TED: Towards Discovering Top-k Edge-Diversified Patterns in a Graph Database

ABSTRACT

With an exponentially growing number of graphs from disparate repositories, there is a strong need to analyze a graph database containing an extensive collection of small- or medium-sized data graphs (*e.g.,* chemical compounds). Although subgraph enumeration and subgraph mining have been proposed to bring insights into a graph database by a set of subgraph structures, they often end up with similar or homogenous topologies, which is undesirable in many graph applications. To address this limitation, we propose the *Top-k Edge-Diversified Patterns Discovery problem* to retrieve a set of subgraphs that cover the maximum number of edges in a database. To efficiently process such query, we present a generic and extensible framework called TED which achieves a guaranteed approximation ratio to the optimal result. Three optimization strategies are further developed to improve the performance, and a lightweight version called TEDLITE is designed for even larger graph databases. Experimental studies on real-world datasets demonstrate the superiority of TED to traditional techniques.

1 INTRODUCTION

The graph database that contains a large collection of small- or medium-sized data graphs has become increasingly prevalent in a variety of domains such as biological networks, drug discovery, and computer vision. Analyzing and mining such a database nurtures many applications, including graph search and classification. While graph analysis varies from application to application, a common phenomenon in these applications is that some subgraph structures (*also known as* graph patterns) play a vital role in characterizing the underlying graph database and building intuitive models for better understanding complex structures. Consequently, subgraph enumeration, which aims to enumerate all subgraphs in a graph database, has been extensively studied in the literature [2–6]. Subgraph enumeration is known to be computationally challenging and memory-consuming since the number of subgraphs in a graph database is exponential to the database size. Therefore, complete enumeration and persistence of all subgraphs in a graph database are infeasible. For instance, more than a million compounds are available from sources such as PUBCHEM [1] and EMOLECULES [2].

Frequent subgraph mining alleviates this problem by generating only frequent subgraphs instead of all subgraphs [7–12]. Given a minimum support threshold sup_{min} [3], a subgraph g is frequent if the fraction of data graph G containing g (*i.e., g* is a subgraph of G) in a database D is no less than sup_{min}. Intuitively, as the threshold decreases, the number of resulting subgraphs increases dramatically. In contrast, the number of subgraphs decreases as the threshold increases, making the resulting subgraphs topologically similar to each other with common substructures and no longer representational. In other words, the results lack diversity whose importance has been advocated in the literature [14–17].

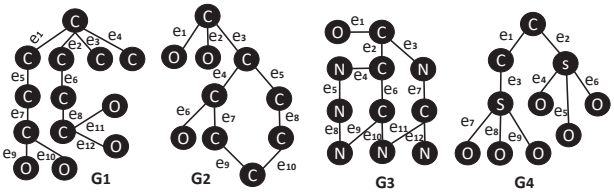

Figure 1: A sample graph database.

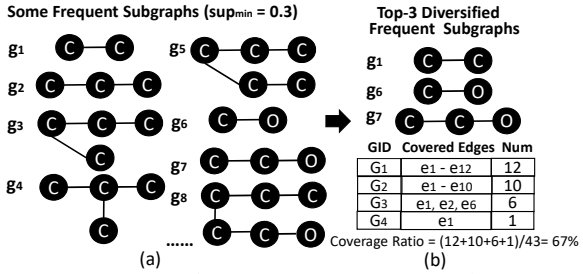

Figure 2: Frequent (resp. diversified frequent) subgraphs.

EXAMPLE 1. *To illustrate this, consider a graph database containing G_1 to G_4 in Figure 1. Let the minimum support $sup_{min} = 0.3$. The database contains many frequent subgraphs, some of which are shown in Figure 2(a). All these subgraphs except g_6 share a common subgraph g_1, which is homogenous and thus redundant. A possible way to alleviate this problem is to select a limited number (*e.g., *k*) of diversified ones from all frequent subgraphs such that the maximum number of edges in the database can be covered. For example, if we select the top-3 diversified frequent subgraphs (*i.e., *g_1, g_6 and g_7) shown in Figure 2(b), they will cover a maximum number of edges (*i.e., *67% edges) in all data graphs from G_1 to G_4. As a comparison, if we just randomly select 3 subgraphs, for example g_3, g_4 and g_5, users cannot obtain any information on graphs G_3 and G_4 since they contain none of the subgraphs.* ∎

Although these diversified frequent subgraphs g_1, g_6 and g_7 cover all data graphs ($G_1 - G_4$, Figure 1) and 67% of their edges, no edge in G_4 (except e_1) is covered. Further, g_7 does not cover new edges that are not covered by g_1 and g_6 (see Figure 2(b)). If we replace g_7 with an infrequent subgraph that contains nodes "S", "O" and an edge between them, the percentage of covered edges will increase from 67% to 81%. This observation motivates us to retrieve, instead of top-k frequent subgraphs, the top-k diversified subgraphs, also known as edge-diversified patterns, that cover a maximum number of edges in the graph database. Note that edge-diversified patterns can contain both frequent and infrequent subgraphs, as shown in the following example.

[1] https://pubchem.ncbi.nlm.nih.gov/
[2] https://www.emolecules.com/
[3] $sup_{min} \in [0, 1]$ is a user-specified parameter, which is used to eliminate infrequent subgraph g whose frequency of occurrences in a database D is less than sup_{min}.

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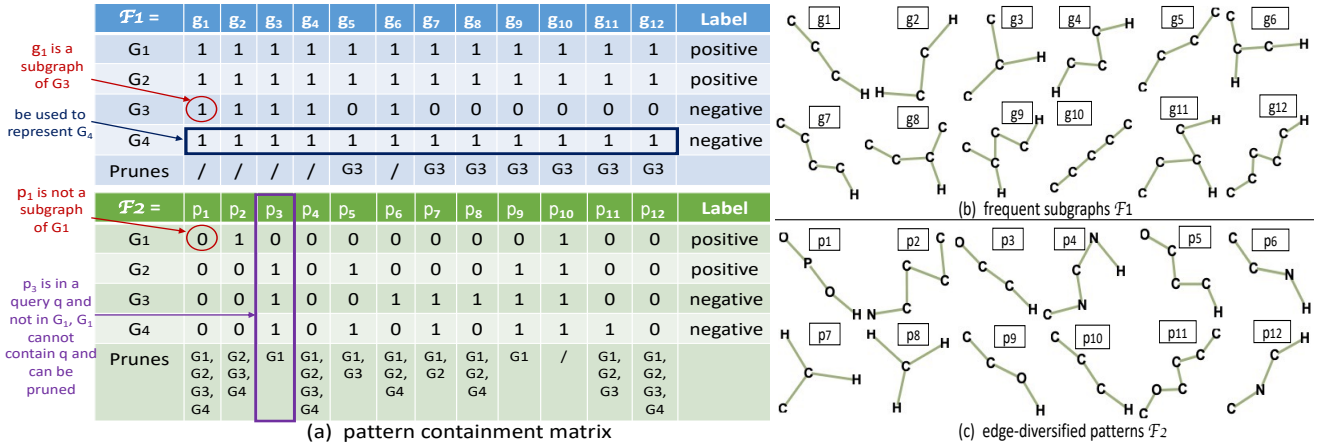


$\mathcal{F}_1$ =	g_1	g_2	g_3	g_4	g_5	g_6	g_7	g_8	g_9	g_{10}	g_{11}	g_{12}	Label
G1	1	1	1	1	1	1	1	1	1	1	1	1	positive
G2	1	1	1	1	1	1	1	1	1	1	1	1	positive
G3	1	1	1	1	0	1	0	0	0	0	0	0	negative
G4	1	1	1	1	1	1	1	1	1	1	1	1	negative
Prunes	/	/	/	/	G3	/	G3	G3	G3	G3	G3	G3	

$\mathcal{F}_2$ =	p_1	p_2	p_3	p_4	p_5	p_6	p_7	p_8	p_9	p_{10}	p_{11}	p_{12}	Label
G1	0	1	0	0	0	0	0	0	0	1	0	0	positive
G2	0	0	1	0	1	0	0	0	1	1	0	0	positive
G3	0	0	1	0	0	1	1	1	1	1	0	0	negative
G4	0	0	1	0	1	0	1	0	1	1	1	0	negative
Prunes	G1, G2, G3, G4	G2, G3, G4	G1	G1, G2, G3, G4	G1, G3	G1, G2, G4	G1, G2	G1, G2, G4	G1	/	G1, G2, G3	G1, G2, G3, G4	

Figure 3: (a) The pattern containment matrix where each entry indicates if a pattern (*i.e.,* g_i or p_i) is a subgraph of data graphs, (b) top-k frequent subgraphs $\mathcal{F}_1$, and (c) edge-diversified patterns $\mathcal{F}_2$.

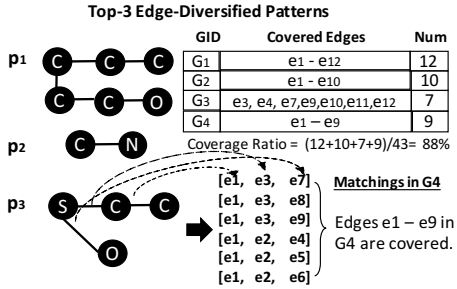


Figure 4: Top-k edge-diversified patterns.

Example 2. *Reconsider Example 1. Figure 4 presents top-3 edge-diversified patterns* (i.e., p_1, p_2 *and* p_3) *for the sample database in Figure 1. Only* p_1 *is a frequent subgraph while* p_3 *(resp.* p_2*) exists in* G_4 *(resp.* G_3*) only. Although* p_3 *is infrequent, it has 6 matchings in* G_4 *and contributes 9 edges to the total edge coverage, as shown in the figure. As such, the top-3 edge-diversified patterns can cover almost 88% edges in all 4 graphs in the sample database.* ∎

Motivated by the aforementioned examples, in this paper, we study the top-k edge-diversified patterns discovery problem, which finds k connected subgraphs from a graph database such that the maximum number of edges in the graph database can be covered. The main difference between frequent subgraphs and edge-diversified patterns lies in that a frequent subgraph g must be contained by multiple (at least sup_{min}) different data graphs even if g has only one occurrence in a data graph G, whereas an edge-diversified pattern can be frequent (*e.g.,* p_1 in Figure 4) or infrequent (*e.g.,* p_2 or p_3 in Figure 4), as long as it can reach a wider edge coverage by covering different parts of data graphs with multiple occurrences. In other words, a frequent subgraph is measured independently by its frequency, whereas edge-diversified patterns are jointly measured by the total edge coverage (see Definition 3). Since the latter patterns can supplement the former with infrequent subgraphs covering remaining edges in the graph database, it naturally provides a more comprehensive summary of the database than using frequent subgraphs alone.

Therefore, top-k edge-diversified patterns discovery can be applied in a wide range of applications such as graph indexing and graph classification. Graph indexing and classification have been widely studied in the literature [25, 42] and adopted in different real-world graph databases (*e.g.,* PubChem and eMolecules).

- **Graph Indexing.** Subgraph query, which finds data graphs that contain a query subgraph q, is a popular query type. As a subgraph query needs to execute subgraph isomorphism tests (see Definition 1), it is an NP-complete problem [25]. Since it is time-consuming to process a query q over each data graph G in a database, one can build pattern-based graph indices to filter out those data graphs that cannot contain q and only execute subgraph isomorphism tests on the remaining graphs. A graph index is commonly defined as a map from a pattern p to each data graph G that contains this pattern. If a query q contains a particular pattern p while G does not contain p, G cannot contain q and can be pruned directly.
- **Graph Classification.** Graph classification, which predicts class labels of data graphs, is an important problem. Despite its increasing importance, many popular feature-based classifiers cannot be applied simply due to the lack of vector representation of graphs. Subgraph patterns can serve as features to vectorize these graphs and embrace feature-based classifiers.

The following examples illustrates the advantage of top-k edge-diversified patterns over top-k frequent patterns for graph indexing and classification. Such advantage also exists in other applications (*i.e.,* visual subgraph query formulation and exploratory subgraph search), which will be elaborated in Section 7.

Example 3. *Figures 3(b) and (c) present the top-12 frequent subgraphs (*$sup_{min} = 0.3$*)* $\mathcal{F}_1 = \{g_1, g_2, ..., g_i, ..., g_{12}\}$ *and edge-diversified patterns* $\mathcal{F}_2 = \{p_1, p_2, ..., p_i, ..., p_{12}\}$ *in PubChem database, respectively.* G_1*,* G_2*,* G_3 *and* G_4 *are data graphs where the class label of* G_1 *and* G_2 *is "positive", and that of* G_3 *and* G_4 *is "negative". Figure 3(a) (top, resp. bottom) shows the pattern containment matrix of these data graphs over* $\mathcal{F}_1$ *(resp.* $\mathcal{F}_2$*). For example,* G_3 *contains* g_1*,* g_2*,* g_3*,* g_4 *and* g_6*, so the corresponding entries* (i.e., *4th row, 2nd-5th and 7th columns) in the matrix are* 1.

1) Graph Indexing. Consider a common query q [4] *that contains all g_i in $\mathcal{F}_1$, p_3, p_5, and $p_7 - p_{11}$ in $\mathcal{F}_2$. If a graph index $\mathcal{I}$ is built on $\mathcal{F}_1$ (denoted by $\mathcal{I}_{\mathcal{F}_1}$), it can filter out G_3. This is because g_5 (or $g_7 - g_{12}$) is a subgraph of q but not a subgraph of G_3 (Figure 3(a), top). Thus, q is not a subgraph of G_3. As such, three subgraph isomorphism tests are needed* (i.e., *testing q over G_1, G_2 and G_4). Moreover, $\mathcal{I}_{\mathcal{F}_1}$ can reduce at most one subgraph isomorphism test* (i.e., *q over G_3) no matter what the query q is (see the last row of the top table in Figure 3(a)). On the other hand, if the graph index $\mathcal{I}$ is built on $\mathcal{F}_2$ (denoted by $\mathcal{I}_{\mathcal{F}_2}$), it can filter out all these data graphs. This is because q contains p_3, p_5, and $p_7 - p_{11}$, which jointly filter out $\{G_1, G_2, G_3, G_4\}$. For example, p_3 can filter out G_1 and p_5 can prune $\{G_1, G_3\}$ (see the last row of the bottom table in Figure 3(a)). Therefore, no subgraph isomorphism test is needed.*

2) Graph Classification. If $\mathcal{F}_1$ is used as vector representations of data graphs, the feature vector of G_1 will be $[1, ..., 1]$ since G_1 contains all g_i in $\mathcal{F}_1$ (see 2nd row of the top table in Figure 3(a)). If $\mathcal{F}_2$ is used as vector representations of data graphs, the feature vector of G_1 will be $[0, 1, 0, ..., 0, 1, 0, 0]$ since G_1 contains p_2 and p_{10} in $\mathcal{F}_2$ (see 2nd row of the bottom table in Figure 3(a)). Given the $\mathcal{F}_2$-based feature vectors, a simple and yet effective classification rule can be obtained: a graph (e.g., *G_3 or G_4) which contains $\{p_3, p_7, p_9, p_{10}\}$ can be negative. But it is hard to find such a good classification rule with $\mathcal{F}_1$-based feature vectors, since the negative graph G_4 has the same representation as that of G_1 or G_2.*

As both frequent (*e.g.*, p_3) and infrequent patterns (*e.g.*, p_8) play an important role in graph indexing and graph classification, edge-diversified patterns show their advantage over frequent patterns.

However, *top-k edge-diversified patterns discovery* problem introduces non-trivial challenges. First, it is NP-hard. Second, adapting existing subgraph enumeration and frequent subgraph mining techniques to this problem is inadequate since they fall short in handling large databases or guaranteeing patterns' quality. In this paper, we address these challenges and propose a novel solution for top-k edge-diversified patterns discovery problem. We make the following contributions.

- To the best of our knowledge, we are the first to study *top-k edge-diversified patterns discovery problem* and address it with two adapted baseline solutions.
- We further present a generic and extensible framework called TED for this problem which requires limited memory and achieves a guaranteed approximation ratio.
- Three optimization strategies are developed to improve the performance and a lightweight version called TEDLITE is designed to handle even larger graph databases.
- By using real-world data graph repositories, extensive experimental evaluations are provided to show the superiority of our methods over two baseline solutions.

The rest of this paper is organized as follows. In Section 2, we provide some preliminaries and the problem statement. In Section 3, two baseline solutions are proposed for top-k edge-diversified patterns discovery problem. In Section 4, our proposed novel framework TED is presented, followed by three optimization strategies in Section 5 and a lightweight version TEDLITE in Section 6. In Section 7, we employ the demonstration system called VISCENT to illustrate the application potentials of edge-diversified patterns. Section 8 shows extensive experimental results. Related work are in Section 9 and conclusions are made in Section 10. Proofs of all theorems and lemmas are given in Appendix A.

[4] https://pubchem.ncbi.nlm.nih.gov/compound/2244

Table 1: List of key notations.

Notation	Description
g, G, D	a subgraph, a graph, a graph database
$V(G), E(G)$	vertex set of graph G, edge set of graph G
$p, \mathcal{P}$	a pattern, a pattern set
k	number of edge-diversified patterns
sup_{min}	minimum support
$Cov(G_i, G_j)$	cover set of G_i over G_j
$\|Cov(G_i, G_j)\|$	coverage of G_i over G_j
E_{max}	maximum number of edges in an edge-diversified pattern
S, S_{fre}	a set of subgraphs, a set of frequent subgraphs

2 PRELIMINARIES

Table 1 lists the notations and acronyms used in this paper.

2.1 Key Concepts

A simple graph G is represented as $G = (V, E)$ where V is a set of vertices and $E \subseteq V \times V$ is a set of edges. For ease of presentation, we assume G is an undirected connected graph whose vertex $v \in V$ is labeled with $l(v)$ and edge $e \in E$ is labeled with $l(e)$ [5]. In this paper, we focus on a graph database containing a large collection of graphs (denoted as D), each of which is with either dozens or hundreds of nodes (up to 801, see Table 2, Section 8.1). Therefore, this paper follows related works [17, 18] to call them small- or medium-sized graphs. A unique *index* (*i.e.,* ID) is assigned to each graph in D. We denote a graph with index i as $G_i \in D$.

DEFINITION 1 (**SUBGRAPH ISOMORPHISM**). Given two graphs G_1 and G_2, a subgraph isomorphism is an injection $f: V(G_1) \rightarrow V(G_2)$ such that 1) $\forall v \in V(G_1)$, $l(v) = l'(f(v))$ and 2) $\forall (u, v) \in E(G_1)$, $(f(u), f(v)) \in E(G_2)$ and $l(u, v) = l'(f(u), f(v))$ where l and l' are the labeling functions of graph G_1 and G_2, respectively.

G_1 is *subgraph isomorphic to* G_2 if there exists at least one subgraph isomorphism f from G_1 to G_2. We also say that G_2 is *covered* by G_1 or that G_2 *contains* G_1 (denoted by $G_1 \subseteq G_2$). Given a subgraph isomorphism f and the subgraph G' of G_2 consisting of vertices $f(v)$ and edges $(f(u), f(v))$ where $u, v \in V(G_1)$, we say that G' is a **matching** of G_1 in G_2. We may simply say that G' is a matching. The edge $(f(u), f(v))$ is called covered edge.

DEFINITION 2 (**COVER SET AND COVERAGE**). Given two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, if G_1 is subgraph isomorphic to G_2 and the matchings are $\mathcal{F}$, the cover set of G_1 over G_2 is $Cov(G_1, G_2) = \cup_{f \in \mathcal{F}}(f(u), f(v))$ and the coverage is $|Cov(G_1, G_2)|$.

Observe that the cover set of G_1 over G_2 is union of all covered edges. The coverage is cardinality of the cover set. In addition, the cover set of a set of graphs $\mathcal{G}_1 = \{G_1, G_2, ..., G_i, ..., G_n\}$ over $\mathcal{G}_2 = \{G'_1, G'_2, ..., G'_j, ..., G'_m\}$ is defined as $Cov(\mathcal{G}_1, \mathcal{G}_2) = \cup_i \cup_j Cov(G_i, G'_j) = \cup_j \cup_i Cov(G_i, G'_j)$ where $i \in [1, n]$ and $j \in [1, m]$.

[5] For the graph with labeled vertex and unlabeled edge, each edge $e \in E$ is labeled with the concatenation of labels (*i.e.,* a new label joining two labels together) of its two end vertices (*i.e.,* $l(e) = l(u).l(v)$).

2.2 Problem Statement

Definition 3 (**Top-k Edge-Diversified Patterns Discovery**). Given a graph database $D = \{G_1, G_2, \cdots, G_j, \cdots, G_n\}$ and an integer k, top-k edge-diversified patterns discovery is to find k connected subgraphs $\mathcal{P} = \{p_1, p_2, \ldots, p_i, \ldots p_k\}$ from D such that the total coverage of $\mathcal{P}$ over D (denoted by $|Cov(\mathcal{P}, D)|$), *i.e.,* $|\cup_i \cup_j Cov(p_i, G_j)|$, is maximized, where $Cov(p_i, G_j)$ is the cover set of p_i over G_j, and the number of edges of p_i (*i.e.,* $|E(p_i)|$) is no more than a given size threshold E_{max}.

Remark. It seems that when $E_{max} = 1$, this problem becomes the (minimum) edge cover problem, which finds a set of edges $\mathbb{C}$ with the smallest possible size such that each vertex in a graph is incident with at least one edge in $\mathbb{C}$. However, given a graph G (*i.e.,* $D = \{G\}$), even if $E_{max} = 1$, they are not the same, as edge-diversified patterns discovery is to find a limited number of edges (*i.e.,* k) such that their matchings in G cover the maximum number of edges, while the (minimum) edge cover problem finds an edge set that covers *all vertices* in G. For example, let $k = 1$ and $D = \{G_1\}$ in Figure 1, top-k edge-diversified patterns are the edge between two "C", but (minimum) edge cover of G_1 is $\{e_3 - e_6, e_9 - e_{12}\}$. In addition, note that $|E(p_i)|$ is not allowed to be larger than a given threshold E_{max}. The reasons are two-fold. First, if some graphs in D are apparently larger than other graphs, there is a likelihood that selecting those graphs as the top-k edge-diversified patterns is already an optimal solution. Thus, we don't have to discuss the problem here. Second, in most applications, such as visual subgraph query formulation, patterns should not be too large [17], since pattern budget (e.g., minimum size, maximum size and number of patterns) is pre-defined for pattern mining.

Theorem 1. *The top-k edge-diversified patterns discovery problem is NP-hard.*

When $k = 1$, the problem can be reduced from maximum coverage problem [22]. We prove the theorem by reduction from it.

3 BASELINE SOLUTIONS

In this section, we present two baseline solutions for this problem. The first one, named as ALL_g, is to enumerate all subgraphs S from the database D, and then conduct a greedy search. Given a minimum support threshold sup_{min}, the second solution named as FSG_g first generates all frequent subgraphs S_{fre} whose support are no less than sup_{min}, instead of all subgraphs. It then adopts the same greedy strategy as ALL_g to find top-k edge-diversified patterns.

3.1 Baseline Solution ALL_g

By adopting greedy search, we come up with the first baseline solution ALL_g, whose pseudo-code is shown in Algorithm 1. Given a graph database $D = \{G_1, G_2, ...G_n\}$ and an integer k, it first enumerates all subgraphs $S = \{s_1, s_2, ...\}$ from D such that $|E(s_i)| \leq E_{max}$ (Line 1), by using an existing subgraph enumeration method [2–6]. Then, MaxCover is invoked to generate top-k edge-diversified patterns (Line 2). MaxCover follows a iterative procedure (Lines 6-8). In each iteration, it greedily selects a pattern p from S such that the cover set of p contains a maximum number of uncovered edges, *i.e.,* $|Cov(p', D) \setminus Cov(\mathcal{P}, D)|$ (Line 7). Once the resulting pattern p is selected, it will be removed from S to pattern set $\mathcal{P}$ (Line 8).

Algorithm 1 Baseline solution ALL_g

Input: graph database $D = \{G_1, G_2, ...G_n\}$, integer k, and E_{max}
Output: Near-optimal top-k edge-diversified patterns
1: $S \leftarrow$ EnumAllSub(D, E_{max})
2: $\mathcal{P} \leftarrow$ MaxCover(S, k) ▷ call procedure MaxCover
3: **return** $\mathcal{P}$
4: **procedure** MaxCover(S, k)
5: $\quad\mathcal{P} \leftarrow \phi$
6: $\quad$**for** iter = 1 to k **do**
7: $\quad\quad p \leftarrow argmax_{p' \in S} |Cov(p', D) \setminus Cov(\mathcal{P}, D)|$
8: $\quad\quad \mathcal{P} \leftarrow \mathcal{P} \cup \{p\}, S \leftarrow S \setminus p$
9: $\quad$**return** $\mathcal{P}$

Algorithm 2 Baseline solution FSG_g

Input: graph database $D = \{G_1, G_2, ...G_n\}$, integer k, and E_{max}
Output: Heuristic top-k edge-diversified patterns
1: $S_{fre} \leftarrow$ EnumFreSub(D, E_{max})
2: $\mathcal{P} \leftarrow$ MaxCover(S_{fre}, k) ▷ MaxCover in Algorithm 1
3: **return** $\mathcal{P}$

Observe that MaxCover follows the same greedy strategy used for solving the max k-cover problem [22]. Therefore, it can achieve an approximation ratio of $1 - \exp(-1)$.

Lemma 1. *Worst case time and space complexities of* ALL_g *are* $O(|D|2^{max(V(G))^2} + k|S||D|max(V(G))^{E_{max}})$ *and* $O(max(E(G))|D| + E_{max}|S|)$, *respectively, where* $max(V(G))$ *(resp.* $max(E(G))$*) is maximum number of vertices (resp. edges) in graph* $G \in D$, *and* $|D|$ *(resp.* $|S|$*) is number of graphs in* D *(resp.* S*).*

3.2 Baseline Solution FSG_g

Note that ALL_g requires searching all subgraphs which may incur large computational overload. To address this, we further propose the second baseline solution FSG_g, whose procedure is shown in Algorithm 2. Instead of enumerating all subgraphs from graph database D, FSG_g first adopts frequent subgraph mining methods [7–12] to generate frequent subgraphs S_{fre} (Line 1). Then MaxCover in Algorithm 1 is invoked to find a pattern set on S_{fre} (Line 2).

Since only frequent subgraphs instead of all subgraphs are selected from the underlying database for generating final patterns, the computational cost of FSG_g is thus reduced.

Lemma 2. *Worst case time and space complexities of* FSG_g *are* $O(|D|2^{max(V(G))^2} + k|S_{fre}||D|max(V(G))^{E_{max}})$ *and* $O(max(E(G))|D| + E_{max}|S_{fre}|)$, *respectively, where* $max(V(G))$ *(resp.* $max(E(G))$*) is maximum number of vertices (resp. edges) in graph* $G \in D$, *and* $|D|$ *(resp.* $|S_{fre}|$*) is number of graphs in* D *(resp.* S_{fre}*).*

3.3 Limitations of Baseline Solutions

Observe that ALL_g provides an approximation ratio of $1 - \exp(-1)$ for final patterns, but it is computationally challenging. Compared to ALL_g, FSG_g significantly reduces the computational cost by selecting frequent subgraphs, based on which the final patterns are derived. However, the pattern quality is not guaranteed since no approximation bound can be provided as only frequent subgraphs are considered. Moreover, they suffer from the following problems:

(1) *Excessive memory consumption.* Both ALL_g and FSG_g need to store all subgraphs or a subset of all subgraphs in memory. However, the number of subgraphs in a graph database is exponential in database size. As a graph database continues to grow rapidly in size, storing those subgraphs in memory will lead to excessive

memory consumption. As will be shown in Section 8 (Fig. 13, Exp 2), even the subgraphs of 5,000 graphs in PubChem database are not easy to be kept in memory.

(2) *A mass of unnecessary computations.* Since the (frequent) subgraph enumeration and MaxCover procedure are performed sequentially, all (frequent) subgraphs, no matter whether they can improve the total coverage of final patterns $\mathcal{P}$, are computed and stored before invoking MaxCover procedure. Therefore, there are a mass of unnecessary computations.

4 TED: A NOVEL FRAMEWORK

To address aforementioned limitations, we propose a novel framework called Ted (*i.e.,* Top-k Edge-Diversified patterns discovery). The main idea is to integrate the search process for top-k patterns into subgraph enumeration. Specifically, it maintains only k candidate patterns $\mathcal{P}$ in memory. These candidates are supposed to potentially maximize the total coverage. When a new subgraph g is enumerated and considered as a *promising candidate* (see Sec. 4.1), it will be added to $\mathcal{P}$ by swapping out one of the patterns. Compare to the above two baseline solutions, Ted has the following advantages:

(i) *Limited memory consumption.* Ted always maintains only k patterns in memory to avoid excessive memory consumption for storing all subgraphs. As can be seen in Theorem 2, the space complexity of Ted is $O(max(E(G))|D|)$ which is far less than that of all$_g$ ($O(max(E(G))|D| + E_{max}|S|)$, Lemma 1) and fsg$_g$ ($O(max(E(G))\ |D| + E_{max}|S_{fre}|)$, Lemma 2).

(ii) *Guaranteed pattern quality.* Ted can achieve an approximation bound of 1/4 and better performance in experimental study. To this end, it provides a swapping criteria such that each newly generated subgraph g is deliberately swapped with one existing pattern in $\mathcal{P}$.

(iii) *Effective pruning strategies.* Ted is able to prune subgraph search space by integrating the search process for top-k patterns into subgraph enumeration.

(iv) *Desirable scalability.* Ted and its lightweight version, namely TedLite, are capable of handling large databases.

In what follows, we begin with a basic Ted algorithm (denoted by Ted_base) in this section, which can achieve both (i) and (ii). Then, three optimization strategies are developed to further realize (iii) (Section 5). Finally, we present TedLite, which is a lightweight version of Ted and able to accomplish (iv) (Section 6).

4.1 The Basic Ted Algorithm

The basic Ted algorithm (Ted_base) generates top-k edge-diversified patterns by alternately performing subgraph enumeration and a search process for top-k patterns. For subgraph enumeration, it adopts a depth-first search (dfs) strategy to traverse the search space. For example, $g_{1,1}, g_{2,1}, g_{3,1}$, and $g_{4,1}$ in Figure 5 are traversed sequentially. Although Apriori-like approaches [7, 8] that adopt breadth-first search (bfs) strategy have been widely studied, they require generating a lot of duplicated candidates and testing subgraph isomorphism. In contrast, depth-first search (dfs) combines the pattern generating and isomorphism checking into one process to address this problem. For top-k pattern search on the enumerated subgraphs, a swapping-based strategy is adopted for maintaining patterns with limited memory consumption.

Algorithm 3 A basic Ted algorithm (Ted_base)

Input: graph database $D = \{G_1, G_2, ...G_n\}$, integer k, and E_{max}
Output: Near-optimal top-k edge-diversified patterns
1: $\mathcal{P} \leftarrow \phi$
2: $S_p \leftarrow$ EnumSub$(D, |E| = 1)$
3: **for** each $g \in S_p$ **do**
4: $\quad S_p \leftarrow S_p \setminus g$
5: $\quad \mathcal{P} \leftarrow$ PatternMaintain$(\mathcal{P}, g, D)$
6: $\quad \mathcal{P}_g \leftarrow$ RightMostExtend(g, D, E_{max})
7: $\quad S_p \leftarrow \mathcal{P} \cup \mathcal{P}_g$
8: **procedure** PatternMaintain$(\mathcal{P}, g, D)$
9: $\quad$ **if** $|\mathcal{P}| < k$ **then**
10: $\quad\quad \mathcal{P} \leftarrow \mathcal{P} \cup \{g\}$
11: $\quad\quad$ **return** $\mathcal{P}$
12: $\quad$ Score$_L, p_t \leftarrow$ min(genLossScore$(\mathcal{P})$)
13: $\quad$ Score$_B \leftarrow$ genBenefitScore(g)
14: $\quad$ **if** Score$_B > (1+\alpha)$Score$_L + \frac{(1-\alpha)|Cov(\mathcal{P},D)|}{k}$ **then**
15: $\quad\quad \mathcal{P} \leftarrow \mathcal{P} \setminus p_t \cup \{g\}$
16: $\quad$ **return** $\mathcal{P}$

Ted_base is outlined in Algorithm 3. Given a graph database $D = \{G_1, G_2, ...G_n\}$ and an integer k, it first enumerates all 1-sized subgraphs (*i.e.,* edges) and appends them into the set S_p (Line 2). Then, an iterative process (Lines 3-7) is performed to generate final patterns $\mathcal{P}$ by taking S_p and D as inputs. Specifically, each subgraph $g \in S_p$ is first considered and removed from S_p (Lines 3-4). Then, the procedure PatternMaintain is performed to update top-k edge-diversified patterns $\mathcal{P}$ with newly enumerated subgraph g (Line 5). After that, the right-most extension method (Procedure RightMostExtend) extends each subgraph $g \in S_p$ with one more edge (Line 6) so that its supergraphs will be considered in the next iteration. The process repeats until S_p is empty. More details about the two main procedures, PatternMaintain and RightMostExtend, are discussed below.

4.1.1 Pattern Maintenance (PatternMaintain). As discussed above (Section 3), the max k-cover problem is a subproblem of top-k edge-diversified patterns discovery. However, greedy-search based solutions typically find entire subgraphs and store them in memory and hence cannot be effectively exploited for large databases. To address this, PatternMaintain maintains only k patterns in memory with a swapping-based method motivated by existing maximum coverage solver in the context of streaming scenario [23–25]. We first introduce the concepts of *loss score* and *benefit score* below to facilitate exposition.

Definition 4 (**Loss score**). Given a pattern set $\mathcal{P}$ and a database D, the **loss score** of a pattern $p \in \mathcal{P}$ is the decrease of total coverage caused by removing p from $\mathcal{P}$, i.e.,

$$\text{Score}_L(p, \mathcal{P}, D) = |\cup_{p\in\mathcal{P}} Cov(p, D) \setminus \cup_{p'\in\mathcal{P}\setminus p} Cov(p', D)|.$$

Definition 5 (**Benefit score**). Given a pattern set $\mathcal{P}$ and a database D, the **benefit score** of a pattern $g \notin \mathcal{P}$ is the increase of total coverage caused by adding g to $\mathcal{P}$, i.e.,

$$\text{Score}_B(g, \mathcal{P}, D) = |\cup_{p'\in\mathcal{P}\cup\{g\}} Cov(p', D) \setminus \cup_{p\in\mathcal{P}} Cov(p, D)|.$$

PatternMaintain first greedily selects k patterns into the pattern set $\mathcal{P}$ (Lines 9-11, Algorithm 3). When a new subgraph g is generated, a swapping-based process is developed to determine if g should be swapped into $\mathcal{P}$ (Lines 12-15). Specifically, it first calculates and ranks loss scores for each pattern $p \in \mathcal{P}$, and then records the pattern p_t and its pattern score Score$_L$ such that p_t has a minimum loss score (Line 12). Meanwhile, the benefit score

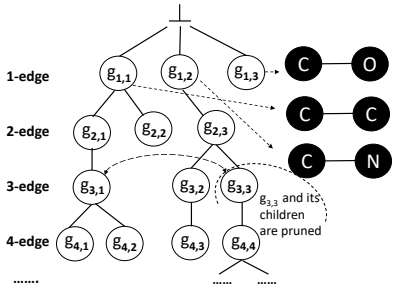


Figure 5: The DFS search space.

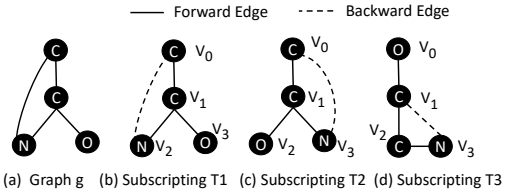


Figure 6: A graph G (a) and its subscriptings (b-d).

SCORE_B of g is also recorded (Line 13). The subgraph g is considered as a **promising candidate** and swapped into $\mathcal{P}$ (Lines 14-15) if the following *swapping criteria* is satisfied:

$$\text{SCORE}_B > (1+\alpha)\text{SCORE}_L + (1-\alpha)|Cov(\mathcal{P}, D)|/k \quad (1)$$

where $\alpha \in [0, 1]$ is a *swapping threshold* for balancing the loss score SCORE_L and average coverage of patterns in $\mathcal{P}$ (*i.e.,* $|Cov(\mathcal{P}, D)|/k$). Note that there are three variants of the swapping criteria, namely, $Swap_1$ [23], $Swap_2$ [24], and $Swap_\alpha$ [25] where $\alpha = 1$, $\alpha = 0$, and $\alpha \in (0, 1)$, respectively. By default, we set $\alpha = 1$ and compare it with other variants in Section 8. The pattern p_t is swapped out once g is swapped in. The pattern set $\mathcal{P}$ is hence updated (Line 15).

4.1.2 Right-Most Extension (RIGHTMOSTEXTEND). TED_BASE adopts a depth-first search (DFS) strategy to enumerate all possible subgraphs by iteratively performing right-most extension (*i.e.,* RIGHTMOSTEXTEND). Figure 5 outlines the DFS search space, where each node represents an m-edge graph (denoted by $g_{m,i}$, *i.e., i*-th graph with m edges). Each link between two nodes represents a possible right-most extension, *i.e.,* a desirable way to extend m-edge graph to $(m+1)$-graph, which is first proposed in gSpan [10]. For example, $g_{1,1}, g_{2,1}, g_{3,1}$, and $g_{4,1}$ in Figure 5 are traversed sequentially. $g_{4,1}$ is a right-most extension of $g_{3,1}$. We begin with the DFS subscripting technique for encoding a graph to illustrate right-most extension.

DFS Subscripting. Given a graph g, we can perform DFS on it and generate the corresponding DFS trees. For example, for graph g in Figure 6(a), there are at least three DFS trees as the solid lines show in Figure 6(b)-(d). The subscript of each vertex in a DFS tree is sequentially built in the process of DFS traversal. That is, V_i is visited before V_j if $i < j$. As a result, each DFS tree T can be represented as vertices sequence. The DFS tree for Figure 6(b) is (V_0, V_1, V_2, V_3). The graph g subscripted with a DFS tree T is denoted by g_T and hence T is named a DFS subscripting of g. Given g_T, *root vertex* is the first visited vertex (*i.e.,* V_0) and *right-most vertex* is the last visited vertex (*i.e.,* $V_{|V(g)|-1}$). The *right-most path* is then defined as the straight path from root vertex to right-most vertex. For example, Figure 6(b)-(d) present three DFS subscriptings whose root vertices are all V_0 and right-most vertices are V_3. The right-most path for Figure 6(b) (resp. (c)) and (d) are (V_0, V_1, V_3) and (V_0, V_1, V_2, V_3), respectively.

Moreover, the *forward edge* contains all edges in the DFS tree T (denoted by E_T^f). The *backward edge* consists of all other edges (denoted by E_T^b). It is obvious that $(V_i, V_j) \in E_T^f$ if $i < j$, and $(V_i, V_j) \in E_T^b$ otherwise. In Figure 6(b), (V_0, V_1) and (V_2, V_0) are a forward edge and backward edge, respectively.

Right-Most Extension. The straightforward method for extending an m-edge graph to an $(m+1)$-edge graph is to add a new edge to any position of the m-edge graph. It is inefficient since there are m positions for extending which will incur a lot of duplicated graphs. Right-most extension is an efficient method to extend a graph with one more edge by restricting the extension positions.

DEFINITION 6 (**RIGHT-MOST EXTENSION**). Given an m-edge graph g and a DFS tree T, right-most extension is to extend g to an $(m+1)$-edge graph g' with an edge e such that at least one of the following rules is satisfied: 1) *forward extension. e* is extended from vertices on the right-most path such that an additional vertex is introduced and 2) *backward extension. e* is extended from right-most vertex to other vertices on the right-most path.

For example, given the graph g in Figure 6(a) and the DFS tree T in Figure 6(b), the forward extension of an edge e can be edges extending from either V_0, V_1 or V_3 to a newly introduced vertex. The backward extension should be (V_3, V_0). Since each graph has various subscriptings which will cause multiple extensions, the subscripting with minimum lexicographic order is selected as base subscripting for extending [10]. As a result, the node (*e.g.,* $g_{3,3}$ in Figure 5) and its descendants in the search space are pruned if the subscripted graph in the node has non-minimum subscripting.

Remark. The completeness of results generated by right-most extension is guaranteed [10]. As will be seen later (THEOREM 4), the quality of final patterns (*i.e.,* coverage) is theoretically guaranteed.

4.2 Fast Pattern Maintenance

A naive method for computing loss score (Line 12, Algorithm 3) and benefit score (Line 13, Algorithm 3) is to directly calculate cover set $Cov(\cdot)$ according to their definitions, which is obviously inefficient. In this section, we propose the FASTMAINTAIN algorithm (Algorithm 4) to facilitate fast pattern maintenance. To begin with, the Private-Edge-Set Index (denoted by PES-Index) is developed to accelerate loss score and benefit score computation. PES-Index consists of five components:

- $|Cov(\mathcal{P})|$: total coverage of $\mathcal{P}$ over D (*i.e.,* $|Cov(\mathcal{P}, D)|$).
- $|pCov(p)|$: *private coverage* of p. $pCov(p)$ is the set of edges in D, which is in the cover set of p but not in the cover set of $p' \in \mathcal{P} \setminus p$, *i.e.,* $pCov(p) = Cov(p, D) \setminus Cov(\mathcal{P} \setminus p, D)$.
- $rCov(e)$: *reverse cover set* of an edge e. It refers to a subset of patterns that contain e in the cover set. That is, $rCov(e) = \{p | p \in \mathcal{P}, e \in Cov(p, D)\}$.
- $rCnt(i)$: *reverse counting set* of number of edges. It refers to a set of patterns such that each pattern p's private coverage is i. That is, $rCnt(i) = \{p | p \in \mathcal{P}, |pCov(p)| = i\}$ where $i \in [0, \sum_{G \in D} |E(G)|]$.
- p_{min}: the pattern $p \in \mathcal{P}$ with minimum private coverage $|pCov(p)|$.

Moreover, four operations, INSERT, DELETE, UPDATE and SELECT, are developed on PES-Index. Specifically, INSERT operation is to insert a newly enumerated subgraph into current pattern set and update PES-Index; DELETE aims to remove a pattern from current pattern set and update PES-Index; UPDATE is a combination operation that sequentially calls DELETE and INSERT operations; SELECT supports fast computations for loss score and benefit score.

Given a graph database D, a pattern set $\mathcal{P}$ and each enumerated graph g, if the number of existing patterns is less than k, INSERT operation is performed to update $\mathcal{P}$ (Line 1, Algorithm 4), and g is directly inserted into $\mathcal{P}$ (Line 8). For each edge e covered by g (*i.e.,* $e \in Cov(g, D)$), its reverse cover set is updated by adding g (Lines 9-10). If its reverse cover set only contains g (*i.e.,* $|rCov(e)|$==1), it indicts that e is only covered by g. Hence, both g's private coverage $|pCov(g)|$ and the total coverage $Cov(\mathcal{P})$ increase by 1 (Line 12). If its reverse cover set contains another pattern p, the private coverage of p (*i.e.,* $|pCov(p)|$) should be decreased by 1 since e is also covered by g (Line 14). Once $|pCov(p)|$ is updated, the reverse counting set $rCnt(i)$ is updated by moving p from $rCnt(|pCov(p)|+1)$ to $rCnt(|pCov(p)|)$ (Line 15). The process repeats until all $e \in Cov(g, D)$ are considered. Then, $rCnt(|pCov(g)|)$ is also updated (Line 16). Based on all computed $rCnt(i)$, we can directly figure out which pattern has minimum loss score by selecting one pattern p_{min} in $rCnt(i) \neq \phi$ such that i is minimum (Line 17). With the constructed PES-Index, the minimum loss score (*i.e.,* SCORE_L) and the corresponding pattern (*i.e.,* p_t) can be easily obtained ($\text{SCORE}_L = |pCov(p_{min})|$ and $p_t = p_{min}$, Lines 2 and 27). The benefit score SCORE_B is calculated by counting the cases where the reverse cover set $|rCov(e)|$ of $e \in Cov(g, D)$ is 0 (Lines 3 and 28), as $|rCov(e)| = 0$ indicates that e is not covered by existing patterns.

If the swapping criterion is satisfied (Line 4), the UPDATE operation is performed by sequentially calling DELETE operation for p_t and INSERT operation for g (Line 5). Firstly, p_t is directly removed from $\mathcal{P}$ and $rCnt(|pCov(p_t)|)$ (Line 19). For each edge $e \in Cov(p_t, D)$, the corresponding $rCov(e)$ should be maintained by removing p_t, and the total coverage should be decreased by 1 if $|rCov(e)|$ is 0 (Lines 20-22). In addition, if the $|rCov(e)|$ of e contains only one pattern p, the $|pCov(p)|$ should be increased by 1, and the reverse counting set $rCnt(i)$ should be updated by moving p from $rCnt(|pCov(p)|-1)$ to $rCnt(|pCov(p)|)$ (Lines 23-25).

Remark. Note that PES-Index is motivated by the existing PNP-Index [46], which was designed for diversified top-k clique search. The main difference lies in that PNP-Index is to build the relationship between the enumerated clique and the vertices in a single large data graph. Each clique is exactly one matching in the data graph and only the vertices in the matching are indexed. In contrast, PES-Index aims to index the cover set (*i.e.,* a set of edges) of a particular edge-diversified pattern over a graph database containing a set of graphs. Each pattern here has multiple matchings in a graph.

EXAMPLE 4. *Let $\alpha = 1$, $k = 3$, and the current pattern set $\mathcal{P} = \{g_1, p_1, p_3\}$ where g_1 and p_1 (resp. p_3) are shown in Figure 2(a) and Figure 4, respectively. $|pCov(g_1)|$, $|pCov(p_1)|$ and $|pCov(p_3)|$ are 2, 10, and 8, respectively, where $pCov(g_1) = \{G_3 : e_2, e_6\}$ (*i.e.,* e_2 and e_6 of G_3). In addition, $|Cov(\mathcal{P})| = 33$ and $rCnt(2) = \{g_1\} \neq \phi$. Hence, $p_t = g_1$ and the minimum loss score $\text{SCORE}_L = |pCov(g_1)| = 2$. When the graph p_2 (Figure 4) is newly enumerated, its benefit score $\text{SCORE}_B = 7$, as $Cov(p_2, D) = \{G3 : e_3, e_4, e_7, e_9 - e_{12}\}$ and $|\{e|e \in Cov(p_2, D)$ and $|rCov(e)| == 0\}| = 7$. Since $\text{SCORE}_B > (1+\alpha)\text{SCORE}_L = 4$, g_1 should be removed from $\mathcal{P}$ and then $|Cov(\mathcal{P})| = 31$. In addition, p_2 should be added into $\mathcal{P}$,* i.e., *$\mathcal{P} = \{p_1, p_2, p_3\}$. The total coverage is $|Cov(\mathcal{P})| = 38$ as shown in Figure 4.* ∎

Algorithm 4 Fast pattern maintenance (FASTMAINTAIN)

Input: Graph database $D = \{G_1, G_2, ...G_n\}$, existing patterns $\mathcal{P}$, graph g
Output: Updated patterns

```
1: if |P| < k, P ← INSERT(g), return P
2: SCORE_L, p_t ← SELECT(g, true)
3: SCORE_B ← SELECT(g, false)
4: if SCORE_B > (1+α)SCORE_L + ((1−α)|Cov(P)|)/k then
5:     P ← UPDATE(p_t, g)
6: return P
7: procedure INSERT(g)
8:     P ← P ∪ {g}
9:     for e ∈ Cov(g, D) do
10:        rCov(e) ← rCov(e) ∪ {g}
11:        if |rCov(e)|==1 then
12:            |pCov(g)| ← |pCov(g)| + 1; |Cov(P)| ← |Cov(P)| + 1
13:        if |rCov(e)|==2 then
14:            for p ∈ rCov(e) \ g, |pCov(p)| ← |pCov(p)| − 1
15:            move p from rCnt(|pCov(p)| + 1) to rCnt(|pCov(p)|)
16:    rCnt(|pCov(g)|) ← rCnt(|pCov(g)|) ∪ {g}
17:    p_min ← a pattern in rCnt(i) ≠ φ s.t. i is minimum.
18: procedure DELETE(p_t)
19:    remove p_t from P and rCnt(|pCov(p_t)|)
20:    for e ∈ Cov(p_t, D) do
21:        rCov(e) ← rCov(e) \ p_t
22:        |Cov(P)| ← |Cov(P)| − 1, if |rCov(e)|==0
23:        if |rCov(e)|==1 then
24:            for p ∈ rCov(e), |pCov(p)| ← |pCov(p)| + 1
25:            move p from rCnt(|pCov(p)| − 1) to rCnt(|pCov(p)|)
26: procedure SELECT(g, flag)
27:    if flag is true, return |pCov(p_min)|, p_min
28:    else return |{e|e ∈ Cov(g, D) and |rCov(e)| == 0}|
```

THEOREM 2. *Worst case time and space complexities of TED_BASE are $O(|D|2^{max(V(G))^2})$ and $O(max(E(G))|D|)$, respectively, where $max(V(G))$ (resp. $max(E(G))$) is maximum number of vertices (resp. edges) in graph $G \in D$, and $|D|$ is number of graphs in D.*

5 OPTIMIZATIONS

Recall that TED_BASE integrates the search process for top-k patterns into subgraph enumeration, which guarantees the pattern quality with limited memory consumption. However, it does not explore the potential of reducing the search space and unnecessary computations to boost the overall effectiveness. Therefore, in this section, we further propose three optimization strategies, namely, *Dynamic Support Setting* in Section 5.1, *Promising Right-Most Extension* in Section 5.2, and *Initial Pattern Selection* in Section 5.3. In short, *Dynamic Support Setting* directly filters unpromising patterns with lower support. While *Promising Right-Most Extension* prunes these unpromising patterns based on the covering relationship of a graph and its descendants instead of support. *Initial Pattern Selection* targets on promoting the quality of initial patterns so that better pruning power is introduced in the early stage.

5.1 Dynamic Support Setting

Observe that edge-diversified patterns may not be frequent as illustrated in Section 1. Therefore, for the sake of completeness of final results, TED_BASE considered each subgraph g even it is contained by only one graph $G \in D$. Hence, the search space is huge. Fortunately, we have the following observation:

Algorithm 5 An improved TED algorithm (TED_DSS)

Input: graph database $D = \{G_1, G_2, ...G_n\}$, integer k, and E_{max}
Output: Near-optimal top-k edge-diversified patterns
1: $\mathcal{P} \leftarrow \phi$
2: $S_p \leftarrow$ EnumSub$(D, |E| = 1)$
3: **for** each $g \in S_p$ **do**
4: $S_p \leftarrow S_p \setminus g$
5: **if** dss$(\mathcal{P})$ > count(g) **then**
6: continue
7: $\mathcal{P} \leftarrow$ PatternMaintain$(\mathcal{P}, g, D)$
8: $\mathcal{P}_g \leftarrow$ RightMostExtend(g, D, E_{max})
9: $S_p \leftarrow \mathcal{P} \cup \mathcal{P}_g$

Observation I. *The search space will be significantly reduced as the minimum support (sup_{min}) increases.*

The intuition behind the observation is that the support has anti-monotone property, *i.e.,* the support of a graph never exceeds that of its subgraphs. Therefore, if a graph with low support is definitely not a promising pattern, all descendants of this graph are filtered out. Motivated by this observation, *Dynamic Support Setting* (DSS) is developed. Specifically, it dynamically sets the value for minimum support sup_{min} to filter some unpromising subgraphs as necessary without sacrificing the completeness of the results. Let count(g) be the number of graphs in D containing g, DSS adopts an iterative process to set minimum support: (1) Set a counter $cnt = 1$. (2) If count$(g) = cnt$, the benefit score of g is no more than the maximum number of un-covered edges in cnt graphs, *i.e.,* $\max|\bigcup_{i\in\mathbb{I}}(E(G_i) \setminus Cov(\mathcal{P}, G_i))|$ where $\mathbb{I} \subseteq [1, |D|]$ and $|\mathbb{I}| = cnt$. If $\max|\bigcup_{i\in\mathbb{I}}(E(G_i) \setminus Cov(\mathcal{P}, G_i))|$ is less than $(1+\alpha)$Score$_L$ + $(1-\alpha)|Cov(\mathcal{P}, D)|/k$ (*i.e., g* is unpromising), $cnt = cnt + 1$, go to step (2). Go to step (3), otherwise. (3) Set minimum support $sup_{min} = cnt/|D|$.

Note that $\max|\bigcup_{i\in\mathbb{I}}(E(G_i) \setminus Cov(\mathcal{P}, G_i))|$ can be easily computed by selecting the first $|\mathbb{I}|$ values from a priority queue, where $|E(G_i) \setminus Cov(\mathcal{P}, G_i)|$ is in descending order. As such, DSS can be used to prune unpromising subgraphs by checking support only.

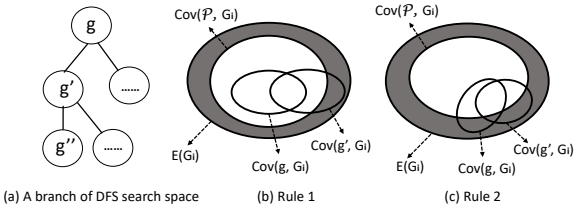
Based on DSS, an improved TED algorithm called TED_DSS, as shown in Algorithm 5, is developed. The difference between TED_DSS and TED_BASE lies in lines 5 and 6 where DSS strategy is introduced. That is, if count(g) is less than dss$(\mathcal{P})$, *i.e.,* the product of minimum support sup_{min} and $|D|$, g is deemed as unpromising and will not be taken into account by pattern maintenance process.

5.2 Promising Right-Most Extension

Recall that in TED_BASE and TED_DSS, graphs are enumerated with right-most extension. As shown in Figure 7(a), an m-edge graph g is extended to an $(m+1)$-edge graph g'. Then, g' is extended to an $(m+2)$-edge graph g''. It is obvious they discard the relationship (see Observation II) between a subgraph and its descendants (*i.e.,* supergraphs).

Observation II. *The benefit score of a subgraph g' over graph G_i is at most the number of uncovered edges in G_i, and the edges in a graph G_i covered by g but not covered by g' will not be covered by g''* (i.e., *a descendant of g'*).

Motivated by this observation, *Promising Right-Most Extension* (PRM) is developed by taking a prudent strategy to extend g to g' (and descendants of g', *e.g.,* g''). Specifically, PRM extends g to g' if and only if one of the following PRM rules is satisfied.



(a) A branch of DFS search space (b) Rule 1 (c) Rule 2

Figure 7: Illustration for PRM.

Algorithm 6 An improved TED algorithm (TED_PRM)

Input: graph database $D = \{G_1, G_2, ...G_n\}$, integer k, and E_{max}
Output: Near-optimal top-k edge-diversified patterns
1: $\mathcal{P} \leftarrow \phi$
2: $S_p \leftarrow$ EnumSub$(D, |E| = 1)$
3: **for** each $g \in S_p$ **do**
4: $S_p \leftarrow S_p \setminus g$
5: $\mathcal{P} \leftarrow$ PatternMaintain$(\mathcal{P}, g, D)$
6: $\mathcal{P}_g \leftarrow$ RightMostExtend(g, D, E_{max})
7: **for** $g' \in \mathcal{P}_g$ **do**
8: **if** prm$(g, g') < (1+\alpha)$Score$_L + \frac{(1-\alpha)|Cov(\mathcal{P},D)|}{k}$ **then**
9: $\mathcal{P}_g \leftarrow \mathcal{P}_g \setminus g'$
10: $S_p \leftarrow \mathcal{P} \cup \mathcal{P}_g$

Definition 7 (**PRM Rules**). *1) Rule 1.* If $g \in \mathcal{P}$, g' extends from g with one edge if $|\cup_{i\in\mathbb{I}}(E(G_i) \setminus Cov(\mathcal{P}, G_i))| \geq (1+\alpha)$Score$_L$ + $(1-\alpha)|Cov(\mathcal{P}, D)|/k$, where $\mathbb{I}$ is the id set of graphs containing g. *2) Rule 2.* If $g \notin \mathcal{P}$, g' extends from g with one edge if $|\cup_{i\in\mathbb{I}}(E(G_i) \setminus (Cov(\mathcal{P}, G_i) \cup (Cov(g, G_i) \setminus Cov(g', G_i))))| \geq (1+\alpha)$Score$_L + (1-\alpha)|Cov(\mathcal{P}, D)|/k$.

Intuitively, PRM rules is a formal explanation of Observation II. Its correctness is guaranteed by the following Theorem 3.

Theorem 3. *Right-most extension with PRM rules has no effect on the quality (*i.e., *coverage) of final patterns.*

Owing to the pruning power of PRM rules, we propose an improved TED algorithm called TED_PRM, as shown in Algorithm 6, by introducing PRM into TED_BASE (Lines 7-9). Specifically, given an m-edge graph g and its all potential $(m+1)$-edge supergraphs $\mathcal{P}_g$, for each $g' \in \mathcal{P}_g$, if g' does not satisfy PRM rules (Line 8), g' will be removed from $\mathcal{P}_g$ for further processing. Note that PRM process (Lines 7-9) can be integrated with RightMostExtend (Line 6), both of them are individually listed here for ease of presentation.

5.3 Initial Pattern Selection

As discussed in Section 4.1, the initial k patterns are selected by traversing the search space in *DFS* manner (Lines 6, Algorithm 3). For example, suppose the search space is shown in Figure 5 and $k = 3$, the initial k patterns are $g_{1,1}$, $g_{2,1}$, and $g_{3,1}$. Observe that all of them contain the same substructure (*i.e.,* $g_{1,1}$), they may cover the same edges in D. Therefore, the minimum loss score Score$_L$ may get small, so that the swapping criterion is easily satisfied (Line 14, Algorithm 3). Although the swapping criterion is satisfied and a pattern g is hence swapped in, the pattern quality may be very low so that g will be swapped out finally. Obviously, frequently swapping patterns does harm to algorithm performance. To address this problem, we develop *Initial Pattern Selection* (IPS) technique motivated by the following observation.

Algorithm 7 An improved TED algorithm (TED_IPS)

Input: graph database $D = \{G_1, G_2, ...G_n\}$, integer k, and E_{max}
Output: Near-optimal top-k edge-diversified patterns
1: $\mathcal{P} \leftarrow$ IPS(D, k)
2: $S_p \leftarrow$ EnumSub$(D, |E| = 1)$
3: **for** each $g \in S_p$ **do**
4: $S_p \leftarrow S_p \setminus g$
5: $\mathcal{P} \leftarrow$ PatternMaintain$(\mathcal{P}, g, D)$
6: $\mathcal{P}_g \leftarrow$ RightMostExtend(g, D, E_{max})
7: $S_p \leftarrow \mathcal{P} \cup \mathcal{P}_g$

Observation III. *The initial k patterns generated by traversing the search space in DFS manner share common substructure and lead to low loss score. While patterns generated with Breadth-First Search* (i.e., *BFS) on the search space tend to be structurally dissimlar to each other and may imply higher loss score.*

Specifically, IPS starts at the first node in first level (*e.g.,* $g_{1,1}$, Figure 5) of the search space. Then, it explores descendant nodes in second level (*e.g.,* $g_{2,1}$) if the extended graph (*e.g.,* $g_{2,1}$) has higher benefit score. The process repeats until no higher benefit score is obtained or the desirable number of edges (*i.e.,* E_{max}) is derived. As a result, the first pattern is obtained. After that, IPS adopts the same technique to generate patterns rooted at the other nodes in first level (*e.g.,* $g_{1,2}$ and $g_{1,3}$, Figure 5). Once all patterns rooted at nodes in first level are generated, the top-k patterns with maximum coverage are selected as initial pattern set.

The improved TED algorithm with IPS (denoted by TED_IPS) is developed as Algorithm 7. The only difference between TED_IPS and TED_BASE lies in line 1 where IPS strategy is introduced.

5.4 Putting Things Together

Algorithm 8 outlines the complete TED algorithm where all three optimizations are integrated. Specifically, IPS (Line 1) is introduced to improve the initial loss score. Then, DSS (Lines 5 and 6) utilizes minimum support to quickly prune unpromising patterns. Finally, PRM takes a prudent strategy to enumerate potential promising subgraphs (Lines 9-11). Theorem 4 ensures that the approximation ratio of our TED algorithm is lower bounded by 1/4.

Algorithm 8 TED algorithm (TED)

Input: graph database $D = \{G_1, G_2, ...G_n\}$, integer k, and E_{max}
Output: Near-optimal top-k edge-diversified patterns
1: $\mathcal{P} \leftarrow$ IPS(D, k)
2: $S_p \leftarrow$ EnumSub$(D, |E| = 1)$
3: **for** each $g \in S_p$ **do**
4: $S_p \leftarrow S_p \setminus g$
5: **if** DSS$(\mathcal{P})$ > COUNT(g) **then**
6: CONTINUE
7: $\mathcal{P} \leftarrow$ PatternMaintain$(\mathcal{P}, g, D)$
8: $\mathcal{P}_g \leftarrow$ RightMostExtend(g, D, E_{max})
9: **for** $g' \in \mathcal{P}_g$ **do**
10: **if** PRM(g, g') < $(1+\alpha)$Score$_L$ + $\frac{(1-\alpha)|Cov(\mathcal{P},D)|}{k}$ **then**
11: $\mathcal{P}_g \leftarrow \mathcal{P}_g \setminus g'$
12: $S_p \leftarrow \mathcal{P} \cup \mathcal{P}_g$

Theorem 4. *Let $\mathcal{P}_{opt}$ be an optimal solution to top-k edge-diversified patterns discovery problem. The approximation ratio of patterns $\mathcal{P}$ generated by TED (and TED_BASE) is bounded by* $\frac{|Cov(\mathcal{P},D)|}{|Cov(\mathcal{P}_{opt},D)|} \geq \frac{1}{4}$.

Theorem 5. *Worst case time and space complexities of TED are* $O(|D|2^{max(V(G))^2})$ *and* $O(max(E(G))|D|)$, *where* $max(V(G))$ *(resp.* $max(E(G))$*) is maximum number of vertices (resp. edges) in graph* $G \in D$, *and* $|D|$ *is number of graphs in* D.

Remark. We admit that the theoretical approximation ratio seems relatively low, but it is the (almost) best known bound for maximum coverage problem in the context of streaming scenarios [23–25]. In practice, we observe better performance (see Section 8.2). Due to the nature of this studied problem, the worst-case time complexity remains high as it is inevitable to enumerate all subgraphs in the worst case. Nevertheless, it heavily reduced the worst-case time complexity of baselines.

6 TEDLITE

Both subgraph enumeration on an entire database and top-k patterns search over all enumerated subgraphs can be computationally expensive for an even larger graph database D. To alleviate this problem, we develop a lightweight TED (denoted by TEDLITE). Intuitively, TEDLITE is to sample a subset of graphs D' from D and then perform TED algorithm on D'. The questions become: how to generate sample graphs and how many graphs should be sampled.

To answer the first question, TEDLITE adopts a random sampling method to sample $|D'|$ graphs from D. Intuitively, the sampled graphs D' are supposed to approximately keep graph property distribution (*e.g.,* label distribution) of original database D. To this end, it first represents each graph as a feature vector, where each entry indicates the frequency of a particular label. Then, graphs are grouped into several clusters by utilizing k-means clustering algorithm. As a result, graphs in each cluster are supposed to have similar label distribution. Therefore, TEDLITE randomly selects $|C_i'|$ graphs (denoted by C_i') from a cluster C_i where $|C_i'|$ should be directly proportional to the size of C_i, *i.e.,* $|C_i'| = |C_i||D'|/|D|$.

For the second question, the intuition of TEDLITE is to ensure that the absolute difference of edge frequency in D' and D are theoretically guaranteed. Formally, given the average edge number of graphs (denoted by $|E_{avg}|$) and an edge e, the absolute difference of its frequency in D' and D is $Dif_{abs} = |fr(e, D) - fr(e, D')|$ where $fr(\cdot)$ is a frequency. The following Theorem 6 shows how to determine a sample size $|D'|$.

Theorem 6. *Given an error bound ϵ and a maximum probability ρ for the absolute difference that exceeds ϵ, the size of the random sample* (i.e., $|D'|$) *is determined by* $|D'| \geq \frac{1}{2\epsilon^2|E_{avg}|} ln\frac{2}{\rho}$.

7 THE VISCENT SYSTEM

In this section, we employ the demonstration system VISCENT to illustrate the application potentials of edge-diversified patterns in visual subgraph query formulation and exploratory subgraph search. VISCENT is built on top of the first exploratory subgraph search framework [19]. Figure 8 shows the architecture of VISCENT, which consists of five modules, Index Constructor, Query Processor, Pattern Generator, Query Editor, and TED Explorer. In particular, Pattern Generator takes as input a graph database D and parameters (*e.g.,* k), and generates top-k edge-diversified patterns $\mathcal{P}_D$, which are displayed on the GUI (*e.g.,* Panel 5, Figure 9). Query Editor provides a canvas (*e.g.,* Panel 4, Figure 9) to users to visually formulate a query Q by dragging-and-dropping patterns $\mathcal{P}_D$

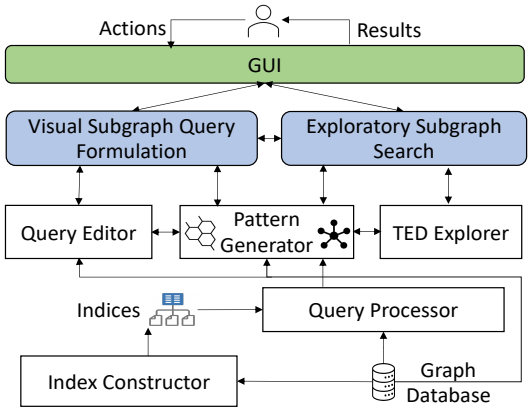


Figure 8: The architecture of VISCENT.

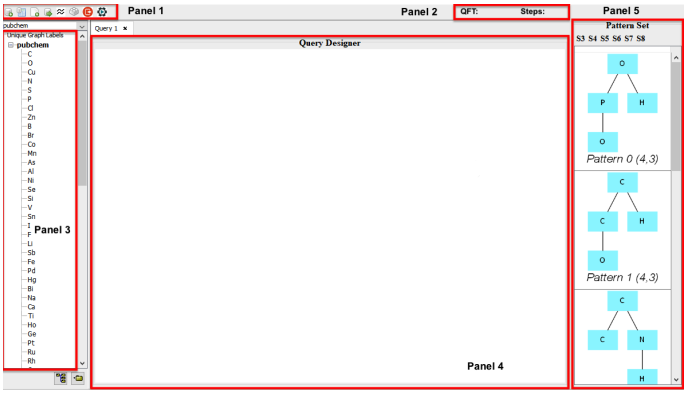


Figure 9: The interface of VISCENT.

and node labels in D (see Section 7.1). Once the query Q is formulated, Query Processor can efficiently process the query with the help of Index Constructor to generate subgraph matching results R. In particular, Query Processor performs subgraph isomorphism checking after Index Constructor filters out irrelevant results with A^2F and A^2I indices [47]. TED Explorer allows users to customize some parameters such as k, invokes Pattern Generator to generate edge-diversified patterns $\mathcal{P}_R$ for the query results R based on these parameters, and finally enables users to explore the summarized query results (*i.e.,* $\mathcal{P}_R$) (see Section 7.2). Based on these modules, the VISCENT system enables users to interactively experience visual subgraph query formulation and exploratory subgraph search, both of which are elaborated as below, with a focus on how edge-diversified patterns play a vital role in generating summary for the underlying database D (*i.e.,* patterns $\mathcal{P}_D$) and query results R (*i.e.,* patterns $\mathcal{P}_R$), respectively.

7.1 Visual Subgraph Query Formulation

Given a query Q and a set of data graphs D, subgraph search/query is to retrieve the data graphs $R = \{G_i\}$ where $G_i \in D$ contains Q (*i.e.,* Q is subgraph isomorphic to G_i). It consists of two steps. The first step is subgraph query formulation (*i.e.,* how to construct the query graph Q). The second step is subgraph query processing (*i.e.,* how to find these matched graphs R, as discussed above).

In contrast to declarative query languages (*e.g.,* SPARQL and *Cypher*), visual subgraph query formulation helps non-programmers to take advantage of graph querying frameworks through a visual query interface (*also known as* GUI) for query construction. The core component of this interface is a set of subgraph patterns that allow users to construct multiple nodes and edges in a query Q by performing a single click-and-drag action (*i.e., pattern-at-a-time mode*) instead of iterative construction of edges one-at-a-time (*i.e., edge-at-a-time mode*). Users are also allowed to delete nodes and edges from a partially constructed query. The *pattern-at-a-time mode* can greatly decrease the time taken to visually construct Q. In VISCENT, as shown in Figure 9, edge-diversified patterns are displayed in Panel 5, and Panel 3 displays the nodes of the underlying database. Users can visually formulate a query by dragging and dropping patterns from Panel 5 and nodes from Panel 3 to Panel 4.

7.2 Exploratory Subgraph Search

Subgraph search focuses on "lookup" retrieval with the assumption that users have a clear query intent (*i.e.,* know the exact structure of query Q) and sufficient knowledge of the underlying database D to accurately construct Q. However, this assumption may become impractical as the graph database evolves. Exploratory subgraph search [19, 20, 48] alleviates this problem by supporting not only lookup retrieval but also exploratory search, which allows users to *iteratively or progressively formulate queries* and *explore the query results*. In this process, an end user becomes more familiar with the content and finally identifies the exact query Q. Suppose an user wants to query Q, she may not have the complete query structure "in her mind" at the very beginning. As VISCENT displays edge-diversified patterns $\mathcal{P}_D$ on the GUI, she may find a pattern p interesting while browsing the pattern set, and initiate her query with p (*i.e.,* $Q_0 = p$). By observing the query results of Q_0, she may iteratively construct $Q_1, Q_2, \ldots$ and finally Q. Without the help of these patterns, such a bottom-up search is not likely to happen.

Edge-diversified patterns can help in this process because the query results R may contain a huge number of graphs, which hinders gaining insights from the results. To address this, VISCENT presents TED Explorer. In particular, for user-specified parameters such as k and maximum (resp. minimum) pattern size MaxE (resp. MinE), TED Explorer invokes Pattern Generator to generate edge-diversified patterns $\mathcal{P}_R$ for query results R, which can be cast as a summary of query results and displayed on the interface for a better exploration experience.

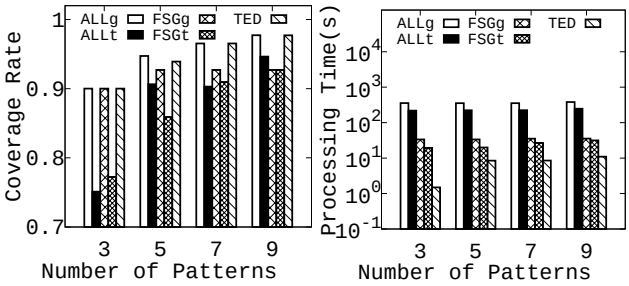
8 PERFORMANCE STUDY

In this section, we investigate the performance of TED and report the key findings. TED is implemented with Java (JDK1.8). All experiments are conducted on a 64-bit Windows desktop with AMD Ryzen 5 3500X 6-Core CPU (3.6GHz) and 32GB of main memory.

8.1 Experimental Setup

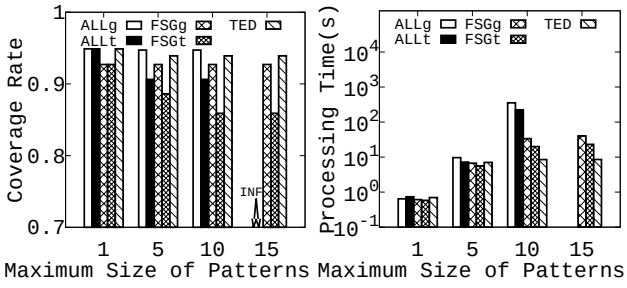
Datasets. The experiments are conducted on three datasets. (1) The dataset AIDS antiviral [6] consists of 40,000 (40K) data graphs. We also use AIDSL to denote the labeled AIDS where each graph

[6] https://wiki.nci.nih.gov/display/NCIDTPdata/AIDS+Antiviral+Screen+Data



(a) Coverage Rate (b) Processing Time

Figure 10: Effect of Number of Patterns.



(a) Coverage Rate (b) Processing Time

Figure 11: Effect of Maximum Size of Patterns.

Table 2: Datasets.

Datasets	E_{max}	V_{max}	E_{avg}	V_{avg}	$\|D\|$
AIDS	251	222	27.3	25.4	40K
eMol	104	100	15.9	15.5	10K
PubChem	838	801	43.8	42.3	1M

is with labeled edges (*i.e.,* bonds). (2) The dataset *PubChem* [7] consists of many chemical compound graphs. Unless otherwise stated, *PubChem* refers to the 23K dataset. Other variants used are 100K, 300K, 500K and 1 million (1M). (3) The dataset *eMol* [8] consists of 10K chemical compounds. Note that <Y><X> are used to denote variants of various datasets, where Y and X refer to the name of the dataset and the number of graphs used, respectively. For example, AIDS10K refers to the dataset AIDS consisting of 10K data graphs. Their statistics are given in Table 2 where E_{max} (resp. V_{max}), E_{avg} (resp. V_{avg}) and $|D|$ indicate maximum number of edges (resp. vertices), average number of edges (resp. vertices), and number of graphs, respectively.

Baselines. We compare TED against the proposed baselines and their variants: (1) enumerating all subgraphs and then performing greedy search (ALL$_g$, Algorithm 1), (2) integrating enumeration of all subgraphs and swapping-based search (ALL$_t$, *i.e.,* a variant of ALL$_g$), (3) enumerating all frequent subgraphs and then performing greedy search (FSG$_g$, Algorithm 2), and (4) integrating enumeration of all frequent subgraphs and swapping-based search (FSG$_t$, *i.e.,* a variant of FSG$_g$). We also compare TED with its variants (BASE, DSS and PRM) where (1) BASE: TED_BASE (Algorithm 3), (2) DSS: BASE + TED_DSS (Algorithm 5), (3) PRM: DSS + TED_PRM (Algorithm 6) and (4) TED (*i.e.,* Algorithm 8): PRM + TED_IPS (Algorithm 7). To illustrate the application potentials of edge-diversified patterns, we further compare TED against (1) CATAPULT [17], the state-of-the-art visual query formulation method, and (2) top-k frequent patterns (denoted as FS).

Parameter settings. Unless specified otherwise, we set $k = 5$ and $E_{max} = 10$.

Performance measures. We use the following measures for performance evaluation: (1) *Processing Time (in second):* time taken to generate the patterns. Note that INF is used to denote the case that a test does not stop in a time limit (10000 seconds) or memory limit. In the experiment, we use log scale for the time. (2) *Coverage Rate:* the coverage rate of patterns to the total number of edges in a database D; (3) *Index Time (in second):* time taken to maintain PES-index; (4) *Index Size (in kilobyte):* space consumption for storing the PES-index. (4) *Query Formulation Time* (QFT): time taken to formulate a query; (5) *Steps*: number of steps taken to formulate a query; (6) *Reduction Ratio* (RR): Ratio of reduced steps by TED, RR = $\frac{Steps_X - Steps_{\text{TED}}}{step_X}$ where $step_X$ and $step_{\text{TED}}$ are the *minimum* number of steps required to construct a query Q when patterns $\mathcal{P}$ derived from the approach X and TED are used, respectively. As we discussed above, X could be CATAPULT or top-k frequent patterns mining. RR > 0 implies that $\mathcal{P}$ derived from TED required fewer steps compared to X. Note that we follow the same assumptions in [17] to estimate $Steps_X$ and $Steps_{\text{TED}}$: (1) a pattern $p \in \mathcal{P}$ can be used to construct the query Q iff $p \subseteq Q$; (2) when multiple patterns are used to construct Q, their corresponding isomorphic subgraphs in Q do not overlap. We shall remove these assumptions in the user study, where users are allowed to modify (*e.g.,* delete nodes/edges) patterns when they are used for query formulations.

8.2 Experimental Results

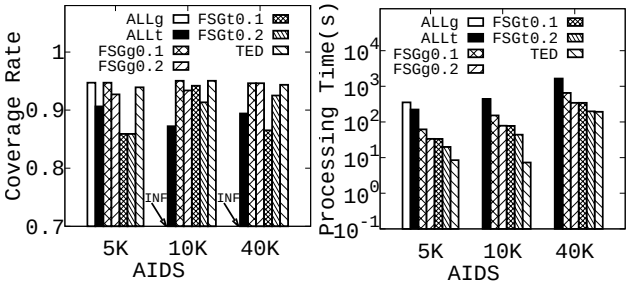
8.2.1 Comparison with Baselines.

Question 1: *How does TED perform compared to the baselines in the default parameter settings? And do different parameters (*i.e., E_{max} *and* k*) affect the results?*

Result 1. TED outperforms baselines in terms of both Processing Time and Coverage Rate in the default parameter settings (see Exp 2). In general, TED is comparable to ALL$_g$ and outperforms other methods in terms of coverage rate, and requires less processing time (see Exp 1).

Exp 1: Setting of Maximum Size and Number of Patterns. To evaluate the performance of TED, we first perform an evaluation to determine parameter settings. We vary the number of patterns (*i.e., k*) on AIDS5K. Figure 10 plots the results. In general, the coverage rate and processing time increase with k, since more patterns are introduced and higher coverage will be obtained as k increases. The methods based on greedy search (*i.e.,* ALL$_g$ and FSG$_g$) generally show better coverage rate and more processing time compared to swapping-based search methods (*i.e.,* ALL$_t$ and FSG$_t$), as the former needs to store all (resp. frequent) subgraphs for further searching. However, TED is always comparable to ALL$_g$ and better than other methods in terms of coverage rate (Figure 10(a)), although it is based on a swapping-based search. As shown in Figure 10(b), TED requires less processing time than other methods on all settings. In the following experiments, we set $k = 5$.

[7] ftp://ftp.ncbi.nlm.nih.gov/pubchem/Compound/CURRENT-Full/SDF/
[8] https://www.emolecules.com/info/plus/download-database



(a) Coverage Rate (b) Processing Time

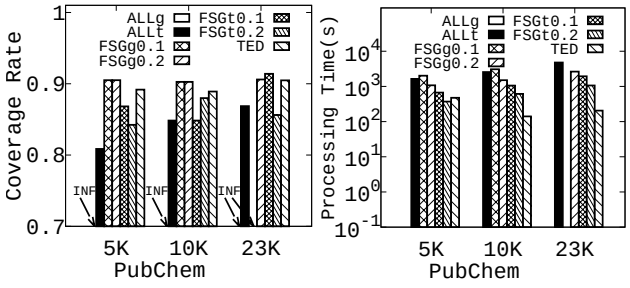
Figure 12: Baseline comparison on AIDS.

We also study the performance of TED with different maximum sizes of patterns (E_{max}) on AIDS5K. As shown in Figure 11, TED is comparable to ALL_g and better than other methods in terms of coverage rate, but requires less processing time in most cases, especially for larger E_{max}. Intuitively, ALL_g can obtain a better coverage rate compared to other methods except TED since all subgraphs are enumerated and stored, which makes it memory- and time-consuming (*e.g.,* INF for $E_{max} = 15$). In addition, as E_{max} increases, the search space is enlarged, and hence the processing time of these methods increases. Note that the coverage rate fluctuates within a narrow range, which is due to the label distribution of edges in the database. We set $E_{max} = 10$ in the following experiments, unless otherwise specified.

Exp 2: Comparison with Baselines. Next, we compare TED with baselines and their variants, *i.e.,* ALL_g, ALL_t, FSG_g, and FSG_t in the default setting, and report the results on AIDS dataset in Figure 12. The results of FSG-based algorithms (*i.e.,* FSG_g and FSG_t) with various supports (0.1 and 0.2) are also reported. As depicted in Figure 12(a), in terms of coverage rate, TED outperforms other baselines and is comparable to ALL_g, which incurs INF on AIDS10K and AIDS40K. As the size of dataset increases from 5K to 40K, processing time of ALL_g increases dramatically, while that of our TED algorithm increases steadily to less than 4 minutes on AIDS40K, as shown in Figure 12(b). We further compare TED with baselines and their variants in two other datasets, *PubChem* and *eMol*. As depicted in Figure 13(a) and Figure 14(a), although FSG_g algorithm often shows comparable coverage rate to TED, its processing time dramatically increases with the size of dataset and even incurs INF (*e.g.,* on PUBCHEM23K), as it adopts greedy search on all frequent subgraphs whose size is data-dependent (Figure 13(b) and Figure 14(b)). In addition, FSG_g cannot theoretically guarantee the quality of the final patterns. Note that ALL_g incurs many INF exceptions on *PubChem* dataset since graphs in the dataset are relatively larger in size (the average and maximum number of edges are 44 and 838, respectively). TED is also compared with baselines on AIDSL dataset and similar results are observed as shown in Figure 15.

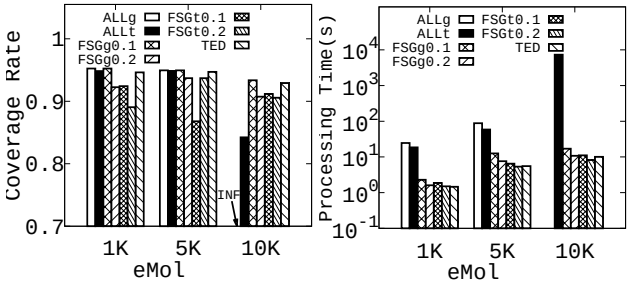
To investigate the effect of maximum number of nodes in a graph, we compare TED with baselines on DS = $\{D_{(0,20]}, D_{(20,50]}, D_{(50,80]}, D_{(80,801]}\}$ [9] where $D_{(r,l]}$ ($|D_{(r,l]}| = 1000$) represents the graphs in *PubChem* whose node sizes are in the range $(r, l]$. Figure 16 depicts the results. In general, TED consistently shows comparable coverage rate to greedy-search based methods, whose processing time dramatically increases with the maximum number of nodes in a graph and even incurs INF. We can also observe that the coverage rate slightly increases with the maximum number of nodes. This is because the total number of edges in each dataset increases more rapidly than the number of uncovered edges.

[9] As shown in Table 2, maximum number of nodes in PubChem is 801.



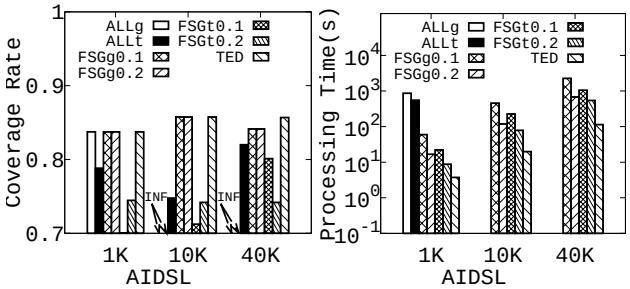
(a) Coverage Rate (b) Processing Time

Figure 13: Baseline comparison on PUBCHEM.



(a) Coverage Rate (b) Processing Time

Figure 14: Baseline comparison on EMOL.



(a) Coverage Rate (b) Processing Time

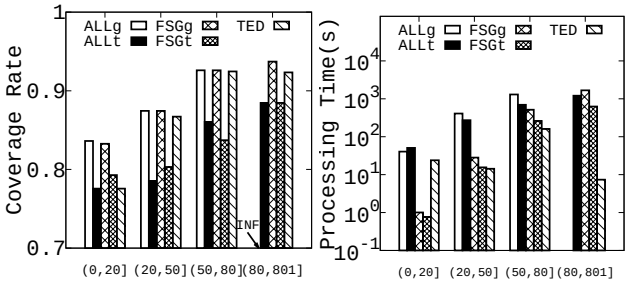
Figure 15: Baseline comparison on AIDSL.

Finally, we compare them with the optimal solutions on small datasets (*i.e., PubChem*100 and *AIDS*100) and report the results in Figure 17. We observe that the ratio of the coverage rate of TED to that of optimal solution (denoted by OPT in the figure) is no less than 0.945, which is far better than the theoretical approximation ratio.

To sum up, TED outperforms baselines in terms of both coverage rate and processing time.

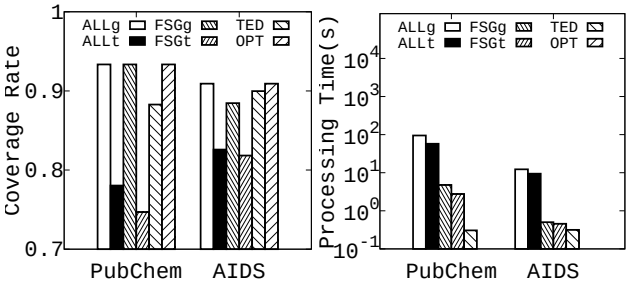
8.2.2 *Effectiveness and Scalability Evaluation.*

Question 2: *Are the presented techniques (optimizations and swapping criteria) effective? Are the proposed framework and indexing technique scalable?*



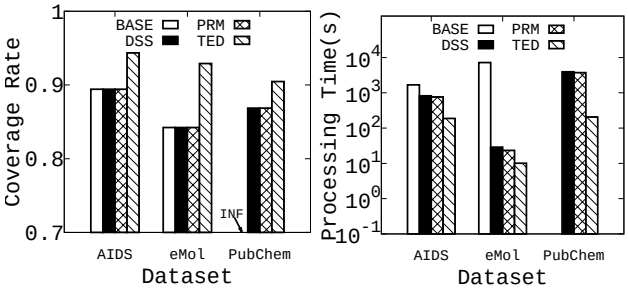
(a) Coverage Rate (b) Processing Time

Figure 16: Impact of Maximum Number of Nodes in a Graph.



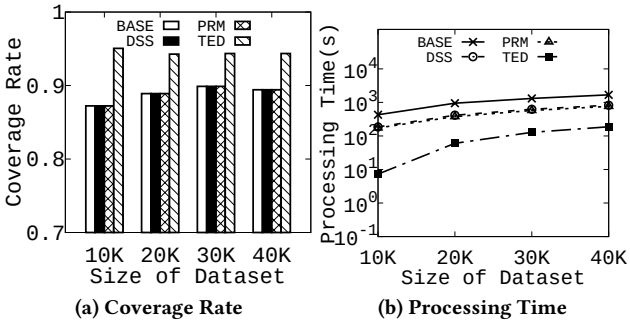
(a) Coverage Rate (b) Processing Time

Figure 17: Baseline comparison on *PubChem*100 and *AIDS*100.



(a) Coverage Rate (b) Processing Time

Figure 18: Effect of Optimization Strategies.



(a) Coverage Rate (b) Processing Time

Figure 19: Effect of Optimization Strategies on AIDS10K-40K.

Result 2. Both optimizations and swapping criteria are effective as the former can reduce processing time without decreasing coverage rate (see Exp 3), and the latter can facilitate TED in coverage rate and processing time, regardless of which swapping threshold is used (see Exp 6). In addition, the space and time taken to store/maintain PES-Index are acceptable (see Exp 4), making TED scalable to handle very large dataset (see Exp 5).

Table 3: Size of PES-Index

Dataset	AIDS		eMol		PubChem	
	10K	40K	5K	10K	10K	23K
Index Size(KB)	234	1008	89	157	428	1157
Index/Graphs (%)	5.39	5.31	5.40	5.39	5.80	7.58

Table 4: Maintenance Time of PES-Index

Dataset	AIDS		eMol		PubChem	
	10K	40K	5K	10K	10K	23K
Index Time(s)	0.5	1.88	0.25	0.37	1.1	2.85
Index Time/Total (%)	6.86	1.00	4.12	3.63	0.78	1.39

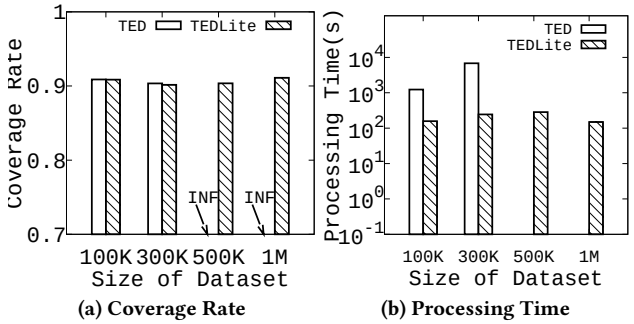
Exp 3: Effect of Optimization Strategies. We further evaluate the effectiveness of optimization strategies by comparing BASE, DSS, and PRM with TED where all optimization strategies are used. The results are presented in Figure 18. Compared to BASE, DSS, and PRM, TED reduces processing time but does not decrease coverage rate, as it eliminates unpromising patterns without sacrificing promising ones. Thanks to all adopted optimization strategies, TED is the best one in terms of coverage rate and processing time compared to BASE, DSS, and PRM. In addition, we can observe that the processing time of BASE, DSS, PRM, and TED shows a decreasing trend, which further justifies the effectiveness of optimization strategies. Similar results are observed on AIDS10K-40K graphs, as shown in Figure 19.

Exp 4: PES-Index Test. In this experiment, we test the size and maintenance time of PES-Index. As presented in Table 3, PES-Index size increases with the size of the dataset. Note that in comparison with the size of dataset, PES-Index size is very small since only five components are stored in PES-Index. In particular, for the larger datasets AIDS40K and PubcChem23K, the space taken to store PES-Index is only 5.31% and 7.58% of the size of the underlying dataset.

We also report the maintenance time of PES-Index in Table 4. Observe that as the size of dataset increases, maintenance time increases accordingly but makes up less than 7% of the total processing time. For example, maintenance time of PES-Index on AIDS40K and PubcChem23K are 1% and 1.39% of the corresponding total processing time, respectively.

Exp 5: Scalability Test. Figure 20 reports the performance of TED and TEDLITE on very large dataset of PUBCHEM. We observe that both of them can efficiently handle large datasets. In particular, TED is able to process up to 300K graphs within about 1.9 hours and achieves high coverage rate (*i.e.,* more than 90%). Compared to TED, TEDLITE has slightly worse results in terms of coverage rate but takes far less processing time (e.g., 150s for 1M graphs in PUBCHEM).

Exp 6: Effect of Swapping Criteria. We investigate the effect of different swapping criteria (see Section 4), namely $Swap_1$, $Swap_2$, and $Swap_\alpha$. The results are reported in Figure 21. In general, TED outperforms the baselines in terms of both coverage rate and processing time, no matter what swapping criteria are used. Although



(a) Coverage Rate (b) Processing Time

Figure 20: Scalability Test.

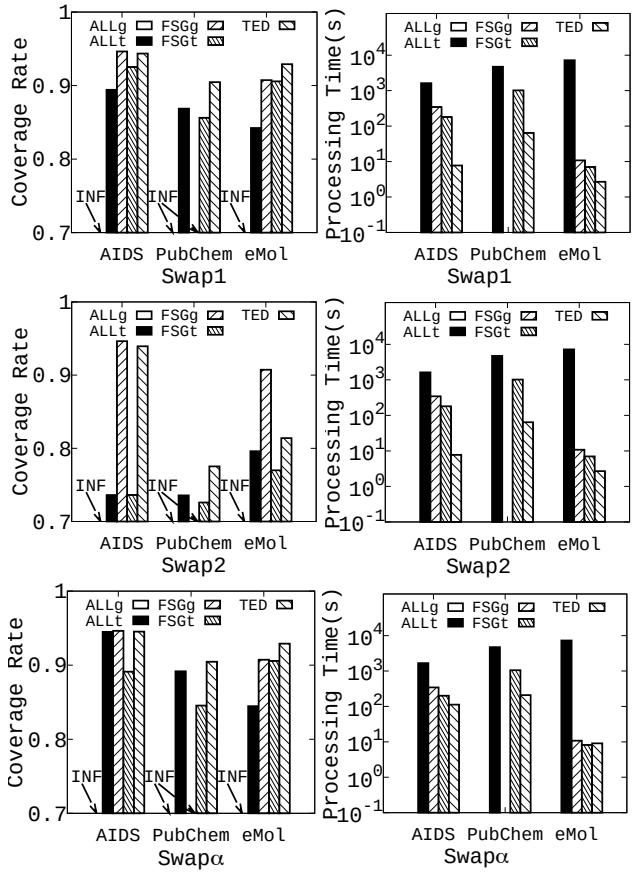


Figure 21: Effect of Swapping Criteria.

FSG_g with $Swap_2$ shows a higher coverage rate in eMol, as discussed in Exp 2, the results generated by FSG_g are data-dependent and are not theoretically guaranteed. Furthermore, it may incur INF in larger datasets (*e.g.,* PubChem). This experiment further justifies the effectiveness of Ted algorithm.

8.2.3 Application Potentials Evaluation.

Question 3: *Whether top-k edge-diversified patterns can facilitate existing or potential applications? These patterns may contain infrequent subgraphs, why do infrequent patterns remain useful?*

Result 3. Top-k edge-diversified patterns can facilitate both visual subgraph query formulation and exploratory subgraph search (see Exp 7). While frequent subgraphs are often useful, infrequent patterns can also facilitate applications where queries are not necessarily frequent (see Exp 8).

Exp 7: User Study. In this section, we conduct user studies based on VISCENT to evaluate the application potentials of edge-diversified patterns. We recruit 15 unpaid volunteers (ages from 20 to 32) in accordance to HCI research that recommends at least 10 participants [27, 28]. Before conducting any user study, all volunteers, who have backgrounds in chemistry, chemical engineering, CS, biology, were trained to use VISCENT. More details on how to use VISCENT are provided in Section 7.

Visual Query Formulation. The first study aims to evaluate the application potential in visual query formulation (VQF). To this end, we compare edge-diversified patterns with canned patterns provided by CATAPULT [17] (the state-of-the-art VQF method), and frequent patterns (denoted as FS). In particular, we first follow the existing work [17] to select 5 queries (see Table 5) of size in the range [30-62], which span a variety of structures (cycles, carbon chains, etc.) and contain different vertex labels. Each query in a dataset (AIDS or *PubChem*) is associated with a unique identifier (*also known as* CID, Table 5) in the *PubChem* repository [10] provided by National Institutes of Health (NIH). Second, each pattern set (TED or CATAPULT or FS) is displayed on the GUI (Panel 5 in Figure 9) for VQF. Volunteers visually formulate the queries by dragging and dropping patterns from Panel 5 and nodes from Panel 3 to Panel 4 to formulate queries. The *Query Formulation Time* (QFT) and *Steps* taken for VQF are recorded in Panel 2 (Figure 9).

Figure 22 reports the results on PubChem and AIDS. We observe that compared to CATAPULT and FS, Ted facilitates more efficient query formulations (shorter QFT and fewer steps). In addition, we can also observe that some queries (*e.g.,* Q_5 in Figure 22(b)) compared to other queries (*e.g.,* Q_1 in Figure 22(b)) benefit more from Ted, *i.e.,* TED can save more QFT and *Steps* taken on Q_5 than those on Q_1 when compared to FS and CATAPULT. The main reason lies in that TED provides more patterns for formulating Q_5 ($|\mathcal{P}_U|$(FS)=2 vs $|\mathcal{P}_U|$(CATAPULT)=3 vs $|\mathcal{P}_U|$(TED)=6) than Q_1 ($|\mathcal{P}_U|$(FS)=1 vs $|\mathcal{P}_U|$(CATAPULT)=2 vs $|\mathcal{P}_U|$(TED)=3), as shown in Table 6. Note that the number of patterns used to formulate a query Q indicates how many patterns can be used to cover different parts of Q so that it can enjoy the *pattern-at-a-time* mode (see Section 7.1) and thus reduce the time/step to visually construct Q.

We also use "Yes" in Table 6 to denote that at least one infrequent ($sup_{min} < 0.2$) edge-diversified pattern can be used in VQF and find that infrequent patterns can also facilitate VQF. This further justifies the rationality of our top-k edge-diversified patterns discovery problem.

Exploratory Subgraph Search. We also conduct a user study on exploratory subgraph search. As exploratory search activities have no predetermined goals and are considered as open-ended [20], in this experiment, queries are user-specified rather than predetermined. As discussed in Section 7.2, volunteers are allowed to enjoy not only the bottom-up search but also TED Explorer, which helps to explore the query results. Therefore, we divide these volunteers into two groups to iteratively construct user-specified queries and explore the query results. The first group uses VISCENT with

[10] https://pubchem.ncbi.nlm.nih.gov/

Table 5: Queries. CID is the unique identifier in the PubChem repository provided by National Institutes of Health (NIH).

Queries	CID, Pubchem (|E|)	CID, AIDS (|E|)
Q_1	169132 (|E| = 34)	135398740 (|E| = 32)
Q_2	20497364 (|E| = 30)	565070 (|E| = 34)
Q_3	493570 (|E| = 47)	102034018 (|E| = 35)
Q_4	135398658 (|E| = 52)	14852846 (|E| = 30)
Q_5	3324 (|E| = 42)	154402349 (|E| = 62)

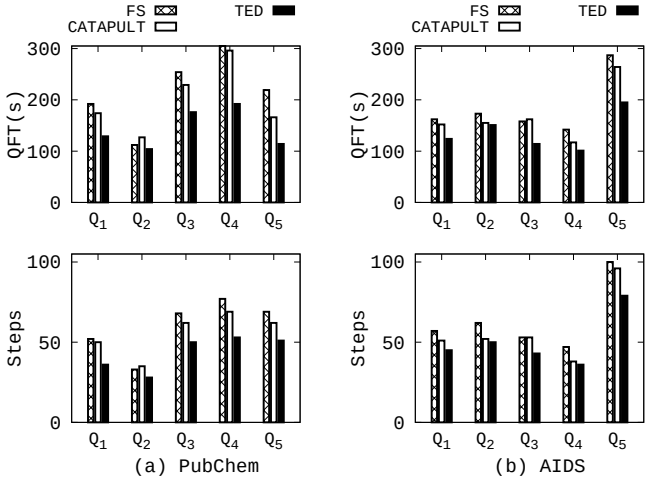


Figure 22: Query Formulation Time (QFT) and Steps.

Table 6: Number of Patterns Used in VQF ($|\mathcal{P}_U|$). "Yes" indicates that at least one infrequent pattern can be used.

Queries	PubChem			AIDS		
	FS	CATAPULT	TED	FS	CATAPULT	TED
Q_1	2	2	**5**	1	2	**3**
Q_2	3	3	**5 (Yes)**	1	1	**2**
Q_3	3	4	**6 (Yes)**	2	1	**4**
Q_4	4	5	**7 (Yes)**	1	2	**3**
Q_5	2	2	**5 (Yes)**	2	3	**6 (Yes)**

TED Explorer displaying patterns (*e.g.*, edge-diversified patterns), while the second group does not use TED Explorer. Compared with the second group, we observe that the first group takes 20% less time when displaying edge-diversified patterns, and only 10%–14% less time when displaying FS and CATAPULT). This means that edge-diversified patterns enhance not only exploration efficiency but also query experience.

Other findings. The most appealing thing to us is that top-k edge-diversified patterns generated by TED contain not only patterns with statistical significance (*e.g.*, frequent patterns) but also patterns with biological importance. In this paper, a pattern is said to have biological importance if it exists in the *PubChem* repository [11], which is maintained by the National Institutes of Health (NIH) and contains millions of chemical molecules and their activities against biological assays. Table 7 reports these patterns' unique identifies (*i.e.*, CID). We can observe that compared to FS, TED and CATAPULT contain more such patterns (8 vs 5). For example, the CID 11473 in TED is an important organic compound *Nitrosobenzene*, which is one of the prototypical organic nitroso compounds. Therefore, TED may open up new opportunities in bioinformatics, drug design, etc.

[11] https://pubchem.ncbi.nlm.nih.gov/

Table 7: Patterns with Biological Importance. CID is the unique identifier in the PubChem repository provided by National Institutes of Health (NIH).

Pattern Set	Patterns with Biological Importance	Total
FS	X-Methylpentane (*e.g.*, CID 7892)), Carbon Chains (*e.g.*, CID 7843), CID 6556, CID 241, CID 6360	5
CATAPULT	Carbon Chains, CID 7282, CID 16665, CID 119440, CID 6380, CID 19660, CID 702, CID 11507	8
TED	Carbon Chains, CID 10903, CID 12230, CID 7964, CID 11473, CID 3034819, CID 702, CID 12338	8

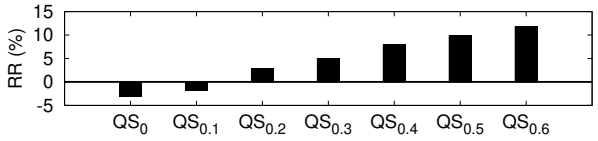


Figure 23: Reduction Ratio (RR).

Exp 8: Effect of Queries. As discussed above, infrequent edge-diversified patterns can also facilitate visual query formulation (VQF). The problem becomes *why infrequent patterns remain useful?* We answer this question by investigating the *ratio of reduced steps* for VQF (*i.e.*, RR = $\frac{Steps_{FS} - Steps_{TED}}{step_{FS}}$, see Section 8.1) between TED and top-k frequent patterns (FS) on the query set QS_ρ ($|QS_\rho| = 100$), where ρ is the fraction of queries that are infrequent. When $\rho = 0$, all queries in QS_ρ are frequent. We vary ρ in $\{0, 0.1, 0.2, ..., 0.6\}$ and plot the results in Figure 23. Obviously, TED underperforms FS on QS_0 (RR < 0) as TED contains a mixture of frequent and infrequent patterns. Nevertheless, RR increases with ρ and is larger than 0 at $\rho = 0.2$. This indicates that in terms of facilitating VQF of infrequent queries, the performance of TED improves as the ratio of infrequent queries increases, which explains the reason why infrequent patterns remain useful.

9 RELATED WORK

Subgraph enumeration listing all subgraphs or counting all instances of a particular graph in a graph database has been extensively studied in the literature. Many of these approaches are based on dynamic programming and techniques such as color coding. [3] develops a simple edge-searching method for listing all triangles, quadrangles, and complete subgraphs. But this method may incur significant disk reads when it is applied to external subgraph enumeration. Compared to [3], [5] presents an enhanced algorithm based on symmetry-breaking technique. In addition, [2] applies the color coding technique and dynamic programming routine for counting non-induced occurrences of subgraph topologies in the

form of trees and subgraphs. A parallel color coding and streaming algorithm for subgraph enumeration in large social contact networks is also designed [6]. To handle the problem that data graphs cannot reside chronically in memory, a disk-based algorithm DualSim [34] is proposed. Since subgraph enumeration is computationally expensive, distributed approaches have been proposed. [29] explores a technique to process subgraph enumeration in a single map-reduce round. Another novel parallel framework named PSgL is built upon Giraph [33]. In addition, Lai et al. develop TwinTwig [32] on MapReduce. Other parallel algorithms [35, 36] for compressing the intermediate results are also considered. Instead of enumerating subgraphs with CPU, GPU-based subgraph enumeration methods [37–39] are also explored. Our top-k edge-diversified patterns discovery problem is orthogonal to these works as subgraph enumeration is a necessary step in our Ted framework.

Instead of enumerating all subgraphs, frequent subgraph mining (FSM) is to generate only frequent subgraphs. Existing FSM methods consider two settings, transactional and single graph such as [13]. The transactional case assumes the graph database contains a set of graphs, which is the same as our setting in this work. Both AGM [7] and FSG [8] methods adopt a BFS-based strategy to generate frequent subgraphs. They first generate a lot of candidates and then perform subgraph isomorphism test to prune false positives. These methods are time-consuming since subgraph isomorphism test is NP-complete and costly. To address this problem, Yan et al. propose gSpan [10] algorithm, which is the first DFS-based method for FSM. Owing to its better performance, it is widely used. FFSM [11] claiming to be competitive with gSpan [10] is the method for efficiently handling the underlying subgraph isomorphism problem in AGM and FSG. Other methods such as [12] adopt the pattern growth strategy. Other than enumerating all frequent subgraphs, MARGIN [40] and CloseGraph [41] generate maximal frequent subgraphs and closed frequent subgraphs, respectively. In addition, [30] and [31] focus on mining representative-based subgraphs, *i.e.,* every non-representative pattern is close to one of the representative patterns, while the representative patterns are diverse from each other. The very nature of these subgraphs/patterns is frequent subgraphs. In contrast, patterns generated by Ted can be frequent and infrequent subgraphs, which is in line with real-world applications such as visual query formulation where subgraph queries are not necessarily frequent in nature as users may frequently pose infrequent subgraph queries. Although there are methods [17, 42, 43] which aim to discover subgraphs that are not necessarily frequent, none of them focus on top-k edge-diversified problems and their solutions can not be directly adapted for it.

Diversity problem is the most germane to this research, which seeks for search results with diversity. [44] presents diversity-aware search method of relevant documents. Fan et al. [14] aims to retrieve diversified top-k matches for a given vertex. The problem of finding redundancy-aware maximal cliques is considered by [45]. In addition, [46] further studies the diversified top-k clique search problem, which is to find k maximal cliques in a data graph so that the maximum number of vertices are included. Given a query graph, [49] retrieves diversified top-k matches to cover more vertices. Other than static graph, diversified pattern mining on temporal network is also studied by [50], which is for finding k diversified *dense temporal subgraphs*. Recent work [51] investigates the problem of diversity-based shortest path. To the best of our knowledge, our work is the first one to study top-k edge-diversified patterns discovery problem.

Top-k edge-diversified patterns discovery problem is also related to the set cover and maximum coverage problems [22]. Given a universal set $\mathcal{U}$ of n elements and a collection $\mathcal{S} = \{S_1, S_2, ..., S_m\}$ of m subsets of $\mathcal{U}$ ($\bigcup_i S_i = \mathcal{U}$), set cover problem is to find as few subsets as possible from $\mathcal{S}$ such that their union covers $\mathcal{U}$. For an integer $k \leq m$, maximum coverage problem finds k subsets from $\mathcal{S}$ such that their union has maximum cardinality. Note that the edge cover problem is a special case of set cover problem, in which the elements of the universe are vertices and each subset covers exactly two elements.

10 CONCLUSION

In this work, we investigate the top-k edge-diversified patterns discovery problem, which is to find k subgraphs from a graph database such that the maximum number of edges in the database are covered. Maximizing total covered edges requires that patterns should have not only high subgraph coverage (*i.e.,* more data graphs are covered by the patterns) but also high diversity (*i.e.,* patterns are diverse to each other to cover different parts of data graphs). This problem may nurture a lot of applications such as visual query formulation where patterns displayed on the GUI should cover more graphs and be diverse to each other to make better use of the limited GUI space. To address this problem, we present a novel framework called Ted and an efficient index structure. In addition, three optimization strategies are developed to improve the performance. To handle even larger graph databases, a lightweight version called TedLite is further designed. Ted requires limited memory and achieves a guaranteed approximation ratio. Extensive experimental results justify the superiority of Ted over baseline solutions.

As for future work, we plan to explore other application potentials of edge-diversified patterns such as drug repositioning. In particular, signaling proteins within a cell act together through linear pathways, cell signaling is often viewed as a network. Understanding signal flow in the network is paramount since some diseases often take effects by altering signaling pathways [21]. Therefore, the discovery of therapeutic drugs from a set of drugs can target these altered signaling pathways to restore the physiological state of a disease network. Since the drug set (*e.g.,* Drugbank) contains more than a million chemical compounds and drugs, testing each drug on the disease network is infeasible. Fortunately, checking each drug on top-k edge-diversified patterns is an alternative way as a drug can target maximum number of edges in the disease network if it can target the top-k edge-diversified patterns. However, the signaling pathway is a directed hypergraph in which an edge can join any number of vertices, which is left for future work.

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A PROOFS

Proof of Theorem 1 (Sketch). Let $k = 1$, the original top-k edge-diversified patterns discovery problem (TED Problem) becomes to find a single edge-diversified pattern, *i.e.,* a graph g that covers maximum number of edges. The reformulated problem (denoted by Simplified TED Problem), *i.e.,* TED Problem with $k = 1$, can be reduced from the maximum coverage problem, which is a classical NP-hard optimization problem [53]. In particular, given a number m and a collection of sets S, the maximum coverage problem aims to find a set $S' \subset S$ such that $|S'| \leq m$ and the number of covered elements is maximized. In Simplified TED Problem, the collection of sets S is the set that consists of all possible edges of the graph dataset D. The subset S' is the cover sets of $g's$ matchings and m is the number of matchings. The number of covered elements corresponds to the number of covered edges in D. In addition, the decision problem of Simplified TED Problem, *i.e.,* whether there exists a set S', *i.e.,* cover sets of m matchings of g in D, such that $|Cov(S', D)| \geq C$ given m and C, is NP since it is possible to guess S' and check its validity in polynomial time. To sum up, Simplified TED Problem is NP-complete. Since Simplified TED Problem is a special case of TED Problem and can be reduced to TED Problem in polynomial time, TED Problem is NP-hard.

Proof of Lemma 1 (Sketch). The worst case time complexity of subgraph enumaration (Line 1, Algorithm 1) is $O(|D|2^{max(V(G))^2})$ [13]. The time complexity of MaxCover (Line 2, Algorithm 1) is due to greedy search for the pattern with maximum marginal coverage (*i.e.,* $|Cov(p', D) \setminus Cov(\mathcal{P}, D)|$). It requires computations for subgraph isomorphism which is a well-known NP-hard problem and takes $O(k|S||D|max(V(G))^{E_{max}})$ time where $max(V(G))^{E_{max}}$ is the time taken for testing subgraph isomorphism [13] and $|S|$ is number of enumerated subgraphs. To sum up, the worst case time complexity of ALL_g (Algorithm 1) is $O(|D|2^{max(V(G))^2} + k|S||D|max(V(G))^{E_{max}})$.

Since the dataset D and all enumerated subgraphs S are stored, the worst case space complexity is $O(max(E(G))|D| + E_{max}|S|)$ where $O(max(E(G)))$ (resp. $O(E_{max})$) is the space for storing a single graph in D (resp. enumerated subgraph in S).

Proof of Lemma 2 (Sketch). In the worst case, *i.e.,* $sup_{min} \times |D| = 1$ (all subgraphs should be enumerated), the worst case time complexity of frequent subgraph mining (Line 1, Algorithm 2) is the same as that of subgraph enumeration, $O(|D|2^{max(V(G))^2})$. As discussed in

Proof of Lemma 1, time complexity of MaxCover on all enumerated frequent subgraphs (Line 2) is hence $O(k|S_{fre}||D|max(V(G))^{E_{max}})$. Overall, the worst case time complexity of FSG_g (Algorithm 2) is $O(|D|2^{max(V(G))^2}+k|S_{fre}||D|max(V(G))^{E_{max}})$. Due to the dataset D and frequent subgraphs S_{fre} are stored, the worst case space complexity is $O(max(E(G))|D| + E_{max}|S_{fre}|)$ where $O(max(E(G)))$ (resp. $O(E_{max})$) is the space for storing a single graph in D (resp. frequent subgraph in S_{fre}).

Proof of Theorem 2 (Sketch). The main time cost is spent on EnumSub($D, |E| = 1$) (Line 2, Algorithm 3), PatternMaintain($\mathcal{P}, g, D$) (Line 5) and RightMostExtend(g, D, E_{max}) (Line 6). In particular, EnumSub($D, |E| = 1$) is to enumerate all edges and thus takes $O(|D|max(E(G)))$ time. PatternMaintain($\mathcal{P}, g, D$) requires computations for loss score and benefit score, which take $O(|D|max(E(G)))$ time (Lines 8-17 and lines 19-25, Algorithm 4). In the worst case, total time cost of RightMostExtend(g, D, E_{max}) is taken on enumerating all subgraph, which takes $O(|D|2^{max(V(G))^2})$ time. Overall, the worst case time complexity is $O(|D|2^{max(V(G))^2})$, since $|D|2^{max(V(G))^2} \gg |D|max(E(G))$.

The space cost is mainly spent on storing the database D, pattern set $\mathcal{P}$ and PES-Index. It is obviously that the former two take $O(max(E(G))|D|)$ and $O(kE_{max}))$ space, respectively. For PES-Index, the main space is spent on storing reverse cover set $rCov(e)$, which consumes $O(max(E(G))|D|)$ space. Therefore, the worst case space complexity is $O(max(E(G))|D|)$ since $max(E(G))|D| \gg kE_{max}$.

Proof of Theorem 3 (Sketch). Let the current patterns be $\mathcal{P}$ and final patterns $\mathcal{P}_{final}$, according to the swapping criteria (Equ. (1), Section 4), only the promising candidate g could be kept in $\mathcal{P}_{final}$. Therefore, given a graph g, we prove that PRM rules have no effect on the quality (*i.e.,* coverage) of final patterns by showing that no promising candidate is filtered out. In particular, 1) for $g \in \mathcal{P}$, $Cov(g, G_i) \subseteq Cov(\mathcal{P}, G_i)$ (see Figure 7(b)), if $|\cup_{i\in\mathbb{I}}(E(G_i) \setminus Cov(\mathcal{P}, G_i))| < (1+\alpha)\text{Score}_L+(1-\alpha)|Cov(\mathcal{P}, D)|/k$, it is impossible that $\text{Score}_B \geq (1+\alpha)\text{Score}_L + (1-\alpha)|Cov(\mathcal{P}, D)|/k$ since $\text{Score}_B \leq |\cup_{i\in\mathbb{I}}(E(G_i) \setminus Cov(\mathcal{P}, G_i))|$ (*i.e.,* all uncovered edges in G_i). 2) for $g \notin \mathcal{P}$, the edges that covered by g but not covered by g' (*i.e.,* $Cov(g, G_i) \setminus Cov(g', G_i)$) will not be covered by descendants of g', hence, the maximum coverage of g's descendants is bounded by $|\cup_{i\in\mathbb{I}}(E(G_i) \setminus (Cov(\mathcal{P}, G_i) \cup (Cov(g, G_i) \setminus Cov(g', G_i))))|$. If $|\cup_{i\in\mathbb{I}}(E(G_i) \setminus (Cov(\mathcal{P}, G_i) \cup (Cov(g, G_i) \setminus Cov(g', G_i))))| < (1+\alpha)\text{Score}_L + (1-\alpha)|Cov(\mathcal{P}, D)|/k$, $\text{Score}_B < (1+\alpha)\text{Score}_L + (1-\alpha)|Cov(\mathcal{P}, D)|/k$. Obviously, no promising candidate is filtered out. Therefore, PRM rules have no effect on the quality (*i.e.,* coverage) of final patterns.

Proof of Theorem 4 (Sketch). We begin by introducing the Max k-cover problem [22]: given a number m and a collection of sets S, the Max k-cover problem aims to find a set $S' \subset S$ such that $|S'| = m$ and the number of covered elements is maximized. This problem has a $\frac{1}{4}$-approximation solution when the swapping strategy is adopted [22]. Observe that the problem has the same setting as our problem if all promising patterns are generated. In our problem, the collection of sets S is the set that consists of all possible edges of the graph dataset D. The subset S' is the cover sets of $\mathcal{P}$' matchings and m is the number of patterns (*i.e.,* $m = k$). The number of covered elements corresponds to the number of covered edges of $\mathcal{P}$ in D. In addition, the same swapping strategy [22] is adopted by default. Hence, the approximation ratio of patterns $\mathcal{P}$ generated by Ted (resp. Ted_base) is bounded by $|Cov(\mathcal{P}, D)| \,/\, |Cov(\mathcal{P}_{opt}, D)| \geq \frac{1}{4}$.

Proof of Theorem 5 (Sketch). Compared to Ted_base, Ted introduces three optimizations, *initial pattern selection* (Line 1, Algorithm 8), *dynamic support setting* (Lines 5-6) and *promising right-most extension* (Lines 9-11). Since time complexity of *initial pattern selection* is not larger than that of subgraph enumeration and its space complexity is $O(kE_{max})$, worst case time and space complexities of Ted will not increase after applying *initial pattern selection*. In addition, worst case time and space complexities of Ted will not increase after applying *dynamic support setting*, as the support of a pattern can be directly derived in the process of right-most extension. The same conclusion is made when applying *promising right-most extension*. Overall, worst case time and space complexities of Ted are $O(|D|2^{max(V(G))^2})$ and $O(max(E(G))|D|)$, respectively.

Proof of Theorem 6 (Sketch). Given the average edge number of graphs (denoted by $|E_{avg}|$) in D and an edge e, the absolute difference of e's frequency in a sample D' and D is $Dif_{abs} = |fr(e, D) - fr(e, D')|$ where $fr(\cdot)$ is a frequency. Given an error bound ϵ and a maximum probability ρ for the absolute difference that exceeds ϵ, we have $Pr[Dif_{abs} > \epsilon] = Pr[|fr(e, D) - fr(e, D')||D'||E_{avg}| > \epsilon|D'||E_{avg}|] < \rho$. According to Chernoff bounds [26, 52], there is an upper bound for the probability ρ, *i.e.,* $\rho = 2exp(\frac{-2(\epsilon|D'||E_{avg}|)^2}{|D'||E_{avg}|})$. Therefore, $|D'|$ is lower bounded by $\frac{1}{2\epsilon^2|E_{avg}|}ln\frac{2}{\rho}$.