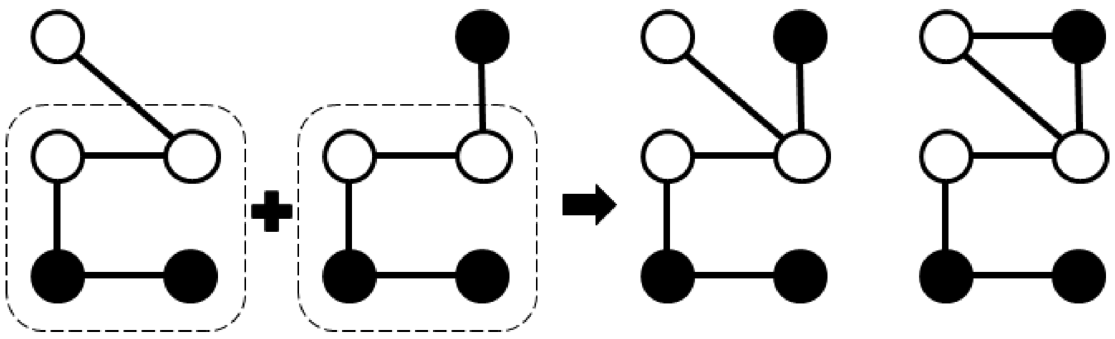


**Fig. 2-1:** AGM: Two graphs generated by joining two paths.

**FSG** (<u>F</u>requent <u>S</u>ub<u>G</u>raph discovery) uses an edge-based candidate generation method that extends the subgraph by one edge at each iteration. Two size-k graphs are joined if and only if they share the same subgraph having k-1 edges. An example of the candidate generation of FSG is shown in Fig. 2-2.

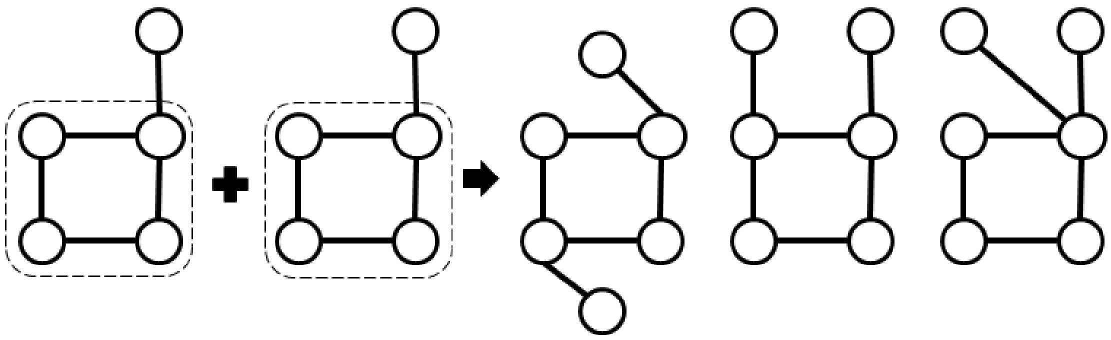


**Fig. 2-2:** FSG: Two graphs and their potential candidates.

Comparatively speaking, AGM finds all frequent induced subgraphs in a graph database while FSG finds all frequent connected subgraphs in a graph database. These two pioneering Apriori-based frequent subgraph mining algorithms at the time when they were proposed, however, both bear three problems, which are later modified and fixed by newer and better ways. These problems include: (1) Huge candidate generation. (2) Multiple scans of database. (3) Difficulties in mining long patterns. Fortunately, non-Apriori-based algorithms have been developed; most adopt the pattern-growth strategy to avoid these problems.

## 2.2 The Pattern-growth Approach

Pattern-growth-based graph mining algorithms include gSpan by Yan and Han. [29], MoFa by Borgelt et al. [33], FFSM by J. Huan et al. [34], and Gaston by Nijssen et al. [30] These algorithms are inspired by the sequence mining algorithm, PrefixSpan [19], and the tree mining algorithms, TreeMinerV [26], FREQT [3]. All of them use a depth-first search for finding candidate frequent subgraphs.

The pattern-growth-based mining algorithms extend a frequent graph by adding a new edge in every possible position. A problem with the edge extension is that the same graph can be discovered many times.

**MoFa** (Molecule Fragment Miner) uses an embedding list to store the information of vertices and the information of edges. Extension is restricted to those graphs, which actually appear in the database. Isomorphism tests in the database can cheaply be done by testing whether an embedding can be refined in the same way. MoFa uses a graph local-numbering scheme to reduce the number of candidates generated from a graph. MoFa sorts the vertices of a graph according to the sequence in which they have been added. When a graph is extended at vertex *v*, later extension may only occur at *v* or at vertices bigger than *v*. Moreover, all extensions that grow from the same vertex *v* are ordered according to increasing vertex and edge labels. Although this local ordering helps, MoFa still generates many isomorphic graphs and then uses standard isomorphism testing to prune duplicates.

**gSpan** (graph-based Substructure pattern mining) uses a canonical representation for graphs, called DFS code. A DFS traversal of a graph defines an order in which the edges are visited. The concatenation of edge representations in that order is the graph's DFS code. Candidate generation is restricted by gSpan with the following rule: graphs can only be extended at vertices that lie on the rightmost path. This restriction reduces the generation of isomorphic candidates, but it cannot fully prevent duplicates from generating. Therefore, gSpan computes the canonical DFS-code for each graph. Graphs with non-minimum DFS code can be pruned. Since instead of embeddings, gSpan only stores appearance lists for each graph, subgraph isomorphism testing must be done on all graphs in these appearance lists.

**FFSM** (Fast Fragment Subgraph Mining) represents graphs as triangle matrices (vertex labels on the diagonal, edge labels on the other positions). The matrix code is the concatenation of all its entries, left to right and row by row. Based on lexicographic ordering, isomorphic graphs have the same canonical code, CAM (Canonical Adjacency Matrix). FFSM joins two matrices of graphs to generate candidates. The extension has a restriction: a new edge-vertex pair can only be added to the last vertex of a CAM. After candidate generation, FFSM permutes matrix line to check whether a generated matrix is canonical. If not, it can be pruned. FFSM stores embeddings to avoid explicit subgraph isomorphism testing. However, FFSM only stores the matching vertices, edges are ignored. This helps speeding up the extension operations since the embedding lists of new graphs can be calculated by set operations on the vertices.

**Gaston** (Graph/sequence/tree extraction) considers graphs that are paths or trees first, and by only proceeding to general graphs with cycles at the end, a large fraction of the work can be done efficiently, since there are efficient ways to enumerate paths and trees. Only in the last phase, Gaston faces the NP-completeness of the subgraph isomorphism problem. Gaston defines a global order on cycle-closing edges and only generates those cycles that are larger than the last one. A graph isomorphism test is then performed on those general graphs with cycles for finding duplicates.

A comparison among these four algorithms of both runtime and memory usage has been done by M. Worlein et al. [38]. The comparison results are shown in Fig. 2-3 and Fig. 2-4. Considering both the runtime and the memory usage, gSpan has the best performance. Therefore, we focus our research on improving gSpan.

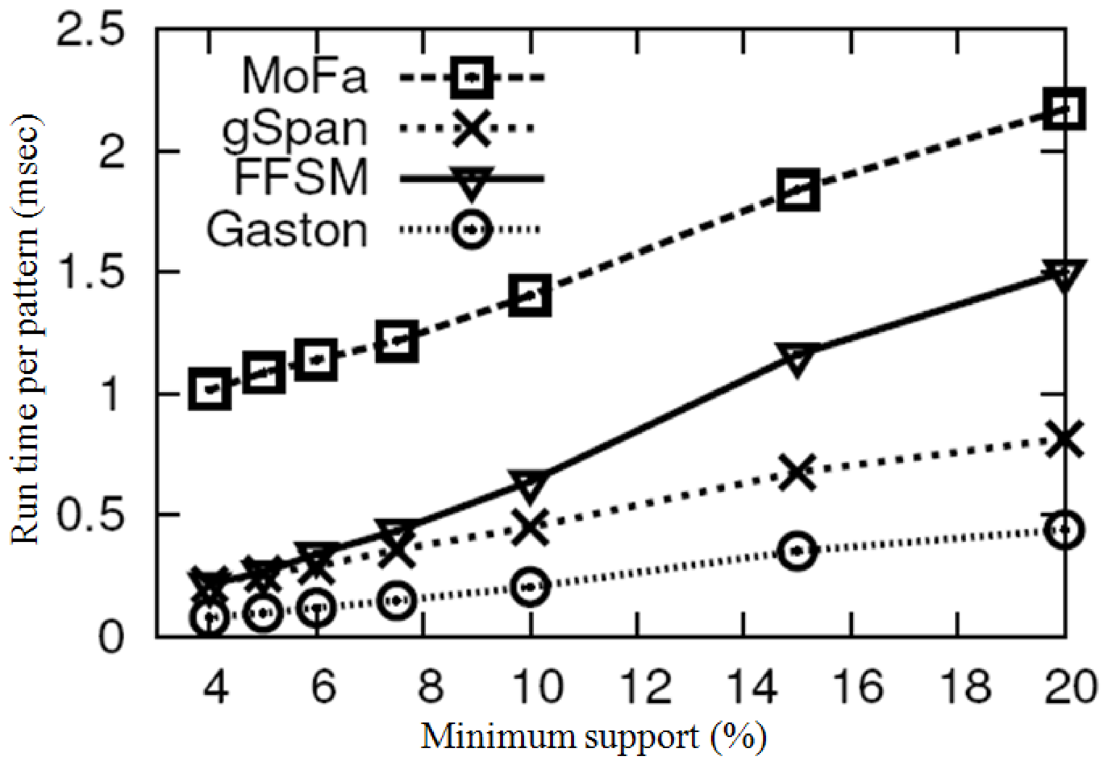


**Fig. 2-3:** Runtime of the four algorithms. [38]

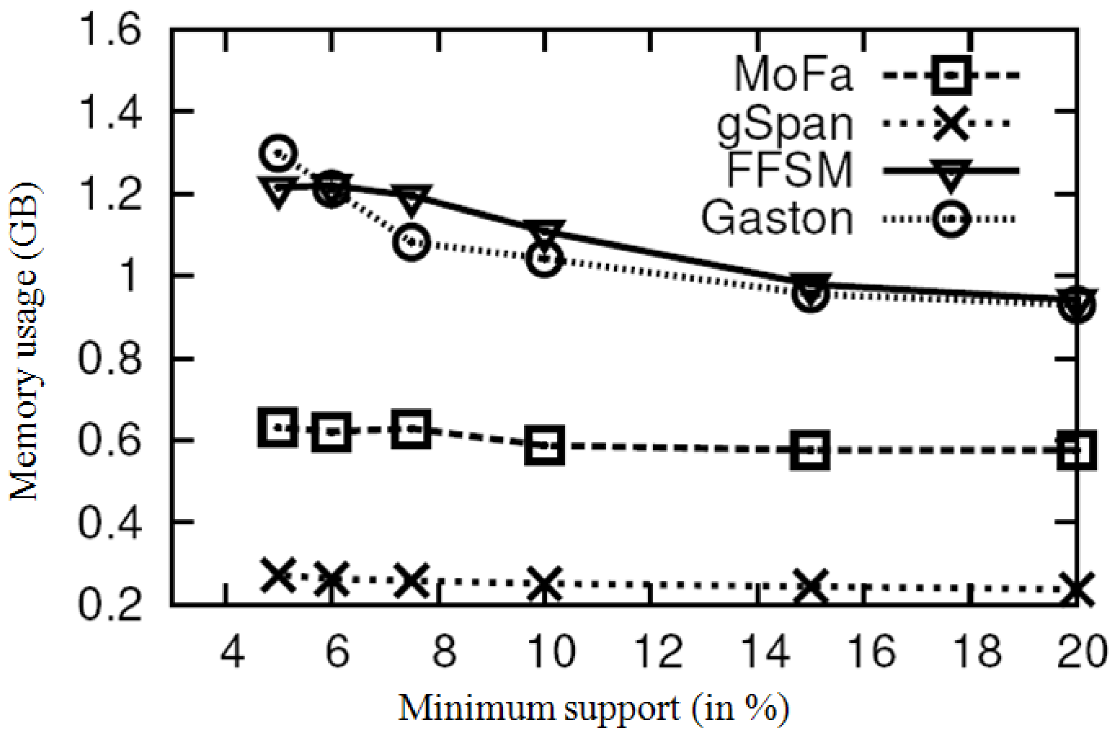


**Fig. 2-4:** Memory usage of the four algorithms. [38]

# Chapter 3

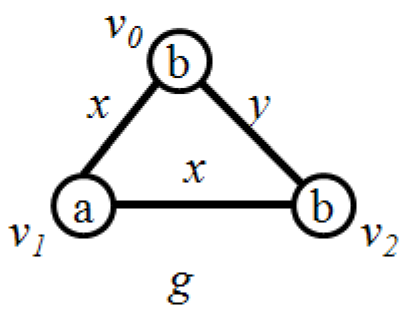
# Problem Definitions

In this chapter, some basic background knowledge with respect to graphs will be described. And then the frequent subgraph mining problem will be defined.

**Definition 1 (Labeled Graph)** *A labeled graph can be represented by a six-tuple, $G = (V, E, L, l_v, l_e)$, where*

*$V$ is a set of vertices,*
*$E \subseteq V \times V$ is a set of edges,*
*$L$ is a set of labels,*
*$l_v : V \rightarrow L$, $l$ is a function assigning labels to the vertices,*
*$l_e : E \rightarrow L$, $l$ is a function assigning labels to the edges.*

In the rest of this thesis, we denote the sets and the functions corresponding to a graph $g$ as $V_g$, $E_g$, $L_g$, $l_{vg}$,and $l_{eg}$. Fig. 3-1 shows an example of a labeled graph $g$. In this example, $l_{vg}(v_0) = b$, $l_{vg}(v_1) = a$, $l_{vg}(v_2) = b$, $l_{eg}(v_0, v_1) = x$, $l_{eg}(v_0, v_2) = y$, and $l_{eg}(v_1, v_2) = x$.



$$V_g = \{v_0, v_1, v_2\}$$
$$E_g = \{(v_0, v_1), (v_0, v_2), (v_1, v_2)\}$$
$$L_g = \{a, b, x, y\}$$

**Fig. 3-1:** A labeled graph

**Definition 2 (Subgraph)** *Given a pair of labeled graphs* $G = (V, E, L, l_v, l_e)$ *and* $G' = (V', E', L', l_v', l_e')$, *G is a subgraph of G' if and only if*

$V \subseteq V'$,
$\forall u \in V, l_v(u) = l'_v(u)$,
$E \subseteq E'$,
$\forall (u,v) \in E, l_e(u,v) = l'_e(u,v)$.

**Definition 3 (Isomorphism)** *A labeled graph* $G = (V, E, L, l_v, l_e)$ *is isomorphic to another graph* $G' = (V', E', L', l_v', l_e')$ *if and only if there exists a bijective function* $f : V \rightarrow V'$, *such that*

$\forall u \in V, l_v(u) = l_v'(f(u))$,
$\forall u,v \in V, (u,v) \in E \Leftrightarrow (f(u),f(v)) \in E'$, *and* $l_e(u,v) = l_e'(f(u),f(v))$.

**Definition 4 (Subgraph isomorphism)** *A labeled graph* $G = (V, E, L, l_v, l_e)$ *is subgraph isomorphic to another graph* $G' = (V', E', L', l_v', l_e')$ *if and only if there exists an injection* $f : V \rightarrow V'$, *such that*

$\forall u \in V, f(u) \in V'$ *and* $l_v(u) = l_v'(f(u))$,
$\forall u,v \in V$, *if* $(u,v) \in E \Rightarrow (f(u),f(v)) \in E'$, *and* $l_e(u,v) = l_e'(f(u),f(v))$.

In other words, a subgraph isomorphism from *G* to *G'* is an isomorphism from *G* to *H*, which is a subgraph of *G'*.

**Definition 5 (Frequent Subgraph Mining)** *Given a graph dataset, GD, and a threshold min_sup, the support of graph G, denoted by* $sup_G$ *is defined as cardinality of graphs in GD to which G is subgraph isomorphic.*

$sup_G = | \{G' | G' \in GD, G \text{ is subgraph isomorphic to } G'\} |$.

*G is frequent if and only if* $sup_G \geq min\_sup$. *The* ***frequent subgraph mining*** *problem is to find every frequent graph in GD.*

An example of subgraph isomorphism is presented in Fig. 3-2. Graph P has four vertices $p_1$, $p_2$, $p_3$, and $p_4$. Graph Q has three vertices $q_1$, $q_2$, and $q_3$. The mapping *f*: $q_1 \rightarrow p_3$, $q_2 \rightarrow p_1$, $q_3 \rightarrow p_2$ represents a subgraph isomorphism from Q to P. Note that the support of Q in GD = {P} is 1, even though there are four subgraph isomorphism from Q to P.

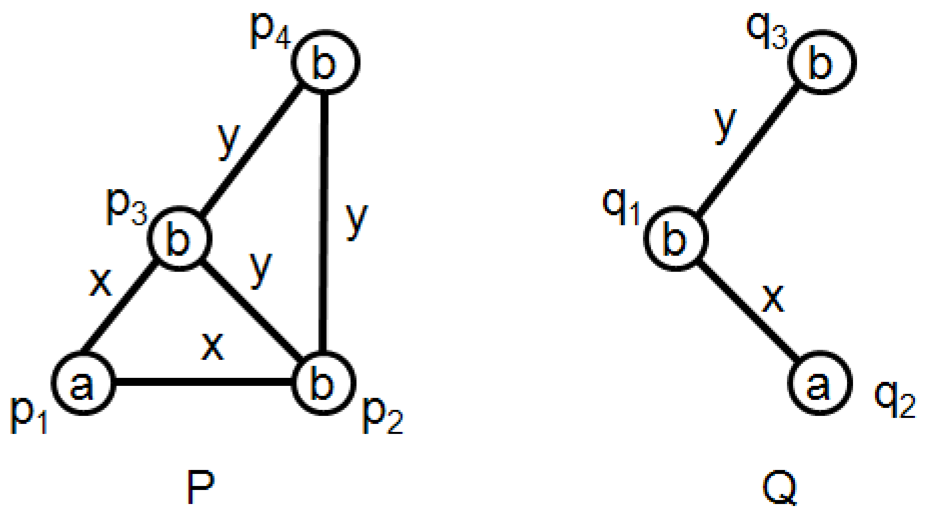


**Fig. 3-2:** An example of subgraph isomorphism.

Fig. 3-3 shows a sample graph data set, and some subgraphs with their supports. In these subgraphs, $g_1$, $g_2$, $g_3$, and $g_4$ are frequent if the minimum support is 2.

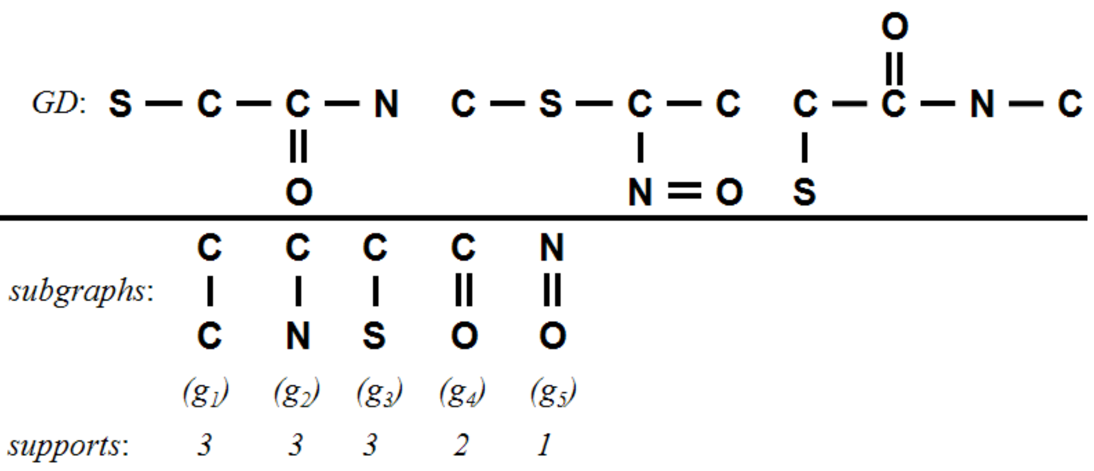


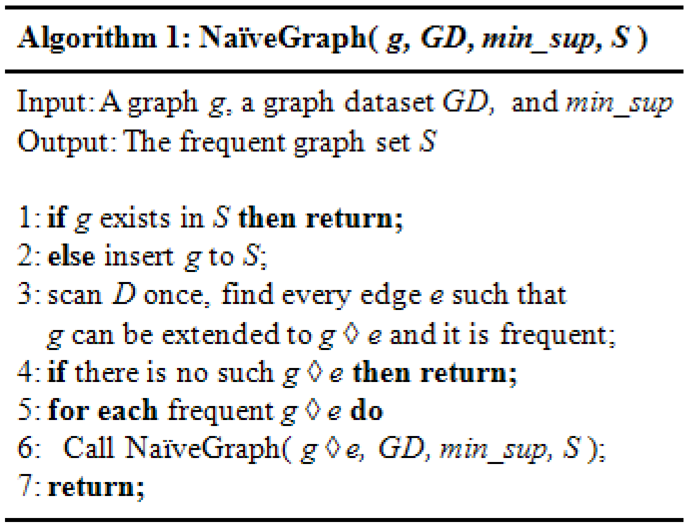
**Fig. 3-3:** An example of the supports of graphs

# Chapter 4

# The Graph Mining Algorithm

The discovery of frequent subgraphs usually consists of two steps. In the first step, we generate frequent subgraph candidates. The frequency of each candidate is checked in the second step. Therefore, the core of any frequent subgraph mining algorithm are two computationally challenging problem: (1) subgraph isomorphism: determine whether a given graph occurs in another graph; and (2) efficient enumeration of all frequent subgraphs. gSpan introduces two techniques to solve these problems: The DFS lexicographic ordering and the right-most extension. In this chapter, we will introduce the general frequent subgraph mining process, and then describe the procedure of gSpan and those techniques of gSapn. Finally, we will formulate our proposed graph mining algorithm.

The general framework of a naïve frequent graph mining algorithm is outlined in Fig. 4-1. We refer to this algorithm as NaïveGraph. In the mining process, a graph *g* can be extended by adding a new edge *e*. Let the new graph denoted by $g \diamond e$. Edge *e* may or may not introduce a new vertex to *g*. For each discovered graph *g*, it performs the extension recursively until all the frequent graphs with *g* embedded are discovered. Line 4 in Algorithm 1 shows the termination condition: When the support of a graph is less than *min_sup*, it is unnecessary to extend it any more.



```
Algorithm 1: NaïveGraph( g, GD, min_sup, S )
Input: A graph g, a graph dataset GD,  and min_sup
Output: The frequent graph set S

1: if g exists in S then return;
2: else insert g to S;
3: scan D once, find every edge e such that
   g can be extended to g ◊ e and it is frequent;
4: if there is no such g ◊ e then return;
5: for each frequent g ◊ e do
6:   Call NaïveGraph( g ◊ e, GD, min_sup, S );
7: return;
```

**Fig. 4-1:** A naïve graph mining algorithm. [29]

**NaïveGraph** is simple, but not efficient. The key issue is the inefficiency of extending *g* to *g* ◊ *e*. The same graph can be extended in different ways. For instance, an n-edge graph may have n different ways to be formed from n different (n-1)-edge graphs if we do not consider isomorphism. As a result, there may be n-1 duplicate graphs. Fig. 4-2 shows a graph *g* and four different ways to generate it. Line 1 in Algorithm 1 gets rid of duplicate graphs. The number of duplicate graphs may be huge. It raises some severe problems. First, the generation and support computation of duplicate graphs waste time. Second, it is nontrivial to tell whether a graph is a duplicate. Third, should we extend *g* if we find *g* a duplicate? If there exists at least one graph that can grow only from this duplicate graph, we still need to extent it. As we can see, these three problems affect the efficiency of the algorithm. gSpan overcomes these problems by using two techniques: (1) the DFS lexicographic ordering; and (2) the right-most extension. It has the following salient properties: (1) it reduces the generation of duplicate graphs; (2) it does not need to search previous discovered frequent graphs in order to detect duplicates; and (3) it never extends any duplicate graph but still guarantees the completeness.

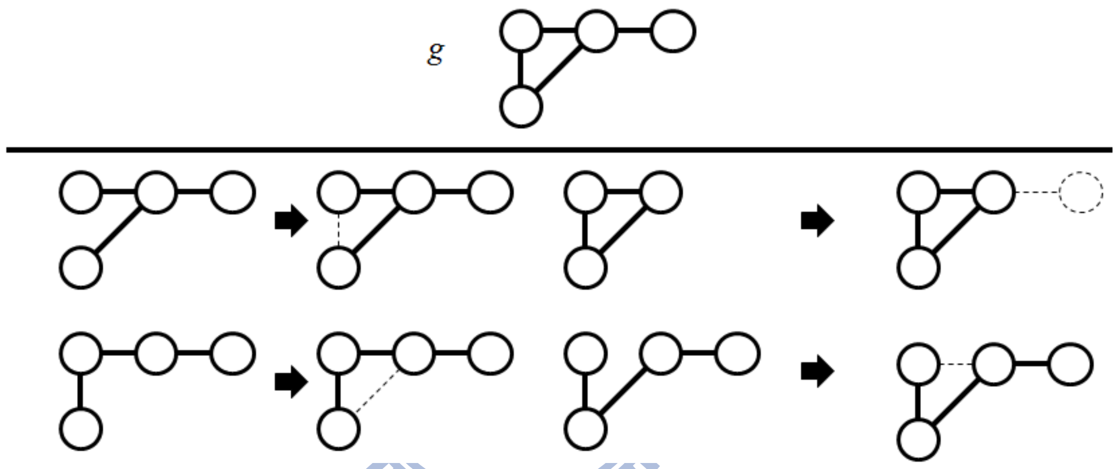


**Fig. 4-2:** Four different ways to generate *g*

In the following two sections, we focus on the background knowledge of the DFS code tree. It includes the two major techniques used in gSpan.

## 4.1 Lexicographic Ordering

This section introduces several techniques developed to represent and extend graphs efficiently. These techniques include mapping a graph to a DFS code, building a lexicographic ordering among these codes, and mining DFS codes based on this lexicographic order.

### 4.1.1 DFS Subscripting

When performing a depth-first search in a graph, a corresponding DFS tree can be constructed. Fig. 4-3 shows a graph and three different DFS trees of it. The graph has four vertices with labels *x, x, y, z* and four edges with labels *a, a, b, b.* The subgraphs with darkened edges in Fig. 4-3(b)-(d) show the DFS trees. For a given graph, there are many ways to construct different DFS trees by selecting different starting points and different growing edges. When building a DFS tree for a graph G, the depth-first discovery of the vertices forms a linear order. If there are n vertices in G, each vertex is assigned a subscript from 0 to n-1 according to the discovery order. i.e. $v_0, v_1, v_2, \ldots, v_{n-1}$. $v_0$ is called the root and $v_{n-1}$ is called the right-most vertex. The straight path from the root to the right-most vertex is named the right-most path. In Fig. 4-3(b)-(d), three different subscriptings are generated for the graph in Fig. 4-3(a). The right-most path is ($v_0, v_1, v_3$) in Fig 4-3(b) and (c), and ($v_0, v_1, v_2, v_3$) in Fig. 4-3(d). Incidentally, the darkened edges are forward edges while the undarkened ones are backward edges. From now on, $(i, j)$ represents an edge from $v_i$ to $v_j$. If $i < j$, it is a forward edge; otherwise, a backward edge. The forward edges of $v_i$ means the forward edges started from $v_i$. The backward edges of $v_i$ means the backward edges started from $v_i$.

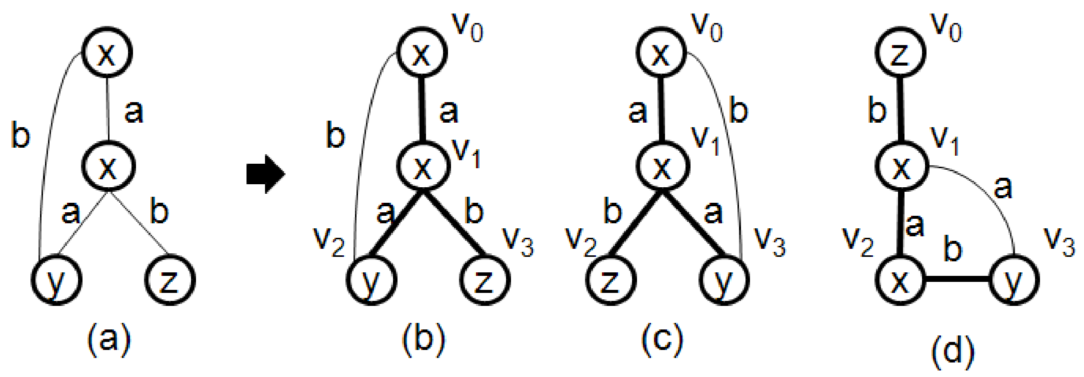


**Fig. 4-3:** DFS subscripting. [29]

### 4.1.2 DFS Code

Since there may be different DFS subscriptings for the same graph, gSpan wants to select one from them as base subscripting. For this purpose, gSpan maps each subscripted graph into an edge sequence. Afterwards, it builds an order among these sequences and selects the subscripting that generates the minimum sequence as its base subscripting. There are two kinds of orders in this process: (1) edge order, which maps edges in a subscripted graph into a sequence; and (2) sequence order, which builds the order among sequences. In the following these two orders will be introduced.

The DFS tree has defined the discovery order of forward edges. For the graph shown in Fig. 4-3(b), the forward edges are discovered in the order (0, 1), (1, 2), (1, 3). Now consider the backward edges, for a given vertex $v$, all of its backward edges should appear just before its forward edges. And its backward edges should appear just after the forward edge where $v$ is the second vertex. For vertex $v_2$ in Fig.4-3(b), its backward edge (2, 0) should appear just after (1, 2). Among the backward edges from the same vertex, gSpan enforces an order: Given $v_i$ and its two backward edges, $(i, j_1)$, and $(i, j_2)$, if $j_1 < j_2$, then edge $(i, j_1)$ will appear before edge $(i, j_2)$. The ordering of the edges in a graph is now completed. Based on this order, a graph can be translated into a sequence. A complete sequence for Fig. 4-3(b) is (0, 1), (1, 2), (2, 0), (1, 3).

gSpan represents an edge by a 5-tuple, $(i, j, l(i), l(i, j), l(j))$, where $l(i)$ and $l(j)$ are the labels of $v_i$ and $v_j$ respectively and $l(i, j)$ is the label of the edge $(v_i, v_j)$. For example, $(v_0, v_1)$ in Fig. 4-3(b) is represented by $(0, 1, X, a, X)$. For two edges $e_1 = (i_1, j_1, l(i1), l(i1,j1), l(j1))$, and $e_2 = (i_2, j_2, l(i2), l(i2,j2), l(j2))$, gSpan defines a linear order, $<_T$, in $R^5$. $e_1 <_T e_2$ holds if one of the following statements is true:

(1) $e_1$ and $e_2$ are forward edges, and $j_1 < j_2$ or $((j_1 = j_2) \wedge (i_1 > i_2))$.
(2) $e_1$ and $e_2$ are backward edges, and $i_1 < i_2$ or $((i_1 = i_2) \wedge (j_1 < j_2))$.
(3) $e_1$ is backward edge and $e_2$ is forward edge, and $i_1 < j_2$.
(4) $e_1$ is forward edge and $e_2$ is backward edge, and $j_1 \leq i_2$.

(5) $i_1 = i_2$, and $j_1 = j_2$ , and $l_{i1} < l_{i2}$ or

$l_{i1} = l_{i2}$ and $l_{(i1,j1)} < l_{(i2,j2)}$ *or*

$l_{(i1,j1)} = l_{(i1,j1)}$ and $l_{j1} < l_{j2}$.

Note that in (1), when $j_1 = j_2$, it is $i_1 > i_2$. In (5), the two edges have the same discovery order, so the labels are considered. Fig. 4-4 shows a graph *g*, and four ways to extend *g*. These extensions add edge *(2, 0), (2, 3), (1, 3),* and *(0, 3)* to *g* respectively. Therefore the order between these edges will be $(2, 0) <_T (2, 3) <_T (1, 3) <_T (0, 3)$.

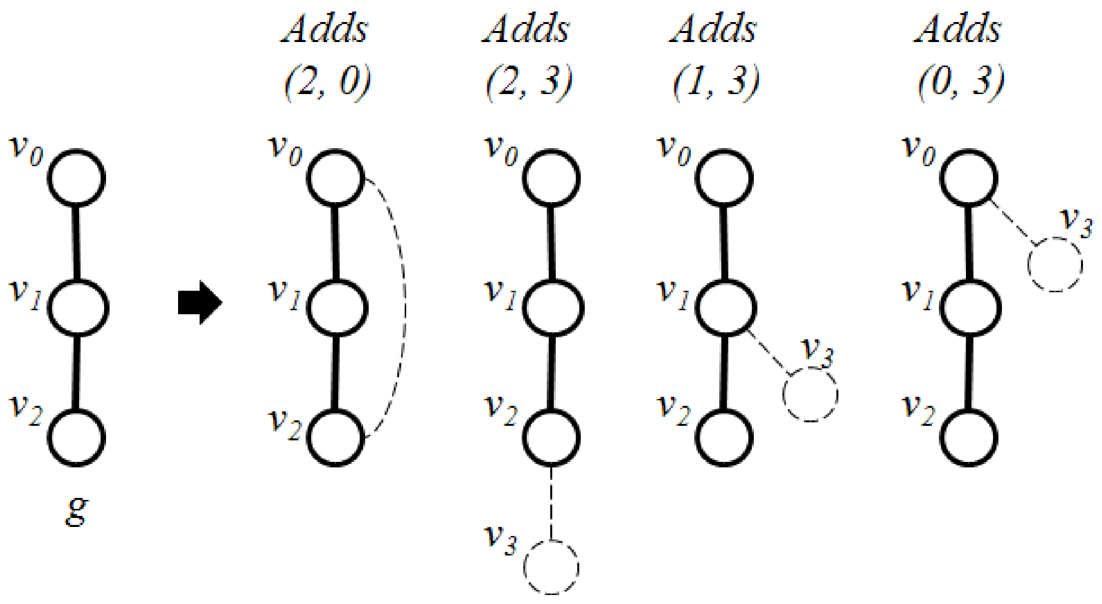


**Fig. 4-4:** An example of edge order.

**Definition 5 (The DFS code)** *Given a DFS tree T for a graph G, an edge sequence* $(e_0, e_1, e_2,\ldots, e_{|E|})$ *can be constructed based on* $<_T$*, such that* $e_i <_T e_{i+1}$*, where* $i = 0,\ldots,|E|-1$*.* $(e_0, e_1, e_2,\ldots, e_{|E|})$ *is called a DFS code, denoted as code(G,T).*

Table 4-1 shows three different DFS codes $\gamma_0$, $\gamma_1$, *and* $\gamma_2$, which are generated by DFS subscriptings in Fig. 4-3(b)-(d). We can see that, for the same graph, different

DFS trees generate different DFS codes. It is a one-to-one mapping between a subscripted graph and a DFS code. Thus, we can treat a subscripted graph and its DFS code as the same. All the notations on subscripted graphs can also be applied to DFS codes. For instance, for a given DFS code $\alpha$, we can use $\alpha \lozenge e$ to represent a possible extension of $\alpha$. The graph represented by a DFS code $\alpha$ is written as $g_\alpha$.

**Table 4-1:** DFS codes for the graphs in Fig. 4-3(b)-(d). [29]

| **Edge** | $\gamma_0$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|
| $e_0$ | $(0,1,X,a,X)$ | $(0,1,X,a,X)$ | $(0,1,Z,b,X)$ |
| $e_1$ | $(1,2,X,a,Y)$ | $(1,2,X,b,Z)$ | $(1,2,X,a,X)$ |
| $e_2$ | $(2,0,Y,b,X)$ | $(1,3,X,a,Y)$ | $(2,3,X,b,Y)$ |
| $e_3$ | $(1,3,X,b,Z)$ | $(3,0,Y,b,X)$ | $(3,1,Y,a,X)$ |

### 4.1.3 DFS Lexicographic Order

gSpan wants to build an order among the DFS codes generated for a graph so that a minimum DFS code can be defined for this graph. The edge order can be extended to a sequence order, which is a linear order on DFS codes. The formal definition of DFS code order is given as follows.

**Definition 6 (DFS Lexicographic Order)** *Given a graph dataset GD, suppose Z = {code(G, T) | G ∈GD, T is a DFS subscripting of G }, i.e., Z is a set containing all DFS codes of all graphs.* ***DFS Lexicographic Order*** *is a linear order defined as follows.*
*If $\alpha$ = code($G_\alpha$, $T_\alpha$) = ($a_0$, $a_1$,…, $a_m$) and $\beta$ = code($G_\beta$, $T_\beta$) = ($b_0$, $b_1$,…, $b_n$), $\alpha$, $\beta \in Z$, then $\alpha < \beta$ if and only if either of the following is true.*

(1) $\exists t$, $0 \leq t \leq min\{m, n\}$, $\forall k < t$, $a_k = b_k$, and $a_t <_T b_t$.
(2) $\forall k$, $0 \leq k \leq m$ , $a_k = b_k$, and $m \leq n$.

**Definition 7 (Minimum DFS Code)** *Given a graph G, C(G) = {code(G,T) | ∀T, T is a DFS tree for G}, based on DFS lexicographic order, the minimum one, min(C(G)), is called* ***Minimum DFS Code*** *of G.*

According to DFS lexicographic order, we can compare the three DFS codes listed in Table 4-1. Code $\gamma_0$ is less than code $\gamma_1$, which is less than code $\gamma_2$. Moreover, $\gamma_0$ is the minimum DFS code of the graph in Fig. 4-3(a). Minimum DFS code can be considered as canonical label.

**Definition 8 (DFS Code Tree)** *In a DFS code tree, each vertex represents a DFS code, the relation between siblings is consistent with the DFS lexicographic order. That is, the pre-order search of DFs code tree follows the DFS lexicographic order.*

DFS code and vertex in the DFS code tree are equivalent in the sense that one can be derived from the other. Any valid DFS code has a unique corresponding vertex in the DFS code tree, and any vertex in the DFS code tree contains a valid DFS code. Some of the vertices contain a minimum DFS code while others do not.

## 4.2 Right-Most Extension

In Algorithm 1, **NaïveGraph** requires extending *g* in any possible position, which will result in a huge number of duplicate graphs. gSpan adopts a more clever way to extend graphs. The extension is restricted as follows: Given *g* and a DFS tree T in *g*, *e* can be extended from the right-most vertex connecting to any other vertices on the right-most path (backward extension); or *e* can be extended from vertices on the right-most path and introduce a new vertex (forward extension). The extension under these restrictions is named *right-most extension*, and it is denoted by $g \lozenge_r e$, where *r* indicates that the extension is a right-most extension. For instance, Fig. 4-5 shows all the potential right-most extensions of the graph of Fig.4-3(b). The darkened edges show the right-most path. The dotted edges are the new edges extended and the dotted vertices are the new vertices added. For simplicity, we omit labels here. The backward extension candidates can be $(v_3, v_0)$. The forward extension candidates can be edges extending from $v_3$, $v_1$, *or* $v_0$ with a new vertex introduced.

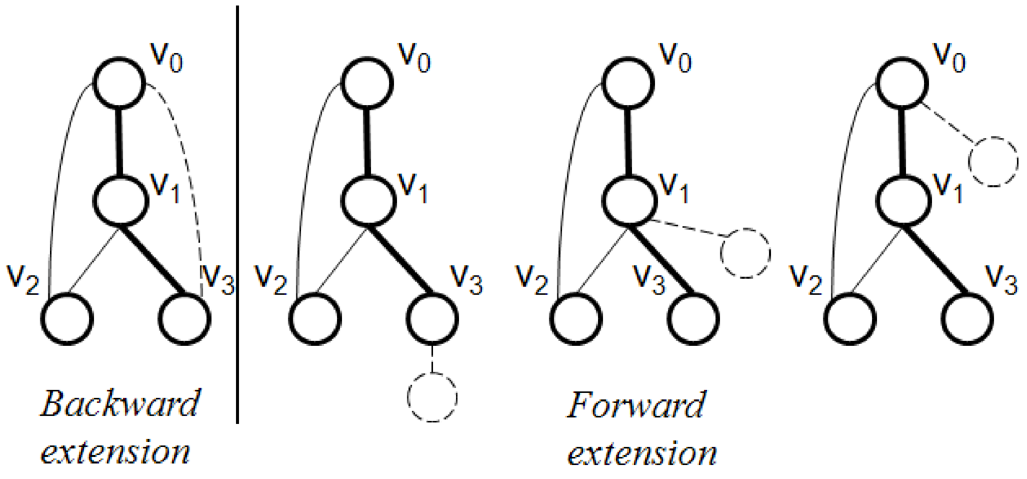


**Fig. 4-5:** The graphs extended from the graph in Fig.4-3(b).

Since a graph may have different DFS subscriptings, the right-most extension may generate many duplicate graphs if we need to extend all the subscriptings. The following theorem shows that we only need to conduct the right-most extension on the base subscripting.

**Theorem 1 (Completeness)** *Performing right-most extension in* **NaïveGraph** *guarantees the completeness of the mining result. Furthermore, performing only the right-most extension on the minimum DFS codes guarantees the completeness of the mining result.*

When performing the right-most extension in **NaïveGraph**, it is possible that a DFS code $\alpha$ is minimum, but $\alpha \lozenge_r e$ is not. For instance, Fig. 4-6 shows a graph $g$ with a minimum DFS code, but one extension of $g$ is not minimum. In this case, we do not need to conduct the right-most extension on this non-minimum DFS code.

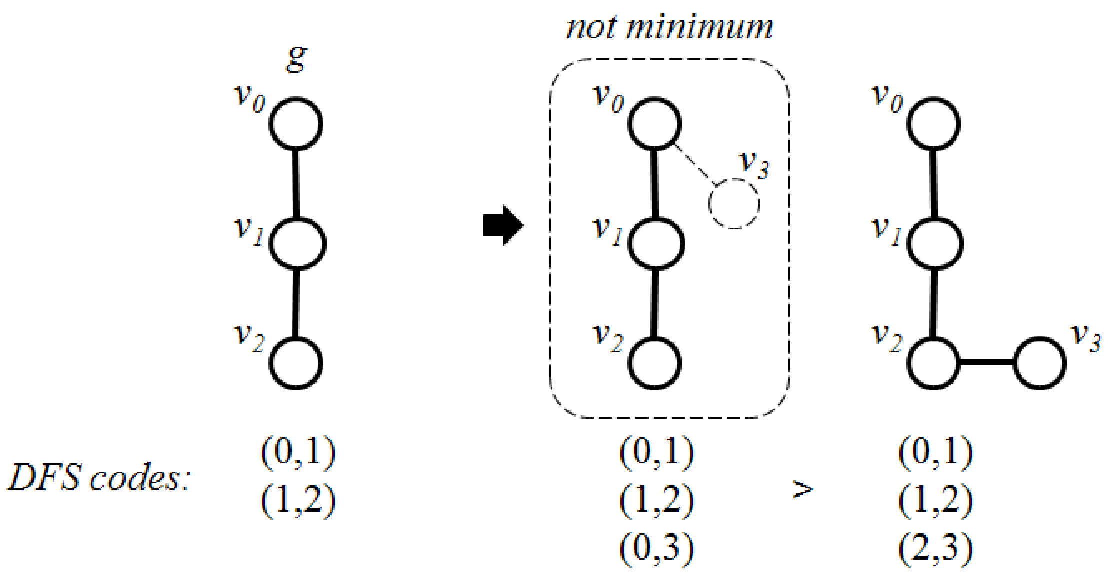


**Fig. 4-6 An example of non-minimum DFS code**

## 4.3 gSpan

In this section, we formulate the algorithm of gSpan based on the DFS lexicographic order and the right-most extension. gSpan uses a sparse adjacency list representation to store graphs. The procedure of gSpan can be illustrated with a DFS code tree. The mining process is equivalent to a pre-order traversal of the DFS code tree, which enumerates all frequent subgraphs of a graph database. The pre-order search of DFS code tree follows the DFS lexicographic order. Fig. 4-7 shows an example of the search space of gSapn, where each vertex of the tree represents a DFS code and each link of the tree represents a possible right-most extension. Fig. 4-8 shows the pseudo code of the framework.

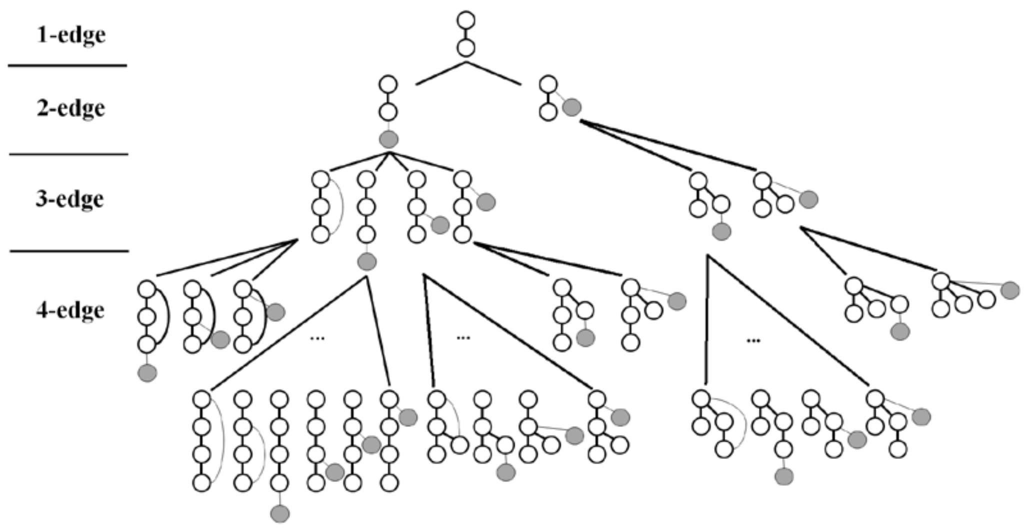


**Fig. 4-7:** A DFS code tree.

```
Algorithm 2: gSpan( s, GD, min_sup, S )

Input: A DFS code s, a graph dataset GD, and min_sup
Output: The frequent graph set S

1: if not isMinimum(s, G_s) then return; // G_s is the graph represented by s
2: else insert s to S;
3: set C to Φ;
4: scan GD once, find every edge e such that
   s can be right-most extended to s ◊_r e and it is frequent;
   insert s ◊_r e into C;
5: if C= Φ then return;
5: sort C in DFS lexicographic order;
6: for each s ◊_r e in C do
7:     Call gSpan( s ◊_r e, GD, min_sup, S );
8: return;
```

**Fig. 4-8:** The pseudo code of gSpan. [28]

The difference between gSpan and **NaïveGraph** is the right-most extension and the termination on non-minimum DFS codes(Algorithm 2 line 1). gSpan replaces the existence judgement in Algorithm 1 Line 1 by checking whether *s* is minimum. Actually, the checking is more efficient to calculate. It prunes all DFS codes which are not minimum. It significantly reduces unnecessary computation on duplicate subgraphs and their descendants. Fig. 4-9 outlines an algorithm for checking whether *s* is minimum. Fig. 4-10 shows the search space of gSpan, If we find two DFS codes *s* and *s'* representing the same graph and *s* < *s'*, by Theorem 1, we can completely stop searching any descendant of *s'*.

**Algorithm 3: isMinimum( s , g )**

```
Input: A DFS code s, and a graph g
Output: A boolean

1: foreach edge sequence w ∈ s do
2:    foreach edge e ∈ g do
3:       if w > e then return false;
4:       if w = e then do
5:          s' := s ; g' := g ;  remove w from s' and remove e from g';
6:          if not isMinimum( s', g') then return false;
7:       end
8:    end
9: end
8: return true;
```

**Fig. 4-9:** The function isMinimum.

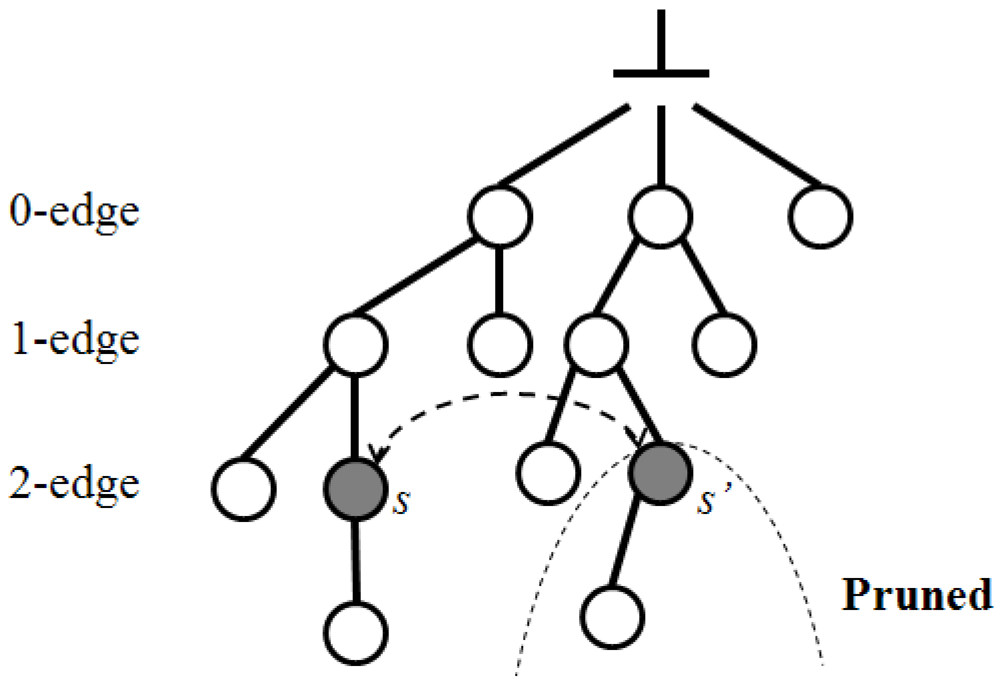


**Fig. 4-10:** The search space of gSpan. [28]

### 4.4 The Proposed Enumeration Method

Given a graph *g* with n vertices, $v_0, v_1, \ldots, v_n$, assume the length of its right-most path is *k*. The right-most path of *g* can be represented by a sequence of $(k+1)$ vertices which starts from $v_0$ and ends at $v_n$. For the sake of simplicity, we denote the vertices of the right-most path as $r_0, r_1, \ldots, r_k$. When performing right-most extension on *g*, we denote the backward extensions as $g \Diamond_{b0} e$, $g \Diamond_{b1} e$, …, $g \Diamond_{b(k-2)} e$ , where $g \Diamond_{bi} e$ means a backward extension of *g* which adds a backward edge $(r_k, r_i)$. Similarly, we denote the forward extension as $g \Diamond_{f1} e$, $g \Diamond_{f2} e$, …, $g \Diamond_{fk} e$,where $g \Diamond_{fi} e$ means a forward extension of *g* which adds a new edge $(r_i, v_{n+1})$ to $r_i$,. Fig. 4-11 shows an example of a graph *g* and the corresponding extensions. The right-most path of *g* is ($r_0$ , $r_1$, $r_2$, $r_3$).

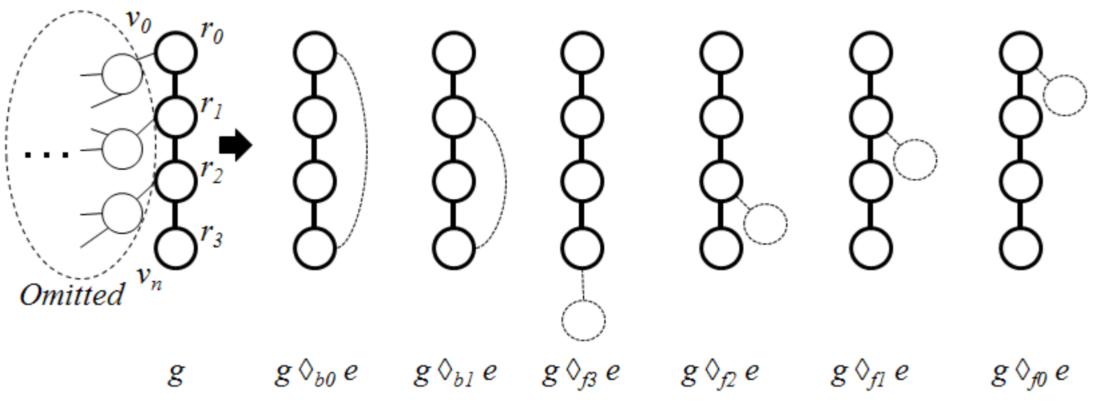


**Fig. 4-11:** A right-most extension.

There are two duplicate graphs in Fig. 4-11, $g \lozenge_{f1} e$ and $g \lozenge_{f0} e$ . In this case, the two extensions are redundant. We want to shrink the search space by removing some redundant extensions from the right-most extension. We propose an additional restriction to the right-most extension. In the following section we will introduce this modified extension.

For a given graph *g* with a right-most path ($r_0$, $r_1$, …, $r_k$), in the forward extensions, the operations $\lozenge_{f0}$, $\lozenge_{f1}$, …, $\lozenge_{f\lfloor k/2 \rfloor}$ are redundant, that is, graphs generated by these operations are duplicate. For instance, in Fig. 4-11, $f_0$ and $f_1$ are not necessary. The backward extensions remain unchanged. In order to prove the completeness of this modified right-most extension, we propose the following theorem.

**Conjecture (Symmetry of Graph)** *Given a graph g, along its right-most path* ($r_0$, $r_1$, …, $r_k$), *we can find a graph g', which is symmetric to g with respect to the center of its right-most path.*

According to this conjecture, for every graph *g*, there exists a graph *g'*, such that $g \Diamond_{f0} e = g' \Diamond_{fk} e$. Thus, we can discard the operation $f_0$ and still guarantee the completeness of the mining result. For the same reason, we can remove all the operation $f_i$, $i=0,1,\ldots,\lfloor k/2 \rfloor$ from the right-most extension.

By replacing the right-most extension of gSpan with this modified right-most extension, the number of candidates is further decreased. I

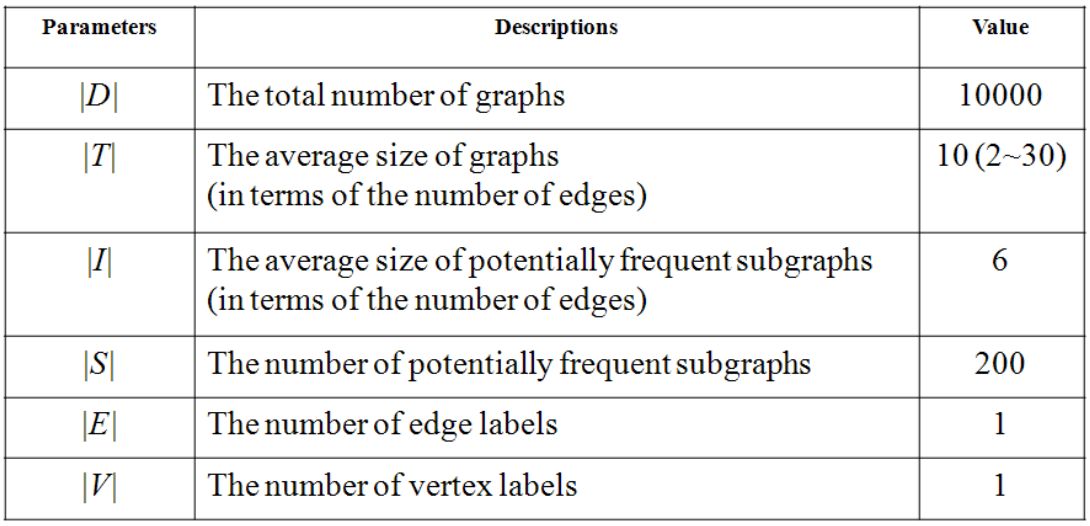
# Chapter 5

# Experimental Results

Since the complexity of graph mining is higher when mines unlabeled graph datasets, we conduct a performance study on unlabeled datasets. On both synthetic and real world datasets, the experiments are performed. We use a synthetic data generator provided by Kuramochi and Karypis[16]. The real data set we tested is a chemical compound dataset with the labels removed. All experiments are done on a 3.0GHz Intel Pentium D PC with 2GB memory, running Windows XP system. Our performance tests show that the number of candidates generated by our algorithm is about 10% less than that generated by gSpan.

We use the data generator provided by Kuramochi. The parameter description of the data generator is shown in Table 5-1. The synthetic datasets are generated using a similar procedure described in [1]. Kuramochi et al. applied a simplified procedure in their graph data synthesis. The details about how to generate the datasets were described in [16]. The generator generates |D| graphs. The size of each graph is a Poisson random variable whose mean is equal to |T|. In our experiments, some parameters of the data generator are fixed value: |T|=10, |I|=6, and |S|=200. Since the datasets are unlabeled graph datasets, which is equivalent to 1-labeled graph datasets, we set $|L_E| = |L_V| = 1$.

**Table 5-1:** Synthetic dataset parameters



| Parameters | Descriptions | Value |
|---|---|---|
| $\|D\|$ | The total number of graphs | 10000 |
| $\|T\|$ | The average size of graphs<br>(in terms of the number of edges) | 10 (2~30) |
| $\|I\|$ | The average size of potentially frequent subgraphs<br>(in terms of the number of edges) | 6 |
| $\|S\|$ | The number of potentially frequent subgraphs | 200 |
| $\|E\|$ | The number of edge labels | 1 |
| $\|V\|$ | The number of vertex labels | 1 |

We test the performance of our algorithm on a synthetic dataset with |D| = 10k. Fig. 5-1 shows the number of candidates generated by our proposed algorithm and gSpan with different minimum supports.

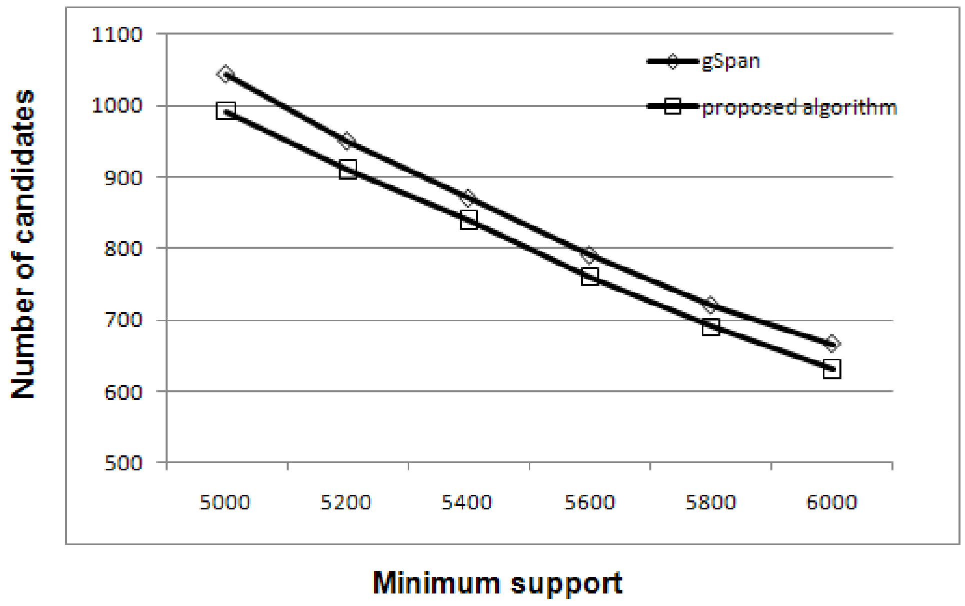


**Fig. 5-1:** Number of candidates (synthetic dataset).

The chemical compound dataset is the same one used in [16,28], This was originally provided for the Predictive Toxicology Evaluation Challenge [36], which contains information on 340 chemical compounds. We set all the labels to a same label to transform this dataset to a unlabeled dataset. There are 340 graphs in total. The average graph size is 27.4 in terms of the number of edges and 27.0 in terms of the number of vertices. There are 26 graphs that have more than 50 edges and vertices. The largest graph contains 214 edges and 214 vertices. We test the performance on this chemical compound dataset. Fig. 5-2 illustrates the number of candidates generated by our algorithm and gSpan with different minimum supports.

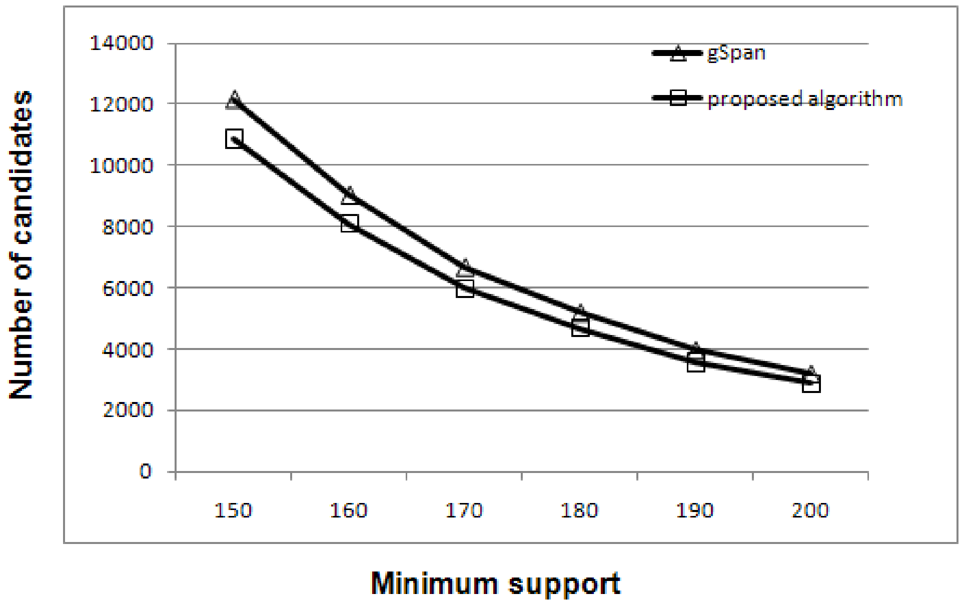


**Fig. 5-2:** Number of candidates (chemical compound dataset).

The experimental results show that the number of candidates generated by our proposed algorithm is about 5%~10% less than that generated by gSpan. In our experiments, the mining result is correct, in other words, the completeness of our proposed enumeration method is fulfilled. Unfortunately, we have not completed a formal proof for the completeness. There is still a possibility that our proposed algorithm works only on some special cases. We require further research and experiment to ensure the completeness of our proposed enumeration method.

# Chapter 6

# Conclusion and Future Works

In this thesis, we analyzed the state-of-the-art graph mining algorithm gSpan and addressed the possible inefficiencies in it. We found that when gSpan deals with large and complex graphs (denser graphs with fewer labels available), especially when deals with unlabeled graphs, the performance of gSpan degrades. Based on gSpan, we proposed a new graph enumeration method, which reduces the candidate generation.

There are still some research issues of our proposed algorithm. First, we have to prove the completeness of our proposed algorithm. Second, there might be a better algorithm to calculate the minimum code when the graph is unlabeled. Third, in order to extend our algorithm to mine labeled graphs, we might require a new lexicographic order. Therefore, to develop a new lexicographic order for our proposed algorithm is a research issue in our future work.

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