Nass: A New Approach to Graph Similarity Search

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ABSTRACT

In this paper, we study the problem of graph similarity search with graph edit distance (GED) constraints. Due to the NP-hardness of GED computation, existing solutions to this problem adopt the filtering-and-verification framework with a main focus on the filtering phase to generate a small number of candidate graphs. However, they have a limitation that the number of candidates grows extremely rapidly as a GED threshold increases. To address the limitation, we propose a new approach that utilizes GED computation results in generating candidate graphs. The main idea is that whenever we identify a result graph of the query, we immediately regenerate candidate graphs using a subset of pre-computed graphs similar to the identified result graph. To speed up GED computation, we also develop a novel GED computation algorithm. The proposed algorithm reduces the search space for GED computation by utilizing a series of filtering techniques, which have been used to generate candidates in existing solutions. Experimental results on real datasets demonstrate the proposed approach significantly outperforms the state-of-the-art techniques.

1 INTRODUCTION

Complex and interconnected data, which are represented by graph models, are used in a wide range of applications such as business process management, pattern recognition, drug design, program analysis, and cheminformatics [13, 18, 20, 21, 25, 27, 29]. Finding graphs similar to a given query is a fundamental operation required in these applications, because inconsistency, natural noises, and different representations are unavoidable in real-world graph data.

To quantify the similarity between graphs, various similarity measures have been developed, such as maximum common subgraphs [2, 18], missing edges and features [24, 31], and graph alignment [19]. Among them, the most commonly used measure in similarity search studies is graph edit distance (GED) [3–6, 14, 16, 17]. The GED between two graphs is the minimum number of edit operations to transform one graph into the other, where an edit operation is insertion, deletion, or relabeling of a single vertex or edge. GED can capture the structural difference between graphs, and it can be applied to many types of graphs [23, 25].

The graph similarity search problem studied in this paper is to retrieve all graphs in a collection of graphs whose GED to a query is within a given threshold. The NP-hardness of GED computation [23] makes this problem challenging, and there has been a rich literature in developing efficient graph similarity search techniques. Existing solutions to the problem have been developed under a filtering-and-verification framework, where candidate graphs are generated using various filtering techniques, and each of the candidates is verified by GED computation. In the filtering-and-verification paradigm, it is crucial to generate a set of candidates as small as possible because the performance of verification relies on the number of candidates. Therefore, the majority of efforts have been aimed at developing candidate generation techniques.

To generate candidates, existing techniques establish a filtering condition between dissimilar graphs by utilizing features of graphs, i.e., substructures of graphs. To eliminate the overhead of extracting features from data graphs and to quickly generate candidates, most techniques build an offline index on features of data graphs. For example, c-star [23] and k-AT [20] build an index on tree-structured features extracted from data graphs. Branch [29, 30] and GSimSearch [26, 27] index branch and path-based g-gram features, respectively. Pars [25, 28] and MLIndex [13] use partitions of graphs as features to be indexed. In contrast to others, a recent technique Inves [9] introduces an online-partitioning algorithm to make use of a partition-based filter in the verification phase. Its partition-based filter plays a role of screening each candidate to reduce the number of candidates passed to GED computation. Hence, this candidate refinement step of Inves can be also considered as a part of candidate generation.

Table 1: Number of candidates vs. number of results of existing algorithms on the AIDS dataset (avg. of 100 queries)

| Threshold (τ) | Candidates | Results |
|--------------|------------|---------|
|              | LF         | GSimSearch | MLIndex | Pars   | Inves   |
| 1            | 13         | 7.6       | 2.7     | 1.3    | 0.5     | 0.22    |
| 2            | 78         | 63        | 37      | 14     | 4.6     | 0.65    |
| 3            | 285        | 273       | 226     | 139    | 59      | 1.26    |
| 4            | 738        | 736       | 691     | 562    | 335     | 2.70    |
| 5            | 1488       | 1487      | 1459    | 1346   | 1035    | 4.91    |
| 6            | 2514       | 2514      | 2493    | 2462   | 2129    | 9.09    |
| 7            | 3780       | 3780      | 3757    | 3751   | 3501    | 18.45   |

An inherent limitation of existing feature-based filtering techniques is that the filtering effect sharply decreases as a GED threshold increases. Table 1 shows the average number of candidates and that of results of existing filtering algorithms on a real dataset AIDS for 100 queries (see Section 6 for details of the dataset and queries). In the table, τ denotes a GED threshold, and LF is a basic filter that utilizes the difference between label multisets of graphs. LF gives an upper bound on the number of candidates. From the results in the table, we observe that the number of candidates grows significantly faster than that of results until it almost reaches an obvious upper bound, i.e., the number of candidates generated by LF.

Motivated by the observation, we propose in Section 3 a fundamentally different filtering approach that makes use of GED computation results in generating candidate graphs. The main idea is that if we identify a graph r as a result of the query, we immediately (re)generate candidate graphs using a subset of pre-computed
graphs similar to \( r \). Unlike existing techniques that strictly separate the filtering phase from the verification phase, our approach makes the filtering phase interact with the verification phase. That is, candidate graphs are continuously regenerated whenever a result of the query is identified in the verification phase.

To compute the GED between a pair of graphs, existing solutions \([9, 13, 15, 23, 25–28, 30]\) perform a best-first search in the space of all possible vertex mappings between the pair, which are organized into a prefix tree. An intermediate node of the prefix tree represents a partial vertex mapping. At each tree node, a GED lower bound of the corresponding partial vertex mapping is computed, and the subtree rooted by the node is pruned if the lower bound is greater than the threshold. In computing a GED lower bound of a partial mapping, all existing solutions exploit label set differences of unmapped vertices and edges. However, a label set-based lower bound tends to be very loose since it cannot reflect structural differences. As a consequence, existing solutions suffer from a huge search space.

To reduce the search space, we formulate the GED computation problem as a repetition of filtering dissimilar subgraphs. Although the existing filtering techniques exhibit poor performance as a threshold increases, we show in Section 4 that they can be effectively used to filter out dissimilar subgraphs during GED computation. Based on the observation, we develop a novel and efficient GED computation algorithm that integrates alternative filtering techniques, which have been used for generating candidates.

In summary, the following are the contributions of this paper.

- We propose a new approach to graph similarity search that exploits GED computation results in generating candidates and utilizes a series of filtering techniques in GED computation.
- We show that candidate graphs can be dynamically regenerated while verifying candidate graphs, and propose a novel graph similarity search algorithm based on the candidate regeneration method.
- We develop an efficient GED computation algorithm that substantially reduces the search space by utilizing a series filtering techniques. We judiciously select filters for GED computation, and carefully apply the selected filters to efficiently prune dissimilar subgraphs.
- We integrate the proposed techniques into a new search framework named \( \text{nass} \) (new approach to graph similarity search), and implement the framework. We conduct extensive experiments on real datasets and show that \( \text{nass} \) outperforms existing techniques by orders of magnitude.

The rest of the paper is organized as follows: Section 2 presents preliminaries and related work. Section 3 proposes a new method to generate candidate graphs via GED verification, and presents our search framework. Section 4 develops an efficient GED computation algorithm that takes advantage of a series filtering techniques. Section 5 presents implementation issues, and Section 6 reports experimental results. Section 7 concludes the paper.

## 2 PRELIMINARIES AND RELATED WORK

### 2.1 Problem Formulation

In this paper, we focus on undirected and labeled simple graphs, though the proposed technique can be easily extended other types of graphs. An undirected and labeled simple graph \( g \) is a triple \((V(g), E(g), l)\), where \( V(g) \) is a set of vertices, \( E(g) \subseteq V(g) \times V(g) \) is a set of edges, and \( l : V(g) \cup (V(g) \times V(g)) \rightarrow \Sigma \) is a labeling function that maps vertices and edges to labels, where \( \Sigma \) is the label set of vertices and edges. \( l(v) \) and \( l(u, v) \) respectively denote the label of a vertex \( v \) and the label of an edge \((u, v)\). If there is no edge between \( u \) and \( v \), \( l(u, v) \) returns a unique value \( \lambda \) distinguished from all other labels. We also define a blank vertex \( \varepsilon \) such that \( l(\varepsilon) = l(\varepsilon, v) = l(\varepsilon, u) = \lambda \). There are no self-loops nor more than one edge between two vertices. For simplicity, in the rest of the paper, we use graph to denote undirected and labeled simple graph.

To measure the similarity between a pair of graphs, we use graph edit distance defined in Definition 1.

**Definition 1 (Graph edit distance).** The graph edit distance (GED) between two graphs \( g_1 \) and \( g_2 \), which is denoted by \( \text{ged}(g_1, g_2) \), is the minimum number of edit operations that transform \( g_1 \) into \( g_2 \), where an edit operation is one of the following:

1. insertion of an isolated labeled vertex
2. deletion of an isolated labeled vertex
3. substitution of the label (i.e., relabeling) of a vertex
4. insertion of a labeled edge
5. deletion of a labeled edge
6. substitution of the label (i.e., relabeling) of an edge.

### Example 1

Consider two graphs \( q \) and \( g_1 \) in Figure 1, where the solid and hollow lines represent edge labels. To transform \( q \) into \( g_1 \), we can perform the following three edit operations on \( q \):

- substitution of the label of the edge between \( a \) and \( b \) (from a hollow edge to a solid edge),
- insertion of a solid edge between \( b \) and \( c \), and deletion of the edge between \( b \) and \( c \). Therefore, \( \text{ged}(q, g_1) = 3 \).

**Lemma 1.** GED defined in Definition 1 is metric \([5]\), and the following properties hold on GED.

- \( \forall g_1, g_2 \quad \text{ged}(g_1, g_2) \geq 0 \).
- \( \forall g_1, g_2 \quad (g_1 = g_2 \iff \text{ged}(g_1, g_2) = 0) \).
- \( \forall g_1, g_2 \quad \text{ged}(g_1, g_2) = \text{ged}(g_2, g_1) \).
- \( \forall g_1, g_2, g_3 \quad \text{ged}(g_1, g_2) \leq \text{ged}(g_1, g_3) + \text{ged}(g_2, g_3) \).

We formulate the problem of graph similarity search in a graph database, as follows.

**Definition 2 (Graph similarity search problem).** For a graph database \( D \) and a query graph \( q \) with a GED threshold \( \tau \), the problem of graph similarity search is to find a result set, denoted by \( R(q, \tau) \), containing all data graphs \( g \in D \) such that \( \text{ged}(q, g) \leq \tau \).
2.2 GED Computation

In this subsection, we provide a general description of existing GED computation methods. A vertex mapping between two graphs $g_1$ and $g_2$ is a bijection of $V(g_1)$ onto $V(g_2)$\(^1\). A vertex mapping is represented by an ordered set of mapped vertex pairs, where the order is imposed by a pre-defined ordering of $V(g_2)$. Given a vertex mapping $m$, $g_1$ can be transformed into $g_2$ by abiding by $m$ as follows. For each mapped vertex pair $u \mapsto v \in m$, we make $u$ and $v$ identical in terms of the labels of the vertices and the labels and connectivity of their adjacent edges. The number of edit operations required in this transformation is called the edit cost of $m$, which is formally stated in Definition 3.

**Definition 3 (Edit cost).** Let $u \mapsto v$ be the last mapped vertex pair in $m$, and $m' = m - \{u \mapsto v\}$. The edit cost of $m$ is defined as:

$$ec(m) = ec(m') + d[l(u), l(v)] + \sum_{u' \mapsto v' \in m'} d[l(u, u'), l(v, v')]$$

where $ec(\emptyset) = 0$ and $d[x, y] = \begin{cases} 0, & \text{if } x = y \\ 1, & \text{otherwise} \end{cases}$.

GED computation is a process to find a vertex mapping having a minimum edit cost among all possible vertex mappings between $g_1$ and $g_2$. To avoid redundant edit cost computation among vertex mappings that shares a prefix, all possible vertex mappings can be organized into a prefix-sharing tree, which is called a search tree.

**Figure 2: Two graphs $g_1$ and $g_2$.**

An example search tree for the graphs in Figure 2 is depicted in Figure 3. In this example, the pre-defined vertex ordering of $g_2$ is $(v_1, v_2, \ldots, v_5)$. Each intermediate node $n$ represents a partial mapping, which is a shared prefix of the vertex mappings in the leaves of the subtree rooted by $n$. Let the $j^{th}$ vertex of $g_2$ be $v$. A tree node containing a vertex $u$ of $g_1$ at level $i$ represents a mapping $m_{ip} \cup \{u \mapsto v\}$, where $m_{ip}$ is the mapping of the parent node, and the mapping of the root is $\emptyset$. In Figure 3, for example, the node indicated by an arrow corresponds to a partial mapping $m = \{u_1 \mapsto v_1, u_2 \mapsto v_2\}$. Since a partial mapping uniquely identifies a node in the search tree, we use a partial mapping interchangeably with the corresponding tree node if clear from the context.

\(^1\)If $|V(g_1)| \neq |V(g_2)|$, we add $|V(g_1)| - |V(g_2)|$ copies of a blank vertex $x$ into $V(g_1)$ or $V(g_2)$ to make $|V(g_1)| = |V(g_2)|$ based on the observation of [30].

**Figure 3: Search tree for graphs in Figure 2.**

**Definition 4 (Lower bound of a partial mapping).** The lower bound of a partial mapping $m$, denoted by $lb(m)$, is a lower limit of the edit costs of the vertex mappings in the leaves of the subtree rooted by $m$.

Given a GED threshold $\tau$, the subtree rooted by $m$ is pruned if $lb(m) > \tau$. To compute $lb(m)$, we first divide each graph participating in $m$ into the following three parts:

- The mapped subgraph of $g$, which is denoted by $g_{\setminus m}$, is an induced subgraph of $g$ defined by the vertices of $g$ participated in $m$.
- The unmapped subgraph of $g$, which is denoted by $g \setminus g_{\setminus m}$, is an induced subgraph of $g$ defined by the vertices in $V(g) \setminus V(g_{\setminus m})$.
- The bridges are edges connecting $g_{\setminus m}$ to $g \setminus g_{\setminus m}$.

Then, $lb(m)$ is computed as the sum of

1. the edit cost required between $g_{\setminus m}$ and $g_{\setminus m}$, which is computed as $ec(m)$ (Definition 3);
2. a lower bound of the GED between $g_{\setminus m}$ and $g_{\setminus m}$, which is computed using the label set-based lower bound (Definition 5);
3. and a lower bound of the number of edit operations required to make the bridges of $g_{\setminus m}$ and $g_{\setminus m}$ identical, which is computed using the bridge cost (Definition 6).

**Definition 5 (Label set-based lower bound [26]).** The label set-based lower bound between two graphs $g_1$ and $g_2$ is defined as:

$$lb_L(r, s) = \Gamma(L_1(r), L_2(s)) + \Gamma(L_2(r), L_1(s))$$

where $L_1(g)$ and $L_2(g)$ denotes the label multisets of vertices and edges of a graph $g$, respectively, and $\Gamma(A, B) = \max(|A|, |B|) - |A \cap B|$.

**Definition 6 (Bridge cost [9]).** Given a partial mapping $m$, the number of bridge operations required in the bridges are at least

$$B(m) = \sum_{u \mapsto v \in m} \Gamma(L^m_B(u), L^m_B(v))$$

where $L^m_B(w)$ denotes the label multiset of the bridges connected to a vertex $w$.

**Example 3.** Consider a partial mapping $m = \{u_1 \mapsto v_1, u_2 \mapsto v_2\}$ between the two graphs in Figure 2. The mapped subgraphs, unmapped subgraphs, and bridges of the graphs are depicted in blue, black, and red lines in the figure, respectively. The edit cost between $g_{\setminus m}$ and $g_{\setminus m}$ is 0 since $ec(m) = 0$. The label multiset of the vertices in $g_{\setminus m}$ is $\{B, C, D\}$, which is the same as that in $g_{\setminus m}$. Similarly, the label multiset of the edges in $g_{\setminus m}$ is identical to that in $g_{\setminus m}$. Hence, $lb_L(g_{\setminus m}, g_{\setminus m}) = 0$. $B(m) = 2$ because the bridge label difference between $u_1$ and $v_1$ is 1 and that between $u_2$ and $v_2$ is also 1. Therefore, $lb_M(m) = 2$. 

**Example 2.** For the graphs in Figure 1, consider a graph database $D = \{g_1, g_2, \ldots, g_s\}$, and a query graph $q$ with a GED threshold $\tau = 2$. The following table shows the GED between $q$ and $g_i$.

| ged($q, g_i$) | $g_1$ | $g_2$ | $g_3$ | $g_4$ | $g_5$ | $g_6$ | $g_7$ | $g_8$ | $g_9$ |
|---------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| $g_1$         | 3     | 1     | 4     | 2     | 4     | 4     | 3     | 1     | 5     |

Hence, the graph similarity search returns $R(q, 2) = \{g_2, g_4, g_6\}$. 

**Table 1: GED values between $q$ and each $g_i$.**
Most of existing solutions traverse the search tree in a best-first fashion based on the lower bound of each node. Initially, the search tree has a root node only. They first expand child nodes of the root node of the search tree. Then, they repeatedly expand child nodes of a node having the lowest lower bound. It is guaranteed that if they meet a leaf node, the vertex mapping for the leaf has the minimum edit cost. If all the subtrees of expanded nodes are pruned, the pair of graphs does not meet the given GED threshold.

2.3 Related Work

Existing filtering techniques utilize features of graphs to establish a necessary condition to meet a GED threshold. Motivated by q-gram idea in string similarity search (e.g., [22]), k-AT [20] defines a q-gram as a tree rooted by a vertex v with all vertices reachable to v in q hops, and GSImSearch [26, 27] defines a path-based q-gram which is a simple path with length q. These techniques are based on the observation that if the GED between two graphs is within a threshold, then the graphs should share at least a certain number of q-grams. c-star [23] and branch [29] structures have been proposed to derive GED lower bounds through bipartite matching. c-star is 1-gram defined by k-AT and branch is a vertex with edges adjacent to the vertex. All of these filtering techniques have focused on developing offline index structures. SEGOS [21] is a two-level index structure proposed to efficiently search star structures.

Recent techniques [9, 13, 25, 28] make use of disjoint substructures of graphs to capture structural differences between graphs. Based on the observation in string similarity search (e.g., [12]) and DNA read mapping techniques (e.g., [10]), they decompose each data graph into partitions, and filter out data graphs dissimilar to the query using the pigeonhole principle. Pars [25, 28] and MLIndex [13] build offline inverted indices on partitioned subgraphs. Mixed [30] utilizes small and large disjoint substructures along with branch structures. Inves [9] develops an online partitioning algorithm that can be used without an index.

The most widely used algorithm for GED computation is A*-GED [15]. Recently, BLP-GED [11], DF-GEA [1], and CSI_GED [7, 8] have been proposed to improve the performance of GED computation. BLP-GED formulates the problem as a binary linear program, and it is faster and more memory-efficient than A*-GED. DF-GEA traverses the search space in a depth first fashion. It has been found to much more memory-efficient than A*-GED. In contrast, CSI_GED proposed an edge-based depth-first search. It also has been found to be both much faster and more memory-efficient than A*-GED.

The verification phase of graph similarity search techniques has been developed based on the A*-GED algorithm. GSImSearch [26] has suggested that the lower bound computation of A*-GED be improved by utilizing the label set differences. This is much faster than the bipartite heuristic used in A*-GED. Inves [9] has introduced a bridge-based lower bound estimation technique, which substantially reduces the search space. Inves and GSImSearch also exploited effective vertex orderings for improving the performance of GED computation.

3 SIMILARITY SEARCH FRAMEWORK

In this section, we present a new approach to graph similarity search. We first show that candidates of a query can be generated through GED verification, then develop a novel graph similarity search algorithm. We analyze the proposed approach to show it can substantially reduce the number of candidates.

3.1 Candidate Generation Method

In this subsection, we show that candidates of a query can be generated from the similarity search results of a data graph. After we define a candidate set in Definition 7, we formally state our observation in Lemma 2.

**Definition 7 (Candidate set).** For a graph database $\mathcal{D}$ and a query graph $q$ with a GED threshold $\tau$, a candidate set $C$ of the query is any subset of $\mathcal{D}$ that satisfies $\mathcal{R}(q, r) \subseteq C$.

**Lemma 2.** Consider a graph database $\mathcal{D}$ and a query graph $q$ with a GED threshold $\tau$. Given a data graph $g \in \mathcal{D}$ such that $\text{ged}(q, g) = \delta \leq \tau$, the following inclusion relationships hold.

\[ \mathcal{R}(q, r) \subseteq \mathcal{R}(g, r + \delta) \]
\[ \mathcal{R}(g, r - \delta) \subseteq \mathcal{R}(q, r) \]

**Proof.** For every graph $r \in \mathcal{R}(q, r)$, the triangle inequality $\text{ged}(g, r) \leq \text{ged}(q, r) + \text{ged}(g, r)$ holds by Lemma 1. Since $\text{ged}(q, r) \leq r$ and $\text{ged}(g, r) = \delta$, $\text{ged}(g, r) \leq r + \delta$, which implies $r \in \mathcal{R}(g, r + \delta)$. It can be similarly proved that every graph $r' \in \mathcal{R}(g, r - \delta)$ is included in $\mathcal{R}(q, r)$.

Lemma 2 suggests that as soon as we identify a result of the query, we can generate a candidate set. It also suggests that some candidate graphs can be directly determined as results of a query without any verification. For every pair of graphs $g_1$ and $g_2$ in $\mathcal{D}$, $\text{ged}(g_1, g_2)$ can be pre-computed and materialized to immediately obtain $\mathcal{R}(q, r + \delta)$ and $\mathcal{R}(g, r - \delta)$ stated in Lemma 2. We use the pre-computed results as an index for generating candidates of a query. For example, Figure 4 shows pre-computed GEDs for the graphs in Figure 1. We will discuss how to implement such an index in Section 5.1. Example 4 demonstrates our candidate generation.

**Example 4.** In Figure 1, consider the query graph $q$ with a GED threshold $\tau = 2$. $g_2$ is a result of the query because $\text{ged}(q, g_2) = \delta = 1$. As soon as $g_2$ is identified as a result, $\mathcal{R}(g_2, r + \delta) = \{g_1, g_2, g_6, g_8\}$ becomes a candidate set of the query by Lemma 2. Among the candidates, $g_8$ is identified as a result of the query without verification, because $\mathcal{R}(g_2, r - \delta = 1) = \{g_2, g_8\}$ (by Lemma 2).
3.2 Search Algorithm

For a query graph $q$ with a GED threshold $\tau$, let $\mathcal{A}$ be a set of results identified so far (initially, $\mathcal{A} = \emptyset$). For the ease of presentation, we abuse a candidate set to denote any subset $C$ of the database $\mathcal{D}$ that satisfies $(R(q, \tau) - \mathcal{A}) \subseteq C$.

Using the label-set-based lower bound in Definition 5, we first generate an initial candidate set $C_0 = \{q' \in \mathcal{D} \mid \text{lb}_q(q') \leq \tau\}$. Then, we repeatedly regenerate a candidate set using Lemma 2 whenever we find a result from the current candidate set, which is initially $C_0$. Definition 8 and Lemma 3 formally state the candidate regeneration. In the following description, we assume that if we find a result $r$ such that $\text{ged}(q, r) = \delta$, we also immediately identify the results in $R(r, \tau - \delta)$ by Lemma 2.

**Definition 8 (Candidate regeneration).** Given a candidate set $C$, let $r$ be the first result identified in $C$, and $\text{ged}(q, r) = \delta$. The refined candidate set $RC(C)$ is defined as:

$$RC(C) = (C - \mathcal{V}(C)) \cap (R(r, \tau + \delta) - R(r, \tau - \delta)),$$

where $\mathcal{V}(C)$ denotes the set of those candidates in $C$ that are verified until the first result $r$ is identified.

**Lemma 3.** The refined candidate set $RC(C)$ in Definition 8 contains all remaining results.

**Proof.** It is obvious that $C - \mathcal{V}(C)$ contains all remaining results. Because, by Lemma 2, $R(r, \tau + \delta)$ is a candidate set of the query and $R(r, \tau - \delta)$ contains identified results, $R(r, \tau + \delta) - R(r, \tau - \delta)$ also contains all remaining results. Therefore, $(C - \mathcal{V}(C)) \cap (R(r, \tau + \delta) - R(r, \tau - \delta))$ contains all remaining results. $\square$

In our method, the total number of candidates is dynamically determined because candidates are repeatedly regenerated while processing a query. Lemma 4 gives a formula to compute the set of total candidates that are verified through GED computation, and Corollary 1 states how to obtain the result set of the query.

**Lemma 4.** Given a candidate set $C$, the set of all candidates that are verified through GED computation is

$$\text{NassCand}(C) = \mathcal{V}(C) \cup \text{NassCand}(RC(C)),$$

where $\text{NassCand}(\emptyset) = \emptyset$.

**Proof.** $\mathcal{V}(C)$ contains all candidates already verified, and RC$(C)$ contains all results requiring GED verification by Lemma 3. Therefore, it can be proved by induction that $\text{NassCand}(C)$ contains all candidates requiring GED verification. $\square$

**Corollary 1.** Let $\{(r_1, \delta_1), \ldots, (r_n, \delta_n)\}$ be the results identified while verifying candidates in $\text{NassCand}(C_0)$, where $C_0$ is an initial candidate set. The result set of the query is $\bigcup_{i=1}^{n} R(r_i, \tau - \delta_i)$.

**Proof.** $R(q, \tau) = \bigcup_{i=1}^{n} (r_i \cup R(r_i, \tau - \delta_i))$ by Lemma 3 and Lemma 4. For all $r_i \in R(r_i, \tau - \delta_i)$, since $\text{ged}(r_i, r_i) = 0$ by Lemma 1 and $0 \leq \delta_i \leq \tau$. Therefore, $\bigcup_{i=1}^{n} r_i \subseteq \bigcup_{i=1}^{n} R(r_i, \tau - \delta_i)$. $\square$

**Example 5.** Consider the query in Example 2 again. The initial candidate set is $C_0 = \{g_1, \ldots, g_8\}$, since $V(C) = \{g_1, \ldots, g_8\}$, but $\text{lb}_q(g_9) = 4 > \tau$. To evaluate the query, we verify $g_1$ and $g_2$ to find the first result $g_2$ because $\text{ged}(q, g_2) = 1$. Therefore, $\mathcal{V}(C_0) = \{g_1, g_2\}$. After $g_2$ is identified as a result, by Definition 8, remaining candidates of the query are refined to

$$RC(C_0) = (C_0 - \mathcal{V}(C_0)) \cap (R(g_2, 2 + 1) - R(g_2, 2 - 1)) = \{(g_1, \ldots, g_8) - \{g_1, g_2\}\} \cap \{(g_1, g_2, g_4, g_6, g_8) - \{g_2, g_8\}\} = \{g_4, g_6\}.$$

Let $C_1 = RC(C_0)$. Given the refined candidate set $C_1$, we identify $g_4$ as the first result in $C_1$ because $\text{ged}(q, g_4) = 2$. Hence, $\mathcal{V}(C_1) = \{g_4\}$ and $C_1$ is refined to

$$RC(C_1) = (C_1 - \mathcal{V}(C_1)) \cap (R(g_4, 2 + 2) - R(g_4, 2 - 2)) = \{(g_4, g_6) - \{g_4\}\} \cap \{(g_1, g_2, g_4, g_6, g_8) - \{g_4\}\} = \emptyset.$$

By Lemma 4, all the verified candidates are contained in

$$\text{NassCand}(C_0) = \mathcal{V}(C_0) \cup \text{NassCand}(RC(C_0)) = \mathcal{V}(C_0) \cup \mathcal{V}(C_1) \cup \text{NassCand}(RC(C_1)) = \{g_1, g_2\} \cup \{g_4\} \cup \text{NassCand}(\emptyset) = \{g_1, g_2, g_4\}.$$

Since $(g_2, 1)$ and $(g_4, 2)$ are identified results from $\text{NassCand}(C_0)$, the result set of the query is $R(g_2, 2 - 1) \cup R(g_4, 2 - 2) = \{g_2, g_8\} \cup \{g_4\} = \{g_2, g_4, g_8\}$ by Corollary 1.

**Algorithm 1: Nass(C, q, \tau)**

**input:** $C$ is a candidate set, $q$ is a query graph, and $\tau$ is a GED threshold. **output:** query results in $C$

1. sort graphs in $C$ by their GED lower bounds;
2. $\mathcal{V} \leftarrow \emptyset$;
3. foreach candidate $g \in C$ do
4. \hspace{1em} $\delta \leftarrow \text{NassGED}(q, g, \tau)$; // refer to Algorithm 3
5. \hspace{2em} $\mathcal{V} \leftarrow \mathcal{V} \cup \{g\}$;
6. \hspace{1em} if $\delta \leq \tau$ then
7. \hspace{2em} \hspace{1em} $\mathcal{A} \leftarrow R(q, \tau - \delta)$;
8. \hspace{2em} \hspace{1em} $C' \leftarrow (C - \mathcal{V}) \cap (R(q, \tau + \delta) - \mathcal{A})$;
9. \hspace{2em} \hspace{1em} return $\mathcal{A} \cup \text{Nass}(C', q, \tau)$;
10. return $\emptyset$;

Algorithm 1 outlines our graph similarity search algorithm based on the proposed candidate generation method. Initially, the algorithm is called with a candidate set generated using the label set-based lower bound. Given a candidate set $C$, the algorithm sorts candidates by their GED lower bounds (Line 1). By sorting the candidates, it first verifies those candidates that are more likely to be results. It computes the GED between the query and each candidate using our GED computation algorithm NassGED, which will be presented in Section 4.3 (Line 4). Candidates verified until the first result is found are appended into $\mathcal{V}$ (Line 5). If the algorithm encounters the first result (Line 6), it appends the results in $R(q, \tau - \delta)$ into $\mathcal{A}$ by Corollary 1 (Line 7), and refines remaining candidates based on Definition 8 (Line 8). Then, it continues to
verify and refine candidates (Line 9). If it cannot find any result from C, it returns an empty set (Line 10).

Correctness of Algorithm 1. Since the algorithm scans the candidate set C sequentially, it always collects the first result along with those results that do not require GED verification by Lemma 2 (Line 7). Then, it regenerates a candidate set which is assured to contain all remaining results requiring verification by Lemma 3 (Line 8). Therefore, it can be proved by induction that the algorithm correctly collects all results.

3.3 Analysis of Our Algorithm

We analyze our algorithm by estimating the number of candidates requiring GED verification. Before we estimate it, we briefly review candidate sets generated by existing solutions. Given a query q with a GED threshold r, all existing candidate generation techniques use a GED lower bound function \( f_{lb} \) to generate a candidate set \( C_{lb}(q,r) = \{ g \mid g \in \mathcal{D} \land f_{lb}(g,q) \leq r \} \). Proposition 1 states the relationship between candidate sets generated by a GED lower bound function \( f_{lb} \).

**Proposition 1.** For any GED lower bound function \( f_{lb} \), the following implication holds:

\[ \forall r_1, r_2 \; r_1 \leq r_2 \implies C_{lb}(q, r_1) \subseteq C_{lb}(q, r_2). \]

**Proof.** For every candidate \( g \in C_{lb}(q, r_1) \), \( f_{lb}(g,q) \leq r_1 \leq r_2 \). Therefore, \( g \in C(q, r_2) \). \( \square \)

Given an initial candidate set, we assume that all results of the query are uniformly distributed in the candidate set. Based on the assumption, Lemma 5 estimates the expected number of candidates requiring GED computation.

**Lemma 5.** Given an initial candidate set \( C_{lb}(q, r) \) generated using the label set-based lower bound \( lb_{L} \), the expected number of candidates generated by Nass that require GED computation is as follows:

\[ |\text{NassCand}(C_{lb}(q, r))| < \frac{|C_{lb}(q, \delta_{min})|}{|R(q, \delta_{min})| + 1} + |R(r, \delta + \delta_{min})|, \]

where \( \delta_{min} = \min_{g \in R(q, \tau)} \text{ged}(q,g) \) and \( r \) is a result of the query such that \( \text{ged}(q, r) = \delta_{min} \).

**Proof.** Since our algorithm sorts initial candidates by their GED lower bounds, candidates in \( C_{lb}(q, \delta_{min}) \) are verified first by Proposition 1. The first result whose distance is \( \delta \) should be contained in \( C_{lb}(q, \delta_{min}) \), where \( \delta_{min} \leq \delta \leq \tau \). Because there are at least \( |R(q, \delta_{min})| \) results in \( C_{lb}(q, \delta_{min}) \), by the uniformity assumption, the algorithm can find the first result after verifying at most \( n_{LG} = \frac{|C_{lb}(q, \delta_{min})|}{|R(q, \delta_{min})| + 1} \) candidates. By the assumption again, a result \( r \) whose distance is \( \delta_{min} \) should be found after verifying \( n_{LG} \) candidates. Therefore, the number of regenerated candidates is less than \( |R(r, \tau + \delta_{min})| \) by Lemma 2 and Lemma 3. \( \square \)

Based on Lemma 5, the following example estimates the number of candidates verified by Nass using the empirical results in Table 1. We note that the candidate generation method using the label set-based lower bound \( lb_{L} \) is the label filtering method LF in Table 1.

**Example 6.** Let’s consider the case where \( \tau = 4 \) and \( \delta_{min} = \tau - 1 = 3 \). In Table 1, \( |C_{lb}(q, \delta_{min})| = 285 \) and \( |R(q, \delta_{min})| = 1.26 \). Therefore, we can expect \( 285 / (1 + 1.26) = 126.1 \) candidates verified until the first result identified. Because the average number of results on threshold \( \tau + \delta_{min} \) is 18.45 in Table 1, the expected total number of candidates verified by our algorithm is at most 126.1 + 18.45 = 144.55, which much less than that of existing techniques on that threshold (i.e., \( \tau = 4 \)).

We remark that any existing filtering method, i.e., lower bound functions, can be used to generate an initial candidate set for Nass. If we use Inves filtering method, for example, the expected number of candidates becomes 44.55 in Example 6. Nonetheless, we use a basic filtering method LF in generating initial candidates because our GED computation algorithm in Section 4 integrates existing filtering techniques.

4 GED COMPUTATION

In this section, we first introduce our GED computation model. Then, we propose a filtering pipeline for GED computation. We finally present the details of our GED computation algorithm.

4.1 Motivation and GED Computation Model

As presented in Section 2.2, existing solutions compute a lower bound of a partial mapping \( m \) between two graphs \( g_1 \) and \( g_2 \) as:

\[ lb_{M}(m) = ec(m) + B(m) + lb_{L}(g_1 \setminus g_{l_{m}}, g_2 \setminus g_{l_{m}}). \]

In the formula, \( ec(m) \) is the tight bound and \( B(m) \) is a relatively precise bound. However, the label set-based lower bound \( lb_{L} \) which is used for the unmapped subgraphs, is very loose because it does not take structural differences into considerations. As a consequence, existing solutions suffer from a huge search space. To address the problem, throughout Section 4, we focus on tightening the lower bound between the unmapped subgraphs by introducing a lower bound function, which exploits a few existing GED lower bounds.

Let \( f_{lb} \) be a GED lower bound function. If \( lb_{M}(m) = ec(m) + B(m) + f_{lb}(g_1 | g_{l_{m}} \setminus | g_{l_{m}} | > \tau \), by Definition 4, we can prune the subtree rooted by \( m \) from the search tree. By rewriting the inequality focusing on \( f_{lb} \), we establish the following filtering condition.

**Condition 1.** Given a partial matching \( m \), we can prune the subtree rooted by \( m \) if \( f_{lb}(g_1 | g_{l_{m}} \setminus g_{l_{m}} | > \tau - (ec(m) + B(m)) \).

Using Condition 1, we model GED computation as a repetition of filtering dissimilar unmapped subgraphs while traversing the search tree. To efficiently obtain a tight \( f_{lb}(g_1 | g_{l_{m}} \setminus g_{l_{m}} | > \tau \), in Section 4.2, we judiciously select and carefully apply a series of existing feature-based lower bound functions, which have been used in generating candidates. As pointed out in Section 1, existing feature-based filtering techniques have a limitation in filtering dissimilar graphs. Nevertheless, we observe that they can be effectively used in pruning dissimilar unmapped subgraphs for GED computation as stated in Claim 1.

**Claim 1.** Given a partial matching \( m \) between \( g_1 \) and \( g_2 \),

\[ Pr[f_{lb}(g_1, g_2) > \tau] \leq Pr[f_{lb}(g_1 | g_{l_{m}} \setminus g_{l_{m}} | > \tau')] \]

for any lower bound function \( f_{lb} \), where \( Pr[p] \) denotes the probability that \( p \) is true, and \( \tau' = \tau - (ec(m) + B(m)) \).
Proof. In this proof, we use an approximate assumption\(^2\) that \(l_{bM}(m_1) \leq l_{bM}(m_2)\) for any mappings \(m_1\) and \(m_2\) such that \(m_1\) is a prefix of \(m_2\). Since an empty mapping \(\emptyset\) is a prefix of any mapping, by the assumption,

\[
l_{bM}(\emptyset) = f_b(g_1, g_2) \\
\leq ec(m) + B(m) + f_b(g_1 | g_1 | m, g_2 | g_2 | m) = f_{bM}(m).
\]

Thus, \(\tau - f_b(g_1, g_2) \geq \tau' - f_b(g_1 | g_1 | m, g_2 | g_2 | m)\), which implies \(Pr\{f_b(g_1, g_2) > \tau\} \leq Pr\{f_b(g_1 | g_1 | m, g_2 | g_2 | m) > \tau'\}\). \(\square\)

Condition 1 also enables us to design a new GED computation algorithm that seamlessly integrates the filtering phase into GED computation. If we apply Condition 1 to the root node of the search tree (i.e., \(m = \emptyset\)), the condition becomes \(f_b(g_1, g_2) > \tau\), which is the condition used in the filtering phase of existing search techniques. For example, if we use the online partitioning-based lower bound of Inves [9] as \(f_b\), and apply it to the root node, we can make a GED computation algorithm that encompases the candidate refinement step of Inves. We remark that existing GED algorithms compute the lower bound of a mapping that has at least one mapped vertex pair. We will present the details of our GED computation algorithm in Section 4.3.

### 4.2 Filtering Pipeline in GED Computation

To tighten \(f_b(g_1 | g_1 | m, g_2 | g_2 | m)\), we apply a series of filtering techniques. There is a trade-off between the efficiency in computing \(f_b\) and the tightness of \(f_b\). Because the number of nodes to visit in the search tree grows exponentially, efficient computation of a lower bound is crucial. With tight lower bounds, on the other hand, we can prune more subtrees in the search tree, and the number of nodes to visit can be reduced substantially. Therefore, the goal here is to judiciously select filtering techniques adequate for reducing the search space, and to carefully apply selected filters for efficient computation. To speed up the computation of \(f_b\), we will also discuss implementation issues in Section 5.2.

We first introduce two existing lower bound functions we select for GED computation. Given a partial mapping \(m\), for simplicity, we use \(g'\) to denote \(g | m\) for a graph \(g\) in this subsection.

**Definition 9 (Compact branch-based lower bound [30]).** Given two vertices \(u\) and \(v\), their branch structures are denoted as \(b_u = (l(u), ES(u))\) and \(b_v = (l(v), ES(v))\), where \(ES(w) = \{l(e)\mid e\ is\ adjacent\ to\ w\}\). The compact distance between \(b_u\) and \(b_v\) is defined as:

\[
bed_C(b_u, b_v) = \begin{cases} 0, & \text{if } l(u) = l(v) \land ES(u) = ES(v) \\ 1/2, & \text{if } l(u) = l(v) \land ES(u) \neq ES(v) \\ 1, & \text{if } l(u) \neq l(v) \end{cases}
\]

Compact branch-based lower bound is defined as:

\[
l_{bC}(g'_1, g'_2) = \min \sum_{b_u \in B(g'_1)} \text{bed}_C(b_u, P(b_u)),
\]

where \(B(g)\) is the multiset of the branches of a graph \(g\), and \(P\) is a bijection from \(B(g'_1)\) to \(B(g'_2)\). If \(|B(g'_1)| < |B(g'_2)|\), \(|B(g'_2)| - |B(g'_1)|\) blank branches are added into \(B(g'_1)\), and vice versa.

**Example 7.** Let’s recall Example 3 in Section 2.2. The label set-based lower bound of the unmapped subgraphs was 0. This lower bound can be tightened by using the compact branch-based lower bound function as follows. Figure 5(a) shows the branch multisets \(B(g'_1') = \{b_{u_1}, b_{u_4}, b_{u_5}\}\) and \(B(g'_2') = \{b_{v_1}, b_{v_4}, b_{v_5}\}\), and the bijection \(P = \{b_{u_1} \mapsto b_{v_1}, b_{u_4} \mapsto b_{v_4}, b_{u_5} \mapsto b_{v_5}\}\) that minimizes \(l_{bC}(g'_1', g'_2')\). The lower bound \(l_{bC}(g'_1', g'_2') = 1\) because \(bed_C(b_{u_1}, b_{v_1}) = 1/2\), \(bed_C(b_{u_4}, b_{v_4}) = 1/2\), and \(bed_C(b_{u_5}, b_{v_5}) = 0\).

To compute \(l_{bC}(g'_1', g'_2')\), we can use an \(O(n \log n)\) algorithm proposed in [30], where \(n = |B(g'_1')|\). The compact branch-based lower bound is used for generating candidate graphs in [30]. Since it is efficiently computed and captures differences in local structures (i.e., branches) of graphs, we select it for GED computation.

**Definition 10 (Partition-based lower bound [9]).** Consider we decompose \(g'_2\) into partitioned subgraphs. The partition-based lower bound is defined as:

\[
l_{bp}(g'_1, g'_2) = |\{p \in P(g'_2) \mid p \nsubseteq g'_1\}|,
\]

where \(P(g'_2)\) denotes the set of partitions of \(g'_2\), and \(p \nsubseteq g'_1\) denotes \(p\) is not subgraph isomorphic to \(g'_1\).

**Example 8.** In Example 3, consider we decompose \(g'_2\) into two partitions \(p_1\) and \(p_2\) as depicted in Figure 5(b). Since \(p_1 \nsubseteq g'_1\) and \(p_2 \nsubseteq g'_1\), the lower bound \(l_{bp}(g'_1, g'_2) = 1\).

To partition \(g'_2\) in Definition 10, we use the online partitioning algorithm proposed in Inves [9]. With partitions of graphs, we can capture structural differences between graphs, and thus we can expect a more accurate bound in general. However, it is expensive to compute \(l_{bp}\) due to subgraph isomorphism tests. In this paper, therefore, we use \(l_{bp}\) only when other lower bound functions cannot filter out \(g'_1\) and \(g'_2\).

Given a partial mapping \(m\) and a GED threshold \(\tau\), to reduce the overhead of computing lower bounds, we incrementally tighten the lower bound of \(m\) as follows.

\[
l_{bM}(m) = \begin{cases} ec(m), & \text{if } ec(m) > \tau \\ ec(m) + B(m), & \text{else if } ec(m) + B(m) > \tau \\ ec(m) + B(m) + f_b(g'_1, g'_2), & \text{otherwise}, \end{cases}
\]

\(^2\)Due to the inaccuracy of the bridge cost, there can be subtle cases that \(l_{bM}(m_1) > l_{bM}(m_2)\), but the assumption is valid in most cases for any lower bound function \(f_b\). For example, in all experiments in Section 6, there was no mapping that violates the assumption (the total number of different mappings was about 2.5 \times 10^7\ in our experiments).

\(^3\)To save computation time, we modified Inves by disabling the rematch functionality and setting \(\alpha\), i.e., the worst case prevention parameter, to 6 (see [9] for the details).
and \( f_L(g'_1, g'_2) \) is defined as:
\[
f_L(g'_1, g'_2) = \begin{cases} 
L(g'_1, g'_2), & \text{if } L(g'_1, g'_2) > \tau' \\
C(g'_1, g'_2), & \text{else if } C(g'_1, g'_2) > \tau' \\
B(g'_1, g'_2), & \text{otherwise},
\end{cases}
\]

where \( \tau' = \tau - (ec(m) + \mathcal{B}(m)) \).

Interestingly, many partial mappings in the search tree have the same unmapped subgraphs. For the graphs in Figure 2, for example, \( m = \{u_1 \rightarrow v_1, u_2 \rightarrow v_2\} \) and \( m' = \{u_1 \rightarrow v_2, u_2 \rightarrow v_1\} \) have the same unmapped subgraphs. Therefore, we can compute \( f_L(g'_1, g'_2) \) once and share the result in those partial mappings having the same unmapped subgraphs. Lemma 6 states the number of partial mappings having the same unmapped subgraphs.

**Lemma 6.** Given a partial mapping \( m \) between two graphs \( g_1 \) and \( g_2 \), there are \( |m|! / n_e! \) partial mappings in the search tree that have the same unmapped subgraphs, where \( n_e \) is the number of copies of \( e \) in \( V(g_1|m) \).

**Proof.** Given two graphs for GED computation, any graph can be \( g_2 \) by the symmetry in Lemma 1. Therefore, we assume, without loss of generality, there is no \( e \) in \( V(g_2) \). Consider a partial mapping \( m' \) between \( g_1 \) and \( g_2 \) such that \( V(g_1|m) = V(g_1|m') \). By the definition of the unmapped subgraph (see Section 2.2), \( m \) and \( m' \) have the same unmapped subgraph of \( g_1 \). Recall that we use a specific ordering of \( g_2 \) for all mappings. Therefore, \( m' \) and \( m \) also have the same vertex set for \( g_2 \), and the same unmapped subgraph of \( g_2 \). There are \( |m|! / n_e! \) distinct permutations of \( V(g_1|m) \), and thus there are \( |m|! / n_e! \) mappings in the search tree that have the same unmapped subgraphs. \( \Box \)

### 4.3 GED Computation Algorithm

Given a partial mapping \( m \), we compute \( lb_M(m) \) as shown in Algorithm 2. If \( m \) survives from \( ec(m) \) and \( \mathcal{B}(m) \) in our filtering pipeline (Lines 1–4), we look up a hash with \( V(g_1|m) \) to share the computation result of \( f_L(g'_1, g'_2) \), if any, based on Lemma 6 (Line 5). We retrieve a pointer to the hash entry, where the hash entry \( e \) has \( e.lb = f_L(g'_1, g'_2) \) and an index \( e.index \) for the lower bound function used in computing \( f_L(g'_1, g'_2) \) (i.e., one of \( lb_L, lb_C, \) and \( lb_B \)). If the lookup fails, the hash makes a new entry \( e \) such that \( e.lb = 0 \) and \( e.index = 0 \), and return the pointer to the entry. If \( m \) also survives from the lower bound from the hash (Lines 5–6) and not all lower bound functions are applied (Line 9), we apply unused lower bound functions to \( m \) (Lines 9–14), and update the hash entry if necessary (Line 10 and Line 12).

Algorithm 3 encapsulates our GED computation algorithm. It first tries to prune the root of the search tree by computing the lower bound of the root node (Line 2). It is worth to remind that NassGED encompasses the refinement step of Inves by applying \( lb_1 \) in Algorithm 2 to the root node. If it fails to prune the root node, it pushes the root node into the priority queue, \( queue \). Then, it repeatedly expands or prunes the search tree by investigating currently active tree nodes, which are contained in the queue, as follows (the while loop in Lines 3–7). The algorithm pops a mapping \( m \) from the queue that has a minimum lower bound (Line 4). If \( m \) is a full mapping (i.e., a mapping having all vertices in \( g_1 \) and \( g_2 \)), it returns \( lb_M(m) \), which is equal to \( ec(m) \) since \( m \) is a full mapping.

```plaintext
Algorithm 2: lb_M(m, \tau)
input: m is a mapping and \tau is a GED threshold
output: a lower bound of m
1 dist ← ec(m);
2 if dist > \tau then return dist;
3 dist ← dist + \mathcal{B}(m);
4 if dist > \tau then return dist;
5 e ← hash.lookup(V(g_1|m));
6 if dist + e.lb > \tau then return dist + e.lb;
7 f_L ← [lb_L, lb_C, lb_B];
8 i ← e.index + 1;
9 while i ≤ |f_L| do
10 e.index ← i;
11 if e.lb < f_L[i](g'_1, g'_2) then
12 e.lb ← f_L[i](g'_1, g'_2);
13 if dist + e.lb > \tau then return dist + e.lb;
14 i ← i + 1;
15 return dist + e.lb;
```

```plaintext
Algorithm 3: NassGED(g_1, g_2, \tau)
input: g_1 and g_2 are graphs, and \tau is a GED threshold
output: NassGED(g_1, g_2)
1 queue ← \emptyset; m_r ← \emptyset;
2 if lb_M(m_r, \tau) ≤ \tau then queue.push(m_r);
3 while queue ≠ \emptyset do
4 m ← queue.pop();
5 if |m| = |V(g_2)| then return lb_M(m, \tau);
6 foreach child node m_c of m do
7 if lb_M(m_c, \tau) ≤ \tau then queue.push(m_c);
8 return \tau + 1;
```

(Lines 5). Otherwise, it expands the search tree using each child mapping of the popped mapping based on the lower bound of the child mapping (Line 7). The algorithm returns \( \tau + 1 \) if it prunes all possible subtrees of the search tree (Line 9).

**Correctness of Algorithm 3.** \( lb_M \) in Algorithm 2 correctly returns a lower bound because (1) each lower bound function correctly calculates a lower bound [9, 30] and (2) the hash returns a correct lower bound (by Lemma 6). Algorithm 3 pushes every node of the search tree whose lower bound is not greater than \( \tau \) (Line 7). It returns if either it finds a full mapping (Line 5) or the queue is empty (Line 8). Since it pops a mapping having the lowest lower bound from the queue, if the mapping popped from the queue is a full mapping, it is guaranteed that the mapping has a minimum edit cost. If the queue is empty, every partial mapping is pruned since the lower bound is greater than \( \tau \), and thus the algorithm returns \( \tau + 1 \) to indicate \( \text{NassGED}(g_1, g_2) > \tau \) (Line 8).
5 IMPLEMENTATION

5.1 Indexing

Given a graph database \( D \), we need to pre-compute and materialize the GED between every pair of graphs in \( D \) to obtain \( R(g, \tau) \) for any graph \( g \in D \) with any distance threshold \( \tau \). However, it is impractical to build such an index. Instead, we assume a pre-defined maximum threshold \( \tau_{\text{max}} \). By Lemma 2, it is sufficient to compute \( R(g, 2\tau_{\text{max}}) \) for each graph \( g \in D \). We use \( \tau_{\text{index}} \) to denote the maximum GED threshold for indexing, i.e., \( \tau_{\text{index}} = 2\tau_{\text{max}} \).

Algorithm 4: \( \text{NassIndex}(D, \tau_{\text{index}}, n)\)

\[
\begin{align*}
\text{input} & : D \text{ is a graph database, } \tau_{\text{index}} \text{ is a threshold for indexing, } n \text{ is the number of threads.} \\
\text{output} & : \text{Index } I \\
1 & I \leftarrow \text{an array of } |D| \text{ empty lists}; \\
2 & \text{repeat } n \text{ times} \\
3 & \quad \text{spawn:} \\
4 & \quad \quad i \leftarrow \text{next_graph_id}(); \quad // \text{synchronous access} \\
5 & \quad \quad \text{if } i \geq |D| \text{ then return;} \\
6 & \quad \quad I[g_i].append(g_i, 0); \\
7 & \quad \quad \text{for } j \leftarrow i + 1 \text{ to } |D| \text{ do} \\
8 & \quad \quad \quad \delta \leftarrow \text{NassGED}(g_i, g_j, \tau_{\text{index}}); \\
9 & \quad \quad \quad I[g_i].append(g_j, \delta); \\
10 & \quad \quad \quad I[g_j].append(g_i, \delta); \\
11 & \text{sync;} \\
12 & \text{return } I;
\end{align*}
\]

Since we need \(|D|\) independent similarity searches to build an index, we implement a straightforward multi-threading to reduce index building time. Our implementation is to spread each data graph to a different thread, and perform similarity searches simultaneously\(^4\). Algorithm 4 shows our indexing algorithm. After initializing the index (Line 1), it spawns \( n \) threads (the loop in Line 2). Each thread synchronously gets a graph id \( i \) (Line 4), which used to indicate the \( i \)th graph \( g_i \) in \( D \), and computes the GED between \( g_i \) and \( g_j \) for \( j > i \) (Lines 7–8). Then, it updates the index entries \( I[g_i] \) and \( I[g_j] \) with the GED (Lines 9–10).

One problem in indexing is that GED computation with \( 2\tau_{\text{max}} \) can be too costly to be practical. We solve the problems by restricting a maximum threshold for an index to \( \tau_{\text{index}} = \tau_{\text{max}} + c \), where \( c \) is a constant less than \( \tau_{\text{max}} \). For a query graph \( q \), if we find a data graph \( g \) such that \( \text{ged}(q, g) \leq c \), by Lemma 2, we can regenerate candidate graphs using the index for all possible thresholds \( 1 \leq \tau \leq \tau_{\text{max}} \). In Table 1, for example, the average number of results is greater than 1 when \( \tau = 3 \). By using \( c = 3 \) for this dataset, therefore, we can expect almost all queries can take advantage of our index.

Another problem is that GED computation of a certain pair of graphs can be intractable even with a reasonably large threshold.

---

\(^4\)There can be alternative implementations, e.g., improving GED computation using multi-threads or improving a similarity search by spreading candidates to different threads. However, parallel graph search is out of the scope of the paper and we will leave this as future work.

---

We solve the problem by allowing an inexact index entry having a GED lower bound for such a pair of graphs. To this end, we assume that the time consumption is proportional to the memory consumption in computing a GED, and we maintain a thread that monitors the real memory consumption of the indexing process. If the memory consumption reaches a pre-defined limit, we select a victim thread that has the largest queue size of \( \text{NassGED} \). The victim thread immediately returns the minimum lower bound among the lower bounds of queued nodes.

Algorithm 5: Replacement of Lines 7–8 of Algorithm 1

\[
\begin{align*}
1 & \text{if } \tau + \delta \leq \tau_{\text{index}} \text{ then } // \text{regenerate a candidate set} \\
2 & \quad A \leftarrow \{ (r, d) \in I[g] \land d = \tau - \delta \land \text{d is exact} \}; \\
3 & \quad R_g \leftarrow \{ (r, d) \in I[g] \land d \leq \tau + \delta \}; \\
4 & \quad C^* \leftarrow (C - \nu) \cap (R_g - A); \\
5 & \text{else } // \text{keep verifying the current candidate set} \\
6 & \quad A \leftarrow \{ g \}; \\
7 & \quad C^* \leftarrow (C - \nu); \\
\end{align*}
\]

To use our index, we modify Lines 7–8 of Algorithm 1 as shown in Algorithm 5. According to Lemma 2, we regenerate candidates only when \( \delta + \tau \leq \tau_{\text{index}} \) (Line 1). For \( R(g, \tau - \delta) \) in Line 7 of Algorithm 1, we include only those graphs having exact GEDs (Line 2). For \( R(g, \tau + \delta) \) in Line 8 of Algorithm 1, which is used to regenerate candidates, we use an approximate set that includes inexact GEDs (Line 3).

Correctness of Algorithm 5. Since an inexact GED is a GED lower bound (i.e., \( R(g, \tau + \delta) \subseteq R_g \)) and uncollected results in Line 2 are included in \( C^* \) (Line 4), \( C^* \) contains all remaining results. Therefore, the algorithm does not miss any result in spite of inexact index entries. If the algorithm cannot use the index (Line 5), it continues to verify the current candidate set (Line 7). Therefore, a restricted \( \tau_{\text{index}} \) does not affect the result set of the query.

5.2 GED Computation

As discussed in Inves [9], a proper vertex ordering of \( g_2 \) is crucial to the performance of GED computation. In this paper, we abide by the vertex ordering of Inves. Because we apply its partitioning technique to the root node of the search tree, we can immediately use the vertex ordering obtained from the partitioning of \( g_2 \) (refer to [9] for the details).

We use a balanced binary search tree to implement the hash for storing \( \text{ibs}(g_1 | q_{1,m}, g_2 | q_{2,m}) \). It can be easily seen that the time complexity for the hash is exactly the same with that for the priority queue used in the GED computation algorithm. A bitmap, which is used as the key for the hash, is created for each mapping \( m \) to represent \( V(g_1 | m) \) as follows. The bitmap has \( |V(g_1)| \) bits, and the \( i \)th bit is 1 if the \( i \)th vertex of \( g_1 \) is included in \( V(g_1 | m) \), otherwise the \( i \)th bit is 0. Apparently, the bitmap of \( m \) is incrementally created using the bitmap of the parent of \( m \) (i.e., the mapping in the parent node of \( m \) in the search tree) by setting one bit for the vertex newly inserted to \( g_1 | m \). Since we focus on small and medium sized graphs, one or two 64-bit integers are sufficient for a bitmap in most cases.
The lower bound of a mapping can be incrementally computed using its parent mapping. Consider a partial mapping $m_p$ and its child $m_c = m_p \cup \{u' \mapsto v'\}$. We compute lower bounds as follows\(^5\).

**Bridge cost.** The label multiset sets of bridges of $u'$ and $v'$ are constructed from the scratch. The label multiset sets of bridges of other vertices are updated as:

$$
\forall u \in V(g_1|m_p), L_{br}^m(u) \leftarrow L_{br}^{m_p}(u) - \{l(u, u')\},
$$

$$
\forall v \in V(g_2|m_p), L_{br}^m(v) \leftarrow L_{br}^{m_p}(v) - \{l(v, v')\}.
$$

Then, $B(m_c)$ is computed using the label multiset sets of bridges constructed for $m_c$.

**Label-based lower bound.** Let $g_1', g_2', g_1''$, and $g_2''$ denote $g_1 \setminus g_1|m_p$, $g_2 \setminus g_2|m_p$, $g_1 \setminus g_1|m_c$, and $g_2 \setminus g_2|m_c$, respectively. The label multiset sets of unmapped subgraphs are incrementally constructed as follows.

$$
L_V(g_1'') \leftarrow L_V(g_1') - \{l(u')\}, \quad L_V(g_2'') \leftarrow L_V(g_2') - \{l(v')\},
$$

$$
L_E(g_1'') \leftarrow L_E(g_1') - \{l(u, u') | u \in V(g_1') \land (u, u') \in E(g_1')\},
$$

$$
L_E(g_2'') \leftarrow L_E(g_2') - \{l(v, v') | v \in V(g_2') \land (v, v') \in E(g_2')\}.
$$

Then, $lb_l$ is computed using the label multiset sets of $g_1''$ and $g_2''$.

**Compact branch-based lower bound.** We remove $b_u'$ and $b_v'$ from $B(g_1')$ and $B(g_2')$, respectively, and compute $lb_c$ again. As we mentioned earlier, we use $O(n \log n)$ algorithm for finding a minimum weighted bipartite matching between $B(g_1')$ and $B(g_2')$, where $n = |B(g_1')|$ (refer to [30] for the details of the algorithm). The algorithm basically merges $B(g_1')$ and $B(g_2')$ after sorting the branch sets. Therefore, the time complexity of $lb_c$ is dominated by the cost for sorting $B(g_1')$ and $B(g_2')$. As we remove $b_u'$ and $b_v'$ from the already sorted branch sets, our incremental implementation requires $O(n)$, which is the cost for merging the sets.

**Partition-based lower bound.** Unlike other lower bounds, it is not straightforward to incrementally compute the lower bound $lb_p$ from parent’s $lb_p$, and thus we do not use parent’s $lb_p$. Instead, we take a different approach to save computation for $lb_p$. Consider $\tau_2' = \tau - (ec(m_1) + 2 |m_1|)$ for a partial mapping $m_1$. As the partitioning technique of Inves increments lower bound of the lower bound, we can save computation by stopping partitioning as soon as $\text{lb}_p = \tau_1' + 1$. Consider $\tau_2'' = \tau - (ec(m_2) + 2 |m_2|)$ for another partial mapping $m_2$ such that the unmapped subgraphs of $m_1$ and $m_2$ are the same. If $\tau_2'' > \tau_1'$, we cannot prune $m_2$ using the $lb_p$ of $m_1$ stored in the hash. Since $lb_p$ may not be tight, we can compute $lb_p$ again for $m_2$. If the stored $lb_p$ is not tight, we can resume partitioning to tighten $lb_p$ instead of computing $lb_p$ from the scratch. It is straightforward to stop and resume partitioning and we omit the details (refer to [9] for the details of the partitioning technique of Inves).

To save the memory, instead of keeping bridge multiset sets, label multiset sets, and branch multiset sets in each mapping, we compute multiset sets for the parent $m_p$ popped from the queue, and use them to incrementally compute label multiset sets of each child of $m_p$.

\(^5\)We note that $\lambda$, which is introduced in Section 2, is not a label. It is used for indicating the absence of an edge or a vertex, and thus, we do not include $\lambda$ in any label multiset discussed in this paper.

# 6 EXPERIMENTS

## 6.1 Experimental Setting

We conducted experiments on two widely used datasets, AIDS and PubChem. AIDS is an antiviral screen compound data set published by NCI/NIH\(^6\). It is a popular benchmark used in most graph search techniques. PubChem is a chemical compound data set\(^7\). It is a subset of chemical compounds published by the PubChem Project. Graphs in the PubChem dataset contain repeating substructures and have less size and label variations compared with the AIDS dataset. Table 2 shows statistics of the datasets. In the table, $|D|$ is the number of graphs in each dataset, $|V|_{avg}$ and $|E|_{avg}$ are the average numbers of vertices and edges, $\sigma_{|V|}$ and $\sigma_{|E|}$ are the standard deviations of the numbers of vertices and edges, and $n_{vl}$ and $n_{el}$ are the numbers of distinct vertex and edge labels.

| Dataset       | $|D|$ | $|V|_{avg}$ | $|E|_{avg}$ | $\sigma_{|V|}$ | $\sigma_{|E|}$ | $n_{vl}$ | $n_{el}$ |
|---------------|------|------------|------------|--------------|--------------|---------|---------|
| AIDS          | 42,689 | 25.60      | 27.60      | 12.2         | 13.3         | 62      | 3       |
| PubChem       | 22,794 | 48.11      | 50.56      | 9.4          | 9.9          | 10      | 3       |

We also used synthetic datasets to evaluate the scalability of Nass (see Section 6.5 for details).

We randomly sampled 100 query graphs from each dataset. If we find a data graph which is the same as a query graph, our index can immediately find all results of the query by Lemma 2 and Lemma 3. Thus, we removed the query graphs from the dataset not to exaggerate the performance gain of Nass. Aggregated results of 100 queries are reported in the experiments. We note that $y$-axis is log-scaled in all experiments. For experiments on the AIDS and PubChem datasets, we set the maximum threshold $\tau_{\text{max}} = 6$.

We implemented Nass in C++, and compiled it using GCC with the -O3 flag\(^8\). We compared Nass with two representative indexing techniques: Pars [25, 28], and MLIndex [13], and two state-of-the-art GED verification techniques: Inves\(^9\) [9] and CSI_GED\(^10\) [7, 8]. Since the indexing techniques, Pars and MLIndex, mainly rely on the outdated $A^* - \text{GED}$ for verification, we used Inves in the verification phase of them, similar to [9]. All experiments were conducted on a machine with 32GB RAM, and an Intel core i7, running a 64-bit Ubuntu OS. Data graphs and indices were kept in memory.

## 6.2 Experiments on Index

We constructed indices by varying the limit of memory consumption for building an index from 1GB to 8GB. On the AIDS dataset, we used $\tau_{\text{index}} = 5 \times \tau_{\text{max}} + 3$ based on the observation that the average number of results of queries is 1.26 when $\tau = 3$. As described in Section 5.1, almost all queries can take advantage of an index built with the $\tau_{\text{index}}$. On the PubChem dataset, we used $\tau_{\text{index}} = \tau_{\text{max}} + 1$ since the average number of results of queries is 0.94 when $\tau = 1$.

We used 8 threads to construct an index.

\(^6\)https://cactus.nci.nih.gov/download/nci/AIDS2DA99.sdz
\(^7\)https://pubchem.ncbi.nlm.nih.gov. Compound_000975001_001000000.sdf
\(^8\)The source code of Nass is available at https://github.com/JongikKim/Nass.
\(^9\)The source code of Inves is obtained from https://github.com/JongikKim/Inves.
\(^10\)The binary code of CSI_GED is obtained from the authors.
Experimental results for indexing is shown in Table 3. In the table, T, I, and N denote the index construction time, the percentage of inexact entries, and the number of indexed entries, respectively.

Table 3: Experimental results on indexing

| Dataset | Memory limit for indexing |
|---------|------------------------|
|         | 1GB        | 2GB        | 4GB        | 8GB        |
| T       | AIDS       | 190379s    | 192211s    | 193319s    | 195267s    |
|         | PubChem    | 83520s     | 114323s    | 152475s    | 192978s    |
| I       | AIDS       | 0.0033%    | 0.0011%    | 0.0006%    | 0.0002%    |
|         | PubChem    | 5.18%      | 2.74%      | 1.72%      | 0.85%      |
| N       | AIDS       | 4220628    | 4220658    | 4220606    | 4220588    |
|         | PubChem    | 105414     | 103596     | 102992     | 102302     |

A similarity search on AIDS and PubChem datasets typically used about 300MB memory in our implementation. However, the search space for GED computation of a certain pair of graphs sharply increased, and required a tremendous amount of memory. By limiting the memory consumption, therefore, we restricted the time for computing GED between such a pair of graphs. Although it takes much time to construct an index, we remark that an index is pre-built offline and many online queries with different thresholds can take advantage of the index (c.f., Pars [25, 28] also spends more than $10^5$ seconds to build an index for the AIDS dataset).

On the AIDS dataset, the percentage of inexact index entries was negligibly small. On the PubChem dataset, it was from 1% to 5% only. The index size can be measured by the number of indexed entries, where each entry contains a graph id with a GED between $0$ and $t_{index}$. If we use a compact representation, an entry requires $\lceil \log_2 |D| + \log_2 (t_{index} + 1) \rceil + 1$ bits, where 1 bit is used to indicate the exactness of the GED. The size of an index can be calculated by multiplying the number of indexed entries by the size of an entry. For example, the PubChem index with 4GB limit requires approximately $10292 \times \lceil \log_2 22774 \rceil + \lceil \log_2 8 \rceil + 1 \rceil = 309KB$. Similarly, the AIDS index with 4GB memory limits requires about 12MB.

Figure 6 shows the query response time for indices constructed with different memory limits. In the figure, No Index denotes Nass without an index (i.e., each graph was directly verified through NassGED). On the AIDS dataset, a similarity search with an index was up to 3 times faster than that without an index as shown in Figure 6(a). On the PubChem dataset, similarly, an indexed search was up to 9 times faster than a search without an index as shown in Figure 6(b). Based on the experiments, we chose the indices with the 4GB memory limit for both datasets. The reported results in the following section are based on the indices.

6.3 Evaluating Graph Similarity Search

Figure 7 shows the query evaluation results of different search algorithms. In the figure, we use P, M, and N to denote Pars+Inves, MIndex+Inves, and Nass respectively. Nass consistently outperformed all existing algorithms for all thresholds as shown in Figure 7(a) and (b). Nass was from 4 to 13 times faster than existing algorithms on the AIDS dataset (Figure 7(a)), and from 4 to 60 times faster on the PubChem dataset (Figure 7(b)).

The improvement of Nass can be explained by the number of candidates$^{11}$ that require GED computation in Figure 7(c) and (d), and the number of mappings pushed into the queue while GED computation in Figure 7(e) and (f). The number of candidates generated by Nass was up to 4 times smaller than that of existing candidates. Interestingly, on the PubChem dataset, the number of candidates generated by Nass was fewer than the number of result graphs when $r = 1$ (Figure 7(d)). This is because Nass can identify some result graphs without verification. Since our index significantly reduced the number of candidates and our GED algorithm effectively prunes the search tree, the number of mappings pushed into the queue was dramatically reduced as depicted in Figure 7(e) and (f). When $r = 5$ on the AIDS dataset, for example, the total number of mappings pushed into the queue by Nass was about 10 times smaller than that of existing techniques. For a low threshold, however, the number of mappings of Nass was slightly greater than that of existing techniques (e.g., $r = 1$ on the AIDS dataset).

$^{11}$The number of candidates of Nass was counted using those candidates that survived from the filtering pipeline in the root node of the search tree (see Section 4.1 and Section 4.3 for the reason).
6.4 Evaluating GED Verification

We compared our GED computation algorithm, denoted by NassGED, with Inves and CSI_GED. We evaluated the performance of GED computation as follows. For each query, we first applied the label filtering to every graph in a dataset, and then directly verified each graph that passed the label filter.

Figure 8: Comparing NassGED with existing GED computation algorithms

Figure 8(a) and (b) show the results on the AIDS and PubChem datasets, respectively. NassGED consistently outperformed Inves and CSI_GED for \( \tau \geq 2 \). On the AIDS dataset, Inves slightly outperformed NassGED when \( \tau = 1 \), but the difference was negligible. On lower thresholds, NassGED and Inves performed much better than CSI_GED. For \( \tau \geq 3 \), NassGED was up to 2.5 times faster than existing algorithms on the AIDS, and up to 6 times faster on PubChem datasets.

Figure 9: Evaluating the filtering pipeline of NassGED

The improvement of NassGED can be explained by the filtering pipeline (Section 4.2) and efficient implementation (Section 5.2). Figure 9(a) and (b) show the effect of the filtering pipeline on AIDS and PubChem. In the figures, +FP and -FP denote NassGED with and without the filtering pipeline, respectively. As shown in the figure, +FP improved GED computation by up to 2.2 times. +FP was slightly slower than -FP for low thresholds (e.g., \( \tau = 1 \) for AIDS and \( \tau \leq 3 \) for PubChem), because of the overhead of lower bound computation. Although +FP requires more computation for lower bounds, we observed that the overhead of lower bound computation did not affect the performance significantly. The total number of mappings pushed into the queue while GED computation was shown in Figure 9. +FP reduced the number of mappings by up to 3.3 times.

6.5 Scalability Test

In this subsection, we report the results of the scalability of Nass. For the experiments, we generated synthetic datasets using a graph generator GraphGen. The generator measures the graph size in terms of the number of edges (\(|E|\)), and the density of a graph as \(|V|(|V|-1)\). We set up the generator as follows: the average size of graphs is 40; the numbers of distinct vertex and edge labels are 5 and 2, respectively; and the density of each graph is 0.2. We initially generated 4k, 8k, 12k, 16k, and 20k datasets. For each graph in a dataset, we generated 4 more graphs by randomly applying 2, 4, 6, or 10 edit operations to the graph 4 times. For scalability test, we used \( \tau_{\text{max}} = 7 \) and \( \tau_{\text{index}} = \tau_{\text{max}} + 1 \). Figure 10 shows the results. For various thresholds, Nass scaled well to large datasets as shown in the figure.

Figure 10: Evaluating the scalability of Nass

7 CONCLUSIONS

In this paper, we proposed a completely different approach to graph similarity search. We generate candidate graphs via GED verification and verify each candidate via various filtering techniques. The proposed search framework Nass substantially reduces the number of candidates by dynamically regenerating candidates while verifying candidates. To efficiently verify each candidate, our GED computation algorithm utilizes various filtering techniques to significantly prune the search space of the prefix tree. We conducted extensive experiments on both real and synthetic datasets, and the results showed that Nass outperformed the state-of-the art algorithms by an order of magnitude.

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