Abstract—The graph edit distance (GED) is a well-established distance measure widely used in many applications. However, existing methods for the GED computation suffer from several drawbacks including oversized search space, huge memory consumption, and lots of expensive backtracking. In this paper, we present BSS_GED, a novel vertex-based mapping method for the GED computation. First, we create a small search space by reducing the number of invalid and redundant mappings involved in the GED computation. Then, we utilize beam-stack search combined with two heuristics to efficiently compute GED, achieving a flexible trade-off between available memory and expensive backtracking. Extensive experiments demonstrate that BSS_GED is highly efficient for the GED computation on sparse as well as dense graphs and outperforms the state-of-the-art GED methods. In addition, we also apply BSS_GED to the graph similarity search problem and the practical results confirm its efficiency.

I. INTRODUCTION

Graphs are widely used to model various complex structured data, including social networks, molecular structures, etc. Due to extensive applications of graph models, there has been a considerable effort in developing techniques for effective graph data management and analysis, such as graph matching [3] and graph similarity search [14, 17, 19].

Among these studies, similarity computation between two graphs is a core and essential problem. In this paper, we focus on the similarity measure based on graph edit distance (GED) since it is applicable to virtually all types of data graphs and can also precisely capture structural differences. Due to the flexible and error-tolerant characteristics of GED, it has been successfully applied in many applications, such as molecular comparison in chemistry [8], object recognition in computer vision [2] and graph clustering [9].

Given two graphs $G$ and $Q$, the GED between them, denoted by $ged(G, Q)$, is defined as the minimum cost of an edit path that transforms one graph to another. Unfortunately, unlike the classical graph matching problem, such as subgraph isomorphism [15], the fault tolerance of GED allows a vertex of one graph to be mapped to any vertex of the other graph, regardless of their labels and degrees. As a consequence, the complexity of the GED computation is higher than that of subgraph isomorphism, which has been proved to be an NP-hard [17] problem.

The GED computation is usually carried out by means of a tree search algorithm which explores the space of all possible mappings of vertices and edges of comparing graphs. The underlying search space can be organized as an ordered search tree. Based on the way of generating successors of nodes in the search tree, existing methods can be divided into two broad categories: vertex-based and edge-based mapping methods. When generating successors of a node, the former extends unmapped vertices of comparing graphs, while the latter extends unmapped edges. $A^\star$-GED [5, 7] and DF-GED [10] are two major vertex-based mapping methods. $A^\star$-GED adopts the best-first search paradigm $A^\star$ [6], which picks up a partial mapping with the minimum induced edit cost to extend each time. The first found complete mapping induces the GED of comparing graphs. However, DF-GED carries out a depth-first search, which quickly reaches a leaf node. The edit cost of a leaf node in fact is an upper bound of GED and hence can be used to prune nodes later to accelerate the GED computation. Different from the above two methods, CSI_GED [4] is a novel edge-based mapping method based on common substructure isomorphism, which works well for the sparse and distant graphs. Similar to DF-GED, CSI_GED also adopts the depth-first search paradigm.

Even though existing methods have achieved promising preliminary results, they still suffer from several drawbacks. Both $A^\star$-GED and DF-GED enumerate all possible mappings between two graphs. However, among these mappings, some mappings must not be optimal, called invalid mappings, or they induce the same edit cost, called redundant mappings. For invalid mappings, we do not have to generate them, and for redundant mappings, we only need to generate one of them so as to avoid redundancy. The search space of $A^\star$-GED and DF-GED becomes oversized as they generate plenty of invalid and redundant mappings.

In addition, for $A^\star$-GED, it needs to store enormous partial mappings, resulting in a huge memory consumption. In practice, $A^\star$-GED cannot compute the GED of graphs with more than 12 vertices. Though DF-GED performing a depth-first search is efficient in memory, it is easily trapped into a local (i.e., suboptimal) solution and hence produces lots of expensive backtracking. On the other hand, for CSI_GED, it adopts the depth-first search paradigm, and hence also faces the expensive backtracking problem. Besides, the search space of CSI_GED is exponential with respect to the number of edges of comparing graphs, making it naturally be unsuitable for dense graphs.

To solve the above issues, we propose a novel vertex-based mapping method for the GED computation, named BSS_GED, based on beam-stack search [11] which has shown an excellent performance in AI literature. Our contributions in this paper are summarized below.
We propose a novel method of generating successors of nodes in the search tree, which reduces a large number of invalid and redundant mappings involved in the GED computation. As a result, we create a small search space. Moreover, we also give a rigorous theoretical analysis of the search space.

Incorporating with the beam-stack search paradigm into our method to compute GED, we achieve a flexible trade-off between available memory and the time overhead of backtracking and gain a better performance than the best-first and depth-first search paradigms.

We propose two heuristics to prune the search space, where the first heuristic produces tighter lower bound and the second heuristic enables to fast search of tighter upper bound.

We have conducted extensive experiments on both real and synthetic datasets. The experimental results show that BSS_GED is highly efficient for the GED computation on sparse as well as dense graphs, and outperforms the state-of-the-art GED methods.

In addition, we also extend BSS_GED as a standard graph similarity search query method and the practical results confirm its efficiency.

The rest of this paper is organized as follows: In Section II, we introduce the problem definition and then give an overview of the vertex-based mapping method for the GED computation. In Section III, we create a small search space by reducing the number of invalid and redundant mappings involved in the GED computation. In Section IV, we utilize the beam-stack search paradigm to traverse the search space to compute GED. In Section V, we propose two heuristics to prune the search space. In Section VI, we extend BSS_GED as a standard graph similarity search query method. In Section VII, we report the experimental results and our analysis. Finally, we investigate research works related to this paper in Section VIII and then make concluding remarks in Section IX.

II. Preliminaries

In this section, we introduce basic notations. For simplicity in exposition, we only focus on simple undirected graphs without multi-edges or self-loops.

A. Problem Definition

Let $\Sigma$ be a set of discrete-valued labels. A labeled graph is a triplet $G = (V_G, E_G, L)$, where $V_G$ is the set of vertices, $E_G \subseteq V_G \times V_G$ is the set of edges, $L : V_G \cup E_G \rightarrow \Sigma$ is a labeling function which assigns a label to a vertex or an edge. For a vertex $u$, we use $L(u)$ to denote its label. Similarly, $L(e(u,v))$ is the label of an edge $e(u,v)$. $\Sigma V_G = \{L(u) : u \in V_G\}$ and $\Sigma E_G = \{L(e(u,v)) : e(u,v) \in E_G\}$ are the label multisets of $V_G$ and $E_G$, respectively. For a graph $G$, $S(G) = (V_G, E_G)$ is its unlabeled version, i.e., its structure. In this paper, we refer $|V_G|$ to the size of graph $G$.

Definition 1 (Subgraph Isomorphism [15]). Given two graphs $G$ and $Q$, $G$ is subgraph isomorphic to $Q$, denoted by $G \subseteq Q$, if there exists an injective function $\phi : V_G \rightarrow V_Q$, such that (1) $\forall u \in V_G$, $\phi(u) \in V_Q$ and $L(u) = L(\phi(u))$, (2) $\forall e(u,v) \in E_G$, $e(\phi(u), \phi(v)) \in E_Q$ and $L(e(u,v)) = L(e(\phi(u), \phi(v)))$.

There are six edit operations can be used to transform one graph to another [12, 20]: insert/delete an isolated vertex, insert/delete an edge, and substitute the label of a vertex or an edge. Given two graphs $G$ and $Q$, an edit path $P = \langle p_1, \ldots, p_k \rangle$ is a sequence of edit operations that transforms one graph to another, such as $G = G^0 \xrightarrow{p_1} \cdots \xrightarrow{p_k} G^k \cong Q$.

The edit cost of $P$ is defined as the sum of edit cost of all operations in $P$, i.e., $\sum_{i=1}^{k} c(p_i)$, where $c(p_i)$ is the edit cost of the edit operation $p_i$. In this paper, we focus on the uniform cost model, i.e., $c(p_i) = 1$ for $\forall i$, thus the edit cost of $P$ is its length, denoted by $|P|$. For $P$, we call it optimal if and only if it has the minimum length among all possible edit paths.

Definition 2 (Graph Edit Distance). Given two graphs $G$ and $Q$, the graph edit distance between them, denoted by $ged(G,Q)$, is the length of an optimal edit path that transforms $G$ to $Q$ (or vice versa).

Example 1. In Figure 1, we show an optimal edit path $P$ that transforms graph $G$ to graph $Q$. The length of $P$ is 4, where we delete two edges $e(u_1,u_2)$ and $e(u_1,u_3)$, substitute the label of vertex $u_1$ with label $A$ and insert one edge $e(u_1,u_4)$ with label $A$.

![Fig. 1: An optimal edit path $P$ between graphs $G$ and $Q$.](image)

B. Graph Mapping

In this part, we introduce the graph mapping between two graphs, which can induce an edit path between them. In order to match two unequal size graphs $G$ and $Q$, we extend their vertex sets as $V^*_G$ and $V^*_Q$ such that $V^*_G = V_G \cup \{v^n\}$ and $V^*_Q = V_Q \cup \{v^n\}$, respectively, where $u^n$ and $v^n$ are dummy vertices labeled with $\varepsilon$, s.t., $\varepsilon \notin \Sigma$. Then, we define graph mapping as follows:

Definition 3 (Graph Mapping). A graph mapping from graph $G$ to graph $Q$ is a bijection $\psi : V^*_G \rightarrow V^*_Q$, such that $\forall u \in V^*_G$, $\psi(u) \in V^*_Q$, and at least one of $u$ and $\psi(u)$ is not a dummy vertex.

Given a graph mapping $\psi$ from $G$ to $Q$, it induces an unlabeled graph $H = (V_H, E_H)$, where $V_H = \{u : u \in V_G \land \psi(u) \in V_Q\}$ and $E_H = \{e(u,v) : e(u,v) \in E_G \land e(\psi(u), \psi(v)) \in E_Q\}$, then $H \subseteq S(G)$ and $H \subseteq S(Q)$.

Let $G^\psi$ (resp. $Q^\psi$) be the labeled version of $H$ embedded in $G$ (resp. $Q$). Accordingly, we obtain an edit path $P^\psi :
Given a graph mapping $\psi$ from graph $G$ to graph $Q$. Let $P_\psi$ be the edit path induced by $\psi$, then $|P_\psi| = C_D(\psi) + C_S(\psi)$.

Example 2. Consider graphs $G$ and $Q$ in Figure [1] Given a graph mapping $\psi : \{u_1, u_2, u_3, u_4\} \rightarrow \{v_1, v_2, v_3, v_4\}$, where $\psi(u_1) = v_1, \psi(u_2) = v_2, \psi(u_3) = v_3$, and $\psi(u_4) = v_4$, we have $H = \{(u_1, u_2, u_3, u_4), (e(u_2, u_4), e(u_3, u_4))\}$. Then $\psi$ induces an edit path $P_\psi : G \rightarrow G' \rightarrow Q'$ shown in Figure [1] where $G' = G$ and $Q' = Q$. By Theorem 1, we compute that $C_D(\psi) = 2, C_I(\psi) = 1$ and $C_S(\psi) = 1$, thus $|P_\psi| = C_D(\psi) + C_I(\psi) + C_S(\psi) = 4$.

Hereafter, for ease of presentation, we assume that $G$ and $Q$ are the two comparing graphs, and $V_G = \{u_1, \ldots, u_{|V_G|}\}$ and $V_Q = \{v_1, \ldots, v_{|V_Q|}\}$. For a graph mapping $\psi$ from $G$ to $Q$, we call it is optimal only when its induced edit path $P_\psi$ is optimal. Next, we give an overview of the vertex-based mapping method for computing $ged(G, Q)$ by enumerating all possible graph mappings from $G$ to $Q$.

C. GED computation: Vertex-based Mapping Approach

Assuming that vertices in $V_G$ are processed in the order $(u_{i_1}, \ldots, u_{i_{|V_G|}})$, $u^n$, where $i_1, \ldots, i_{|V_G|}$ is a permutation of $1, \ldots, |V_G|$ detailed in Section 3. Then, we denote a graph mapping from $G$ to $Q$ as $\psi = \bigcup_{i=1}^{\min(|V_Q|)} \{(u_i \rightarrow v_j)\}$.

The GED computation is always achieved by means of an ordered search tree, where inner nodes correspond to partial graph mappings and leaf nodes correspond to complete graph mappings. Such a search tree is created dynamically at runtime by iteratively generating successors linked by edges to the currently considered node. Let $\psi_r = \{(u_{i_1} \rightarrow v_{j_1}), \ldots, (u_{i_l} \rightarrow v_{j_l})\}$ be the (partial) mapping associated with a node $r$, where $v_{j_l}$ is the mapped vertex of $u_{i_l}$ for $1 \leq l \leq l$, then Algorithm 2 outlines the method of generating successors of $r$.

Algorithm 1 is easy to understand. First, we compute the sets of unmapped vertices $C^*_G$ and $C^*_Q$ in $G$ and $Q$, respectively (line 2). Then, if $|C^*_G| > 0$, for the vertex $u_{i_{|V_G|+1}}$, to be extended, we choose a vertex $z$ from $C^*_G$ or $z^n$ as its mapped vertex, and finally generate all possible successors of $r$ (lines 4–8); otherwise, all vertices in $G$ were processed, then we insert all vertices in $C^*_Q$ into $G$ and obtain a unique successor leaf node (lines 10–11).

Staring from a dummy root node root such that $\psi_{root} = \emptyset$, we can create the search tree layer-by-layer by iteratively generating successors. For a leaf node $r$, we compute the edit cost of its corresponding edit path $P_\psi$ by Theorem 1. Thus, when we generate all leaf nodes, we must find an optimal graph mapping and then obtain $ged(G, Q)$.

### Algorithm 1: Basic Gen Succr

1. $\psi_r \leftarrow \{(u_{i_1} \rightarrow v_{j_1}), \ldots, (u_{i_l} \rightarrow v_{j_l})\}$, $su \leftarrow \emptyset$
2. $C^*_G \leftarrow V_G \backslash \{u_{i_1}, \ldots, u_{i_l}\}$, $C^*_Q \leftarrow V_Q \backslash \{v_{j_1}, \ldots, v_{j_l}\}$
3. if $|C^*_G| > 0$
4. for each $z \in C^*_G$
5. generate successor $q$, s.t., $\psi_q \leftarrow \psi_r \cup \{(u_{i_{l+1}} \rightarrow z)\}$
6. $q \leftarrow succ \cup \{q\}$
7. generate successor $q$, s.t., $\psi_q \leftarrow \psi_r \cup \{(u_{i_{l+1}} \rightarrow v^n)\}$
8. $q \leftarrow succ \cup \{q\}$
9. else
10. generate successor $q$, s.t., $\psi_q \leftarrow \psi_r \cup \bigcup_{z \in C^*_Q} \{(u^n \rightarrow z)\}$
11. $q \leftarrow succ \cup \{q\}$
12. return $q$.

However, the above method Basic Gen Succr used in A*-GED [5] and DF-GED [16] generates all possible successors. As a result, both A*-GED and DF-GED enumerate all possible graph mappings from $G$ to $Q$ and their search space size is $O(|V_Q||V_G|)$ [4]. However, among these mappings, some mappings certainly not be optimal, called invalid mappings, or they induce the same edit cost, called redundant mappings. For invalid mappings, we do not have to generate them, and for redundant mappings, we only need to generate one of them. Next, we present how to create a small search space by reducing the number of invalid and redundant mappings.

III. CREATING SMALL SEARCH SPACE

A. Invalid Mapping Identification

Let $|\psi|$ be the length of a graph mapping $\psi$, i.e., $|V^\psi_G|$. We give an estimation of $|\psi|$ in Theorem 2 which can be used to identify invalid mappings.

### Theorem 2. Given an optimal graph mapping $\psi$ from graph $G$ to graph $Q$, then $|\psi| = \max\{|V^\psi_G|, |V^\psi_Q|\}$.

**Proof:** Suppose for the purpose of contradiction that $|\psi| > \max\{|V^\psi_G|, |V^\psi_Q|\}$. Then $(x \rightarrow v^n)$ and $(u^n \rightarrow y)$ must be present simultaneously in $\psi$, where $x \in V_G$ and $y \in V_Q$. We construct another graph mapping $\psi' = \psi \backslash \{(x \rightarrow v^n), (u^n \rightarrow y)\} \cup \{(x \rightarrow y)\}$, and then prove $|P_{\psi'}| < |P_{\psi}|$ as follows:

Let $H$ and $H'$ be two unlabeled graphs induced by $\psi$ and $\psi'$, respectively, then $V_H = \{u : u \in V_G \land \psi'(u) \in V_Q\} = \{u : u \in V_G \land \psi(u) \in V_Q\} \cup \{x : \psi'(x) = v_Q\} = V_H \cup \{x\}$. Let $A_{x} = \{z : z \in V_H \land \psi(u) \in E_G \land \psi(u,v) \in E_Q\}$, then $E_{H'} = \{e(u,v) : e(u,v) \in E_G \land e(\psi(u),\psi'(v)) \in E_Q\}$.

As $\psi' \leftarrow \psi \backslash \{(x \rightarrow v^n), (u^n \rightarrow y)\}$.

Thus, $|V_{H'}| = |V_H| + 1$ and $|E_{H'}| = |E_H| + |A_{x}|$.

As $C_D(\psi) = |V_G| - |V_H| + |E_G| - |E_H|$ and $C_I(\psi) = |V_Q| - |V_H| + |E_Q| - |E_H|$, we have $C_D(\psi') = C_D(\psi) - (1 + |A_{x}|)$ and
For an edge $e(u, v)$ in $E_H$, $e(\psi(u), \psi(v))$ is its mapped edge in $E_Q$. As $\pi(\psi(u)) = \pi(\psi'(u))$, we have $\psi(u) \sim \psi'(u)$ and then obtain $N_Q(\psi(u)) = N_Q(\psi'(u))$. Thus, we have $e(\psi(u), \psi(v)) \in E_Q$. Similarly, since $\pi(\psi(v)) = \pi(\psi'(v))$, we obtain $\psi(v) \sim \psi'(v)$. Thus, there must exist edges between $\psi(u)$ and $\psi'(u)$, $\psi'(u)$ and $\psi'(v)$ (an illustration is shown in Fig. 2), thus $e(\psi'(u), \psi'(v)) \in E_Q$ and hence we obtain $e(v, u) \in E_{H'}$. Thus, $E_H \subseteq E_{H'}$. Similarly, we also obtain $E_{H'} \subseteq E_H$. So, $E_H = E_{H'}$.

Since $V_H = V_{H'}$ and $E_H = E_{H'}$, we have $H = H'$. Thus, $C_I(\psi) = C_I(\psi')$ and $C_D(\psi) = C_D(\psi')$. Next, we do not distinguish $H$ and $H'$ anymore.

Fig. 2: Illustration of isomorphic vertices.

For any vertex $u$ in $V_H$, we have $L(\psi(u)) = L(\psi'(u))$ as $\psi(u) \sim \psi'(u)$. Thus, $\{|u : u \in V_H \land L(u) \neq L(\psi(u))\} = \{|u : u \in V_H \land L(u) \neq L(\psi(u))\}$. For any edge $e(u, v)$ in $E_H$, since $\psi(u) \sim \psi'(u)$, we know $\psi(v) = \psi'(v)$ and $\psi(u) = \psi'(u)$. Hence, $\{\psi(u), \psi(v) : \psi(u), \psi(v)] = \{\psi'(u), \psi'(v)\}$. Therefore, $C_\psi(\psi') = C_\psi(\psi')$. So, we have $|P_\psi| = |P_\psi'|$.

Example 3. Consider graphs $G$ and $Q$ in Fig. 1. For $Q$, we know that $L(v_1) = L(v_2) = L(v_3) = A$, and $N_Q(v_1) = N_Q(v_2) = N_Q(v_3) = \{v_4, A\}$, thus $v_1 \sim v_2 \sim v_3$. So, we divide $\psi_2$ into equivalent classes $V_Q = \{v_1, v_2, v_3\}$, $V_Q = \{v_4\}$. Given two graph mappings $\psi = \{(u_1 \rightarrow v_1), (u_2 \rightarrow v_2), (u_3 \rightarrow v_3), (u_4 \rightarrow v_4)\}$ and $\psi' = \{(u_1 \rightarrow v_2), (u_2 \rightarrow v_3), (u_3 \rightarrow v_1), (u_4 \rightarrow v_4)\}$, we have $\psi(\psi') = \psi'$. Thus, there must exist edges between $\psi(u)$ and $\psi'(u)$, $\psi'(u)$ and $\psi'(v)$ (an illustration is shown in Fig. 2), thus $e(\psi'(u), \psi'(v)) \in E_Q$ and hence we obtain $e(v, u) \in E_{H'}$. Thus, $E_H \subseteq E_{H'}$. Similarly, we also obtain $E_{H'} \subseteq E_H$. So, $E_H = E_{H'}$.
to a dummy vertex, i.e., $(u \to v^n) \notin \psi$ for $\forall u \in V_G$.

**Rule 1.** If $|C'_G| \leq |C'_Q|$, then $z \in C'_Q$; otherwise $z = v^n$ or $z \in C'_Q$.

Applying rule 1 into the process $\text{GenSuccr}$ of generating successors of each node, we know that if $|V_G| \leq |V_Q|$ then none of the vertices in $V_G$ will be mapped to a dummy vertex otherwise only $|V_G| - |V_Q|$ vertices do. As a result, the obtained graph mapping $\psi$ must satisfy $|\psi| = \max\{|V_G|, |V_Q|\}$.

**Definition 6** (Canonical Code Partial Order). Let $\psi$ and $\psi'$ be two graph mappings such that $\text{code}(\psi) = \text{code}(\psi')$. We define that $\psi \preceq \psi'$ if $\exists 1 \leq l \leq |\psi|$, s.t., $\psi(u_i) = \psi'(u_i)$ for $1 \leq k < l$ and $\psi(u_i) < \psi'(u_i)$.

By Theorem 3 we know that graph mappings with the same canonical code induce the same edit cost, thus among these mappings we only need to generate the smallest according to the partial order defined in Definition 6. For $u_{i+1}$, we only map it to the smallest unmapped vertex in $V_Q^m$, for $1 \leq m \leq \lambda_Q$. This will guarantee that the obtained graph mapping is smallest among those mappings with the same canonical code. Then we establish Rule 2 as follows:

**Rule 2.** $z \in \bigcup_{m=1}^{\lambda_Q} \min\{|C'_Q \cap V_Q^m|\}$.

Based on the above Rule 1 and Rule 2, we give the method of generating successors of $r$ in Algorithm 2 where lines 4–8 corresponds to Rule 2 and lines 9–11 corresponds to Rule 1.

**Algorithm 2: GenSuccr**

1. $\psi \leftarrow \{(u_1 \to v_1), \ldots, (u_l \to v_l)\}$, $\text{succ} \leftarrow \emptyset$;
2. $C'_G \leftarrow V_G \setminus \{(u_1, \ldots, u_l)\}$, $C'_Q \leftarrow V_Q \setminus \{v_1, \ldots, v_l\}$;
3. if $|C'_G| > 0$ then
   4. for $m \leftarrow 1$ to $\lambda_Q$ do
   5. if $C'_Q \cap V_Q^m = \emptyset$ then
   6. $z \leftarrow \min\{|C'_Q \cap V_Q^m|\}$;
   7. generate successor $q$, s.t., $\psi_q \leftarrow \psi_r \cup \{(u_{i+1} \to z)\}$;
   8. $\text{succ} \leftarrow \text{succ} \cup \{q\}$;
   9. if $|C'_G| > |C'_Q|$ then
10. generate successor $q$, s.t., $\psi_q \leftarrow \psi_r \cup \{(u_{i+1} \to u^n)\}$;
11. $\text{succ} \leftarrow \text{succ} \cup \{q\}$;
   12. else
13. generate successor $q$, s.t., $\psi_q \leftarrow \psi_r \cup \{u^n \to z\}$;
14. $\text{succ} \leftarrow \text{succ} \cup \{q\}$;
15. return succ;

**Example 4.** Consider graphs $G$ and $Q$ in Figure 1. Figure 5 shows the entire search tree of $G$ and $Q$ created layer-by-layer by using GenSuccr, where vertices in $G$ are processed in the order $(u_1, u_2, u_3, u_4)$. In a layer, the values inside the nodes are the possible mapped vertices (e.g., $v_1$ and $v_4$ in layer one are the possible mapped vertices of $u_1$). The sequence of vertices on the path from root to each leaf node gives a complete graph mapping. In this example, we totally generate 4 graph mappings, and then easily compute that $\text{ged}(G, Q) = 4$.

| Layer | $V_G$ |
|-------|-------|
| 1     | $u_1$  |
| 2     | $u_2$  |
| 3     | $u_3$  |
| 4     | $u_4$  |

![Fig. 3: Search tree created by GenSuccr.](image)

**D. Search Space Analysis**

Replacing $\text{BasicGenSuccr}$ (see Alg. 1) with GenSuccr to generate successors, we reduce a large number of invalid and redundant mappings and then create a small search tree. Next, we analyze the size of search tree, i.e., the total number of nodes in the search tree.

Nodes in the search tree are grouped into different layers based on their distances from the root node. Hence, the search tree is divided into layers, one for each depth. When all vertices in $V_G$ were processed, for any node in the layer $|V_G|$ (starting from 0), it generates a unique successor leaf node, thus we regard this layer as the last layer. Namely, we only need to generate the first $|V_G|$ layers. For the layer $l$, let $N_l$ be the total number of nodes in this layer. So, the total number of nodes in the search tree can be computed as $S_R = \sum_{l=0}^{N_l} N_l$.

For the layer $l$, the set of vertices in $G$ that have been processed is $B'_G = \{v_1, \ldots, v_l\}$, correspondingly, we must choose $l$ vertices from $V_Q \cup \{v^n\}$ as their mapped vertices. Let $B'_Q = \{v_1, \ldots, v_l\}$ be the $l$ selected vertices, then we use a vector $x = [x_1, \ldots, x_{\lambda_Q+1}]$ to represent it, where $x_m$ is the number of vertices in $B'_Q$ that belong to $V_Q^m$, i.e., $x_m = |B'_Q \cap V_Q^m|$, for $1 \leq m \leq \lambda_Q$, and $x_{\lambda_Q+1}$ is the number of dummy vertices in $B'_Q$. Thus, we have

$$\sum_{m=1}^{\lambda_Q+1} x_m = l,$$

where $0 \leq x_m \leq |V_Q^m|$ for $1 \leq m \leq \lambda_Q$, and $x_{\lambda_Q+1} \geq 0$.

For a solution $x$ of equation (1), it corresponds to a unique $B'_Q$. The reason is as follows: In Rule 2, each time we only select the smallest unmapped vertex in $V_Q^m$ as the mapped vertex, for $1 \leq m \leq \lambda_Q$. Thus, for $x_m$ in $x$, it means that $B'_Q$ contains the first $x_m$ smallest vertices in $V_Q^m$. For example, let us consider the search tree in Figure 3. Let $l = 3$ and $x = [2, 1, 0]$, then $B'_Q$ contains the first 2 smallest vertices in $V_Q^3$, i.e., $v_1$ and $v_2$, and the smallest vertex in $V_Q^2$, i.e., $v_4$, then we have $B'_Q = \{v_1, v_2, v_4\}$.

Let $\Psi_l$ be the set of solutions of equation (1), then it covers all possible $B'_Q$. For a solution $x$, it totally produces $\prod_{m=1}^{\lambda_Q+1} x_m!$ different (partial) canonical codes. For example, for $x = [2, 1, 0]$, it produces 3 partial canonical codes, i.e., $(1, 1, 2), (1, 2, 1)$ and $(2, 1, 1)$. As we know, each (partial) canonical code corresponds to a (partial) mapping from $B'_G$.
to $B^l_Q$, which is associated with a node in the layer $l$, thus

$$N_l = \sum_{x \in \Psi} \frac{l!}{\prod_{m=1}^{\lambda_Q+1} x_m}.$$  \hspace{1cm} (2)

In Rule 1, only when the number of unmapped vertices in $G$ is greater than that in $Q$, we select a dummy vertex $v^*$ as the mapped vertex. As a result, if $|V_G| > |V_Q|$ then the number of dummy vertices in $B^l_Q \setminus V_Q$ is 0 otherwise is $|V_C| - |V_Q|$. Let $l = |V_G|$ and we then discuss the following two cases:

Case 1. When $|V_G| > |V_Q|$. For any $x$, we have $x_{\lambda_Q+1} = |V_G| - |V_Q|$. Then equation (1) is reduced to $\sum_{m=1}^{\lambda_Q} x_m = |V_G|$. Since $\sum_{m=1}^{\lambda_Q} |V_Q^m| = |V_Q|$ and $0 \leq x_m \leq |V_Q^m|$, for $1 \leq m \leq \lambda_Q$, then equation (1) has a unique solution $x = \left( |V_Q^1|, \ldots, |V_Q^\lambda_Q|, |V_G| - |V_Q| \right)$. Thus, $N_{|V_G|} = \frac{|V_Q|!}{(|V_G| - |V_Q|)! \prod_{m=1}^{\lambda_Q} |V_Q^m|!}$. As $N_0 = 1$ and $N_1 \leq \cdots \leq N_{|V_Q|}$, we obtain $S_R \leq \frac{|V_Q|!}{(|V_G| - |V_Q|)! \prod_{m=1}^{\lambda_Q} |V_Q^m|!} + 1$.

Case 2. When $|V_G| \leq |V_Q|$. For any $x$, we have $x_{\lambda_Q+1} = 0$. Then equation (1) is reduced to $\sum_{m=1}^{\lambda_Q} x_m = |V_Q|$. As $|V_G| \leq |V_Q|$, we have $N_{|V_G|} = \sum_{x \in \Psi} \frac{|V_G|!}{|x|! \prod_{m=1}^{\lambda_Q} |V_Q^m|!} \leq \sum_{x \in \Psi} \frac{|V_G|!}{x_{\lambda_Q+1}! \prod_{m=1}^{\lambda_Q} x_m!} = \frac{|V_Q|!}{|V_Q|! \prod_{m=1}^{\lambda_Q} |V_Q^m|!}$. Since $N_0 = 1$ and $N_1 \leq \cdots \leq N_{|V_Q|}$, we have $S_R \leq \frac{|V_Q|!}{|V_G|! \prod_{m=1}^{\lambda_Q} |V_Q^m|!} + 1$.

However, this will overestimate $S_R$ when $|V_G| \ll |V_Q|$. For the layer $l$, if we do not consider the isomorphic vertices in $B^l_Q$, then there are $l!$ mappings from $B^l_Q$ to $B^l_I$. Since there are at most $l!$ possible $B^l_Q$, we have $N_l \leq (l!)! \cdot l! = \frac{|V_G|!}{(|V_Q| - |V_Q|)! \prod_{m=1}^{\lambda_Q+1} x_m} \cdot \frac{(l+1)!}{l!} + 1$. Also, $S_R = \frac{|V_Q|!}{|V_G|! \prod_{m=1}^{\lambda_Q} |V_Q^m|!}$ \leq $2 \frac{|V_Q|!}{(|V_Q| - |V_Q|)! \prod_{m=1}^{\lambda_Q} |V_Q^m|!} + 1$.

In summary, if $|V_G| > |V_Q|$, $S_R = O\left( \frac{|V_Q|!}{|V_G|! \prod_{m=1}^{\lambda_Q} |V_Q^m|!} \right)$; otherwise, $S_R = O(\min\left\{ \frac{|V_G|!}{|V_Q|! \prod_{m=1}^{\lambda_Q} |V_Q^m|!}, \frac{|V_Q|!}{(|V_Q| - |V_Q|)! \prod_{m=1}^{\lambda_Q} |V_Q^m|!} \right\})$.

IV. GED COMPUTATION USING BEAM-STACK SEARCH

The previous section shows that we create a small search space. However, we still need an efficient search paradigm to traverse the search space to seek for an optimal graph mapping to compute GED. In this section, based on the efficient search paradigm, beam-stack search [11], we give our approach for the GED computation.

A. Data Structures

For a node $r$ in the search tree, $f(r) = g(r) + h(r)$ is the total edit cost assigned to $r$, where $g(r)$ is the edit cost of the partial path accumulated so far, and $h(r)$ is the estimated edit cost from $r$ to a leaf node, which is less than or equal to the real cost. Before formally presenting the algorithm, we first introduce the data structures used as follows:

- a beam stack $bs$, which is a generalized stack. Each item in $bs$ is a half-open interval $[f_{min}, f_{max})$, and we use $bs[l]$ to denote the interval of layer $l$. For a node $r$ in layer $l$, its successor $n$ in next layer $l + 1$ is allowed to be expanded only when $f(n)$ is in the interval $bs[l]$, i.e., $bs[l], f_{min} \leq f(n) < bs[l], f_{max}$.
- priority queues open[0], open[|V_G|], where open[l] (0 \leq l \leq |V_G|) is used to store the expanded nodes in layer $l$.
- a table new, where new[$H(r)$] stores all successors of $r$ and $H(r)$ is a hash function which assigns a unique ID to $r$.

B. Algorithm

Algorithm 3 performs an iterative search to obtain a more and more tight upper bound $ub$ of GED until $ub = ged(G, Q)$. In an iteration, we perform the following two steps: (1) we utilize beam search [10] to quickly reach to a leaf node whose edit cost is an upper bound of GED, then we update $ub$ (line 4). As beam search expands at most $w$ nodes in each layer, some nodes are inadmissible pruned when the number of nodes in a layer is greater than $w$, where $w$ is the beam width; Thus, (2) we backtrack and pop items from $bs$ until a layer $l$ such that $bs.top() f_{max} < ub$ (lines 5–6), and then shift the range of $bs.top()$ (line 9) to re-expand those inadmissible pruned nodes in next iteration to search for tighter $ub$. If $l = -1$, it means that we finish a complete search and then obtain $ub = ged(G, Q)$ (lines 7–8).

In procedure Search, we perform a beam search starting from layer $l$ to re-expand those inadmissible pruned nodes to search for tighter $ub$, where PQQL and PQPLL are two temporary priority queues used to record expanded nodes in two adjacent layers. Each time we pop a node $r$ with the smallest cost to expand (line 4). If $r$ is a leaf node, then we update $ub$ and stop the search as $g(z) \geq g(r)$ holds for $\forall z \in PQL$ (line 7); otherwise, we call ExpandNode to generate all successors of $r$ that are allowed to be expanded in next layer and then insert them into PQQL (lines 8–9). As at most $w$ successors are allowed to be expanded, we only keep the best $w$ nodes (i.e., the smallest cost) in PQQL, and the nodes left are inadmissible pruned (lines 11–13). Correspondingly, line 12, we modify the right boundary of $bs.top()$ as the lowest cost among all inadmissible pruned nodes to ensure that the cost of the $w$ successors currently expanded is in this interval.

In procedure ExpandNode, we generate all successors of $r$ that are allowed to be expanded. Note that, all nodes first generated are marked as false. If $r$ has not been visited, i.e., $r.visited = false$, then we call GenSuccr (i.e., Alg. 2) to generate all successors of $r$ and mark $r$ as visited (lines 3–4); otherwise, we directly read all successors of $r$ from new (line 6). For a successor $n$ of $r$, if $f(n) \geq ub$ or $n.visited = true$, then we safely prune it, see Lemma [11]. Meanwhile, we delete all successors of $n$ from new (line 9); otherwise, if $bs.top(). f_{min} \leq f(n) < bs.top(). f_{max}$, we expand $n$. If all successors of $r$ are safely pruned, we safely prune $r$, and delete $r$ from open[l] and its successors from new, respectively (line 13).
Lemma 1. In ExpandNode, if \( f(n) \geq ub \) or \( n.\text{visited} \) = true, i.e., line 8, we safely prune \( n \).

Proof: For the case \( f(n) \geq ub \), it is trivial. Next we prove it in the other case.

Consider \( bs \) in the last iteration. Assuming that in this iteration we perform Search starting from layer \( k \) (i.e., backtracking to layer \( k \) in the last iteration, see lines 5-6 in Alg. 3), and node \( r \) and its successors \( n \) are in layers \( l \) and \( l + 1 \), respectively, then \( k \leq l \) and \( bs[m].f_{\text{max}} \geq ub \) for \( l + 1 \leq m \leq |V_G| \). If \( n.\text{visited} \) = true, then we must have called ExpandNode to generate successors of \( n \) in the last iteration. For a successor \( x \) of \( n \) in layer \( l + 2 \), if \( x \) is inadmissible pruned, then \( f(x) \geq bs[l + 1].f_{\text{max}} \geq ub \), thus we safely prune \( x \); otherwise, we consider a successor of \( x \) and repeat this decision process until a leaf node \( z \). Then, it must satisfy that \( f(z) = g(z) \geq ub \). Thus, none of descendants of \( n \) can produce tighter \( ub \). So, we safely prune it.

Lemma 2. A node \( r \) is visited at most \( \mathcal{O}(|V_Q|) \) times.

Proof: For a node \( r \) in layer \( l \), it generates at most \( |V_Q| + 1 \) successors by GenSuccessor. In order to fully generate all successors in layer \( l + 1 \), we backtrack to this layer at most \( \mathcal{O}(|V_Q| + 1) \) times as \( |open[l]| \leq w \). After that, when we visit \( r \) once again, all successors of \( r \) are either pruned or marked, thus we safely prune them by Lemma 1. So, \( r \) cannot produce tighter \( ub \) in this iteration and we safely prune it, i.e., lines 12-13 in ExpandNode. Plus the first time when generating \( r \), we totally visit \( r \) at most \( |V_Q| + 3 \) times, i.e., \( \mathcal{O}(|V_Q|) \).

Theorem 4. Given two graphs \( G \) and \( Q \), BSS_GED must return \( ged(G, Q) \).

Proof: By Lemma 2, a node is visited at most \( \mathcal{O}(|V_Q|) \) times, thus all nodes are totally visited at most \( \mathcal{O}(|V_Q| + |S_R|) \) times (see \( S_R \) in Section III-D), which is finite. So, BSS_GED always terminates. In Search, we always update \( ub = \min \{ub, g(r)\} \) each time. Thus, \( ub \) becomes more and more tight. Next, we prove that \( ub \) converges to \( ged(G, Q) \) when BSS_GED terminates by contradiction.

Suppose that \( ub > ged(G, Q) \). Let \( r \) and \( n \) be the leaf nodes whose edit cost is \( ub \) and \( ged(G, Q) \), respectively. Let \( x \) in layer \( l \) be the common ancestor of \( r \) and \( n \), which is farthest from root. Let \( z \) in layer \( l + 1 \) be a successor of \( x \), which is the ancestor of \( n \). Then \( f(z) \leq f(n) = ged(G, Q) < ub \).

For \( z \), it is not in the path from root to \( r \), thus it must be pruned in an iteration, i.e., \( f(z) \geq ub \) or \( z.\text{visited} = \text{false} \). Line 8 in ExpandNode (if \( z \) has been inadmissible pruned, we backtrack and shift the range of \( bs[l] \) to re-expand it until that \( z \) is pruned or marked). For the case \( f(z) \geq ub \), it contradicts that \( f(z) < ub \), and for the other case, we conclude that \( f(n) \geq ub \) by using the same analysis in Lemma 1, which contradicts that \( f(n) < ub \). Thus, \( ub = ged(G, Q) \).

V. SEARCH SPACE PRUNING

In BSS_GED, for a node \( r \), if \( f(r) = g(r) + h(r) \geq ub \), then we safely prune \( r \). As \( g(r) \) is the irreversible edit cost, the upper bound \( ub \) and lower bound \( h(r) \) are the keys to perform pruning. Here, we give two heuristics to prune the search space as follows: (1) proposing an efficient heuristic function to obtain tighter \( h(r) \); (2) ordering vertices in \( G \) to enable to fast find of tighter \( ub \).

A. Estimating \( h(r) \)

Let \( P \) be an optimal edit path that transforms \( G \) to \( Q \), then it contains at least maximum of \[ |V_G|, |V_Q| - |\Sigma V_G \cap \Sigma V_Q| \] edit operations performed on vertices. Next, we only consider the edit operations in \( P \) performed on edges. Assuming that we first delete \( \gamma_1 \) edges to obtain \( G_1 \), then insert \( \gamma_2 \) edges to
obtain $G_2$, and finally change $\gamma_3$ edge labels to obtain $Q$.

When transforming $G$ to $G_1$ by deleting $\gamma_1$ edges, we have $\Sigma_{E_G1} \subseteq \Sigma_{E_G}$, thus $|\Sigma_{E_G} \cap \Sigma_{E_G1}| \geq |\Sigma_{E_G1} \cap \Sigma_{E_G}|$. When transforming $G_1$ to $G_2$ by inserting $\gamma_2$ edges, for each inserted edge, we no longer change its label, thus $|\Sigma_{E_G2} \cap \Sigma_{E_G1}| = |\Sigma_{E_G1} \cap \Sigma_{E_G}| + \gamma_2$. When transforming $G_2$ to $Q$ by changing $\gamma_3$ edge labels, we need to substitute at least $|\Sigma_{E_G2} \cap \Sigma_{E_G}| + (\gamma_2 + \gamma_3) = |\Sigma_{E_G1} \cap \Sigma_{E_G}|$. So, we have

$$\gamma_3 \geq |\Sigma_{E_G} \cap \Sigma_{E_G1}| + \gamma_2 + \gamma_3 \geq |E_G|.$$ 

(3)

Let $lb(G, Q) = \max\{|V_G|, |V_Q|\} - |\Sigma_{V_G} \cap \Sigma_{V_Q}| + \sum_{i=1}^{3} \gamma_i$, then $gcd(G, Q) \geq lb(G, Q)$. Obviously, the lower bound $lb(G, Q)$ should be as tight as possible. In order to achieve this goal, we utilize the degree sequence of a graph.

For a vertex $u$ in $G$, its degree $d_u$ is the number of edges adjacent to $u$. The degree sequence $\delta_G = \{d_G[1], \ldots, d_G[V]|\}$ of $G$ is a permutation of $d_1, \ldots, d_{|V|}$ such that $d_G[i] \geq d_G[j]$ for $i < j$. For unequal size $G$ and $Q$, we extend $\delta_G$ as $\delta_Q$ as $\delta_G = \{d_G[1], \ldots, d_G[V]|, 0, 0, \ldots, 0|\} - |V| - |V_Q| \}$ and $\delta_Q = \{\delta_Q[1], \ldots, \delta_Q[V]|, 0, 0, \ldots, 0|\}$, resp., where $|V| = \max\{|V_G|, |V_Q|\}$. Let $(\Delta G, Q) = \{\sum_{|V_G[i]| > \delta_G[i] - \delta_G[i]}/2 \}$ and $(\Delta Q, G) = \{\sum_{|V_Q[i]| < \delta_Q[i] - \delta_Q[i]}/2 \}$. For $1 \leq i \leq |V|$, then we give the respective lower bounds of $\gamma_1$ and $\gamma_3$ as follows:

**Theorem 5** (13). **Given two graphs** $G$ and $Q$, we have $\gamma_1 \geq \Delta (G, Q)$ and $\gamma_3 \geq \Delta (G, Q)$.

Based on inequality (3) and Theorem 5, we then establish the following lower bound of GED in Theorem 6.

**Theorem 6**. **Given two graphs** $G$ and $Q$, we have $gcd(G, Q) \geq LB(G, Q)$, where $LB(G, Q) = \max\{|V_G|, |V_Q|\} - |\Sigma_{V_G} \cap \Sigma_{V_Q}| + \max\{\Delta (G, Q), \Delta (Q, G)\} + |E_G| - |\Sigma_{E_G} \cap \Sigma_{E_Q}|$. 

Next, we discuss how to estimate $h(r)$ based on Theorem 6. Let $\psi_i = \{(u_i \rightarrow v_j), \ldots, (u_i \rightarrow v_j)\}$ be the partial mapping associated with $r$, then we divide $G$ into two parts $G_1$ and $G_2$, where $G_1$ is the mapped part of $G$, s.t., $V_{G_1} = \{u_1, \ldots, u_i\}$ and $E_{G_1} = \{e(u_i, v) : u, v \in V_{G_1} \land e(u, v) \in E_G\}$, and $G_2$ is the unmapped part, s.t., $V_{G_2} = V_{G} \setminus V_{G_1}$ and $E_{G_2} = \{e(u, v) : u, v \in V_{G_2} \land e(u, v) \in E_G\}$. Similarly, we also obtain $Q_1$ and $Q_2$. For $r$, by Theorem 6, we know that $LB(G_2, Q_2)$ is the lower bound of $gcd(G_2, Q_2)$ and hence can adopt it as $h(r)$. However, for the potential edit cost on the edges between $G_1$ (resp. $Q_1$) and $G_2$ (resp. $Q_2$), $LB(G_2, Q_2)$ has not covered it.

**Definition 7** (Outer Edge Set). **For a vertex** $u$ in $G_1$, we define its outer edge set as $O_u = \{e(u, v) : v \in V_{G_2} \land e(u, v) \in E_G\}$, which consists of edges adjacent to $u$ that neither belong to $E_G$ nor $E_{G_2}$.

Correspondingly, $O_\psi(u)$ is the outer edge set of $\psi(u)$. Note that, if $\psi(u) = v^a$, then $O_\psi(u) = \emptyset$. Thus, $\Sigma_{O_u} = \{L(e(u, v)) : e(u, v) \in O_u\}$ is the label multiset of $O_u$.

In order to make $O_u$ and $O_\psi(u)$ have the same label multiset, assuming that we first delete $\xi_1^u$ and then insert $\xi_2^u$ edges on $u$, and finally substitute $\xi_3^u$ labels on the outer edges adjacent to $u$. Similar to the previous analysis of obtaining $\xi_2$, we have

$$|O_u| - \xi_1^u + \xi_2^u = |O_\psi(u)| + \xi_2^u + \xi_3^u \geq |O_\psi(u)|$$

(4)

Thus, $\sum_{i=1}^{3} \xi_i^u \geq |O_\psi(u)| + |O_\psi(u)|$. As $|O_u| + \xi_u^u = |O_\psi(u)| + |O_\psi(u)|$, we have $\sum_{i=1}^{3} \xi_i^u \geq |O_\psi(u)| + |O_\psi(u)| + \xi_2^u \geq |O_\psi(u)| + |O_\psi(u)|$. So, $\sum_{i=1}^{3} \xi_i^u \geq \max\{|O_u|, |O_\psi(u)|\} - |O_\psi(u)| \land |O_\psi(u)|$. Adding all vertices in $G_1$, we obtain the lower bound $LB_2^1$ as follows:

$$LB_2^1 = LB(G_2, Q_2) + \sum_{u \in V_{G_1}} \max\{|O_u|, |O_\psi(u)|\} - \max\{|O_u|, |O_\psi(u)|\}$$

(5)

**Definition 8** (Outer Vertex Set). **For a vertex** $u$ in $G_1$, we define its outer vertex set as $A_u = \{v : v \in V_{G_2} \land e(u, v) \in E_G\}$, which consists of vertices in $G_2$ adjacent to $u$.

Correspondingly, $A_\psi(u)$ denotes the outer vertex set of $\psi(u)$. Note that, if $\psi(u) = v^a$, then $A_\psi(u) = \emptyset$. Thus, $A_{G_2} = \bigcup_{u \in V_{G_1}} A_u$ denotes the set of vertices in $G_2$ adjacent to those outer edges between $G_1$ and $G_2$. Similarly, we obtain $A_{Q_2} = \bigcup_{u \in V_{G_1}} A_u$. As $|A_{G_2}| \leq |A_{Q_2}|$, then we need to insert at least $|A_{G_2}^r| - |A_{Q_2}^r|$ outer edges on some vertices in $G_1$, hence $\sum_{u \in V_{G_1}} \xi_2^u \geq |A_{Q_2}^r| - |A_{G_2}^r|$, considering equation (3) for a vertex $u$ in $G_1$, we have $\xi_1^u + \xi_3^u \geq |O_\psi(u)| + |O_\psi(u)|$ and $\sum_{u \in V_{G_1}} (|O_u| - |O_\psi(u)| - |O_\psi(u)|)\|A_{G_2}^r| - |A_{Q_2}^r|\|$. As $|O_u| + \xi_u^u = |O_\psi(u)| + \xi_u^u$, we have $\sum_{u \in V_{G_1}} (|O_u| + \xi_u^u) \|A_{Q_2}^r| - |A_{Q_2}^r|\|$. So, we obtain the lower bounds $LB_2^1$ and $LB_2^1$ as follows:

$$LB_2^1 = LB(G_2, Q_2) + \sum_{u \in V_{G_1}} (|O_u| - |O_\psi(u)| - |O_\psi(u)|)$$

(6)

$$LB_2^1 = LB(G_2, Q_2) + \sum_{u \in V_{G_1}} (|O_u| - |O_\psi(u)| - |O_\psi(u)|)$$

(7)

Based on the above lower bounds $LB_2^1$, $LB_2^1$ and $LB_2^3$, we adopt $h(r) = \max\{LB_2^1, LB_2^1, LB_2^3\}$ as the heuristic function to estimate the edit cost of a node $r$ in BSS_GED.

**Example 5**. Consider graphs $G$ and $Q$ in Figure 4. For a node $r$ associated with a partial mapping $\psi(r) = \{(v_1 \rightarrow v_1)\}$, then $G_2 = \{(u_1, v_2, u_3), \{e(u_3, u_5), e(u_5, u_3)\}\}$, and $Q_2 = \{(v_2, v_3, v_5, v_6), \{e(v_3, v_5), e(v_5, v_6)\}\}$. By Theorem 6, we compute $LB(G_2, Q_2) = 2$. Considering vertices $u_1$ and $u_2$ that have been processed, we have $O_{u_1} = \{e(u_1, u_3), e(u_1, u_4)\}$ and $O_{u_2} = \{e(u_2, u_4)\}$, and then obtain $\Sigma_{O_{u_1}} = \{a, a\}$ and $\Sigma_{O_{u_2}} = \{b\}$. Similarly, we have
In this section, we extend BSS\_GED to solve the GED-based graph similarity search problem: Given a graph database $\mathcal{G} = \{G_1, G_2, \ldots\}$, a query graph $Q$ and an edit distance threshold $\tau$, the problem aims to find all graphs in $\mathcal{G}$ satisfy $ged(G_i, Q) \leq \tau$. As computing GED is an NP-hard problem, most of the existing methods, such as [12], [14], [19], [20], all use the filter-and-verify schema, that is, first filtering some graphs in $\mathcal{G}$ to obtain candidate graphs, and then verifying them.

Here, we also use this strategy. For each data graph $G_i$, we compute the lower bound $LB(G_i, Q)$ by Theorem 6. If $LB(G_i, Q) > \tau$, then $ged(G_i, Q) \geq LB(G_i, Q) > \tau$ and hence we filter $G_i$; otherwise, $G_i$ becomes a candidate graph.

For a candidate graph $G_i$, we need to compute $ged(G_i, Q)$ to verify it. The standard method is that we first compute $ged(G_i, Q)$ and then determine $G_i$ is a required graph or not by judging $ged(G_i, Q) \leq \tau$. Incorporating $\tau$ with BSS\_GED, we can further accelerate it as follows: First, we set the initial upper bound $ub\beta$ as $\tau + 1$ (line 1 in Alg. 3). Then, during the execution of BSS\_GED, when we reach to a leaf node $r$, if the cost of $r$ (i.e., $g(r)$) satisfies $g(r) \leq \tau$, then $G_i$ must be a required graph and we stop running of BSS\_GED. The reason is that $g(r)$ is an upper bound of GED and hence we know that $ged(G_i, Q) \leq g(r) \leq \tau$.

\begin{algorithm}
\caption{DetermineOrder($G$)}
\begin{algorithmic}[1]
\Statex 1 $F[1..|V_G|] \leftarrow \text{false}$, $order[] \leftarrow \emptyset$, count $\leftarrow 1$;
\Statex 2 rank $\leftarrow$ sort vertices in $V_G$ according to the partial order $\preceq$;
\Statex 3 for $i \leftarrow 1$ to $|V_G|$ do
\Statex \hspace{1em} 4 $u \leftarrow \text{rank}[]$;
\Statex \hspace{1em} 5 \hspace{1em} if $F[u] = \text{false}$ then
\Statex \hspace{2em} 6 \hspace{1em} 6 DFS($u, F, \text{rank}, \text{order}, \text{count}$)
\Statex \hspace{1em} \hspace{1em} return order
\Statex \Statex \Statex \Statex procedure DFS ($u, F, \text{rank}, \text{order}, \text{count}$)
\Statex \hspace{1em} 7 \Statex \hspace{1em} order[count] $\leftarrow u$, count $\leftarrow \text{count} + 1$, $F[u] \leftarrow \text{true}$;
\Statex \hspace{1em} 8 $N_u \leftarrow \{v : v \in V_G \land e(u, v) \in E_G\}$;
\Statex \hspace{1em} 9 while $|N_u| > 0$ do
\Statex \hspace{2em} 10 \hspace{2em} $v \leftarrow \arg\min\{\text{rank}[j] : j \in N_u\}$;
\Statex \hspace{2em} 11 \hspace{2em} $N_u \leftarrow N_u \setminus \{v\}$;
\Statex \hspace{2em} 12 \hspace{2em} if $F[v] = \text{false}$ then
\Statex \hspace{3em} 13 \hspace{2em} \hspace{2em} DFS($v, F, \text{rank}, \text{order}, \text{count}$);
\Statex \hspace{1em} \hspace{1em} return;
\end{algorithmic}
\end{algorithm}

VII. Experimental Results

In this section, we perform comprehensive experiments and then analyse the obtained results.

A. Datasets and Settings

We choose several real and synthetic datasets used in the experiment, described as follows:
AIDS \cite{5} It is an antivirus screen compound dataset from the Development and Therapeutics Program in NCI/NIH, which contains 42687 chemical compounds. We generate labeled graphs from these chemical compounds and omit Hydrogen atom as did in \cite{13,14}.

PROTEIN \cite{2} It is a protein database from the Protein Data Bank, constituted of 600 protein structures. Vertices represent secondary structure elements and are labeled with their types (helix, sheet or loop). Edges are labeled to indicate if two elements are neighbors or not.

Synthetic. The synthetic dataset is generated by the synthetic graph data generator GraphGen \cite{6}. In the experiment, we generate a density graph dataset S1K.E30.D30.L20, which means that this dataset contains 1000 graphs; the average number of edges in each graph is 30; the density of each graph is 30%; and the distinct vertex and edge labels are 20 and 5, respectively.

Due to the hardness of computing GED, existing methods, such as A*-GED \cite{5}, DF-GED \cite{16} and CSI-GED \cite{4}, cannot obtain GED of large graphs within a reasonable time and memory. Therefore, for AIDS and PROTEIN, we exclude large graphs with more than 30 vertices as did in \cite{1}, and then randomly select 10000 and 300 graphs to make up the datasets AIDS-10K and PROTEIN-300. For S1K.E30.D30.L20, we use the entire dataset.

As suggested in \cite{1,4}, for each dataset, we randomly select 6 query groups, where each group consists of 3 data graphs having three consecutive graph sizes. Specifically, the number of vertices of each group is in the range: $6 \pm 1, 9 \pm 1, 12 \pm 1, 15 \pm 1, 18 \pm 1$ and $21 \pm 1$.

For the tested database $D = \{D_1, D_2, \ldots \}$ and query group $T = \{T_1, T_2, \ldots \}$, we need to perform $|D| \times |T|$ times GED computation. For each pair of the GED computation, we set the available time and memory be 1000s and 24GB, respectively, and then define the metric average solve ratio as follows:

$$sr = \frac{\sum_{i=1}^{|D|} \sum_{j=1}^{|T|} solve(D_i, T_j)}{|D| \times |T|}.$$ \hspace{1cm} (8)

where $solve(D_i, T_j) = 1$ if we obtain $ged(D_i, T_j)$ within both 1000s and 24GB, and $solve(D_i, T_j) = 0$ otherwise. Obviously, $sr$ should be as large as possible.

We have conducted all experiments on a HP Z800 PC with a 2.67GHz GPU and 24GB memory, running Ubuntu 12.04 operating system. We implement our algorithm in C++, with -O3 to compile and run. For BSS.GED, we set the beam width $w = 15$ for the sparse graphs in datasets AIDS-10K and PROTEIN-300, and $w = 50$ for the density graphs in dataset S1K.E30.D30.L20.

B. Evaluating GenSuccr

In this section, we evaluate the effect of GenSuccr on the performance of BSS.GED. To make a comparison, we replace GenSuccr with BasicGenSuccr (i.e., Alg. \cite{1} and then obtain BSS.GED\textsuperscript{b}, where BasicGenSuccr is the basic method of generating successors used in A*-GED \cite{5} and DF-GED \cite{16}. In BSS.GED\textsuperscript{b}, we also use the same heuristics proposed in Section \hspace{1cm} \cite{7}. Figure 5 shows the average solve ratio and running time.

As shown in Figure 5, the average solve ratio of BSS.GED is much higher than that of BSS.GED\textsuperscript{b}, and the gap between them becomes larger as the query graph size increases. This indicates that GenSuccr provides more reduction on the search space for larger graphs. Regarding the running time, BSS.GED achieves the respective 1x–5x, 0.4x–1.5x and 0.1x–4x speedup over BSS.GED\textsuperscript{b} on AIDS-10K, PROTEIN-300 and S1K.E30.D50.L20. Thus, we create a small search space by GenSuccr.

C. Evaluating BSS.GED

In this section, we evaluate the effect of beam-stack search and heuristics on the performance of BSS.GED. We fix

\begin{itemize}
  \item AIDS
  \item PROTEIN
  \item Synthetic
\end{itemize}
datasets AIDS-10K, PROTEIN-300 and S1K.E30.D30.L20 as the tested datasets and select their corresponding groups 15±1 as the query groups, respectively.

(1). Effect of \( w \)

As we know, beam-stack search achieves a flexible trade-off between available memory and expensive backtracking by setting different \( w \), thus we vary \( w \) to evaluate its effect on the performance. Figure 6 shows the average solve ratio and running time.

![Fig. 6: Effect of \( w \) on the performance of BSS_GED.](image)

By Figure 6, we obtain that the average solve ratio first increases and then decreases, and achieves maximum when \( w = 15 \) on AIDS-10K and PROTEIN-300, and \( w = 50 \) on S1K.E30.D30.L20. There are several factors may contribute to this trend: (1) When \( w \) is too small, BSS_GED may be trapped into a local suboptimal solution and hence produces lots of backtracking. (2) When \( w \) is too large, BSS_GED expands too many unnecessary nodes in each layer. Note that, depth-first search is a special case of beam-stack search when \( w = 1 \). Thus, beam-stack search performs better than depth-first search. As previously demonstrated in [16], depth-first search performs better than best-first search. Therefore, we conclude that the beam-stack search paradigm outperforms the best-first and depth-first search paradigms for the GED computation.

(2). Effect of Heuristics

In this part, we evaluate the effect of the proposed two heuristics by injecting them one by one into the base algorithm. We use the term Basic for the baseline algorithm without applying any heuristics. +h1 denotes the improved algorithm of Basic by incorporating the first heuristics (Section V-A). +h2 denotes the improved algorithm of +h1 by incorporating the second heuristic (Section V-B). Figure 7 plots the average solve ratio and running time.

![Fig. 7: Effect of heuristics on the performance of BSS_GED.](image)

By Figure 7, we know that the average solve ratio of Basic is only 15% of that of +h1. This means that the proposed heuristic function provides powerful pruning ability. Considering the running time, +h1 brings the respective 50x, 2x and 9x speedup over Basic on AIDS-10K, PROTEIN-300 and S1K.E30.D30.L20. Moreover, compared with +h1, the running time needed by +h2 decreases 21%, 30% and 41% on AIDS-10K, PROTEIN-300 and S1K.E30.D30.L20, respectively. Thus, the proposed two heuristics greatly boost the performance.

D. Comparing with Existing GED Methods

In this section, we compare BSS_GED with existing methods A*GED [5], DF-GED [16] and CSI_GED [4]. Figure 8 shows the average solve ratio and running time.

![Fig. 8: Effect of \( \tau \) on the performance of BSS_GED.](image)

By Figure 8, we know that BSS_GED performs the best in terms of average solve ratio. For A*GED, it cannot obtain GED of graphs with more than 12 vertices within 24GB. For DF-GED, it cannot finish the GED computation of graphs with more than 15 vertices in 1000s. Besides, for density graphs in S1K.E30.D30.L20, the average solve ratio of CSI_GED drops sharply as the query graph size increases, which confirms that it is unsuitable for dense graphs.

Regarding the running time, BSS_GED still performs the best in most cases. DF-GED performs better than A*GED, which is consistent with the previous results in [16]. Compared with DF-GED, BSS_GED achieves 50x–500x, 20x–2000x and 15x–1000x speedup on AIDS-10K, PROTEIN-300 and S1K.E30.D30.L20, respectively. Though CSI_GED performs better than BSS_GED on AIDS-10K when the query graph size is less than 9, BSS_GED achieves 2x–5x speedup over CSI_GED when the graph size is greater than 12. Besides, for S1K.E30.D30.L20, BSS_GED achieves 5x–95x speedup over CSI_GED. Thus, BSS_GED is efficient for the GED computation on sparse as well as dense graphs.

E. Performance Evaluation on Graph Similarity Search

In this part, we evaluate the performance of BSS_GED as a standard graph similarity search query method by comparing it with CSI_GED and GSimJoin [19]. For each dataset described in Section VII-A, we use its entire dataset and randomly select 100 graphs from it as query graphs. Figure 9 shows the total running time (i.e., the filtering time plus the verification time).

![Fig. 9: Effect of \( \tau \) on the performance of BSS_GED.](image)

It is clear from Figure 9 that BSS_GED has the best performance in most cases, especially for large \( \tau \). For GSimJoin, it cannot finish when \( \tau \geq 8 \) in AIDS and PROTEIN because of the huge memory consumption. Compared with GSimJoin for \( \tau \) values where it can finish, BSS_GED achieves the respective 1.6x–15000x, 3.8x–800x and 2x–3000x speedup on AIDS, PROTEIN and S1K.E30.D30.L20. Considering CSI_GED, it performs slightly better than BSS_GED when \( \tau \leq 4 \) on AIDS. However, BSS_GED performs much better than CSI_GED when \( \tau \geq 6 \) and the gap between them becomes larger as \( \tau \) increases. Specifically, BSS_GED achieves 2x–28x, 1.2x–10000x and 1.1x–187x speedup over CSI_GED on AIDS, PROTEIN and S1K.E30.D30.L20, respectively. As previously discussed in [4], CSI_GED performs much better than the state-of-the-art graph similarity search query methods. Thus, we conclude that BSS_GED can efficiently finish the graph computation.
GED is an edge-based mapping method through similarity search and runs much faster than existing methods.

VIII. RELATED WORKS

Recently, the GED computation has received considerable attention. A*-GED \cite{5, 7} and DF-GED \cite{16} are two major vertex-based mapping methods, which utilize the best-first and depth-first search paradigms, respectively. Provided that the heuristic function estimates the lower bound of GED of unmapped parts, A*-GED guarantees that the first found complete mapping induces the GED of comparing graphs, which seems very attractive. However, A*-GED stores numerous partial mappings, resulting in a huge memory consumption. As a result, it is only suitable for the small graphs. To overcome this bottleneck, DF-GED performs a depth-first search, which only stores the partial mappings of a path from the root to a leaf node. However, it may be easily trapped into a local suboptimal solution, leading to massive expensive backtracking. CSI_GED \cite{4} is an edge-based mapping method through common substructure isomorphism enumeration, which has an excellent performance on the sparse graphs. However, the edge-based search space of CSI_GED is exponential with respect to the number of edges of comparing graphs, making it naturally be unsuitable for dense graphs. Note that, CSI_GED only works for the uniform model, and \cite{1} generalized it to cover the non-uniform model.

Another work closely related to this paper is the GED based graph similarity search problem. Due to the hardness of computing GED, existing graph similarity search query methods \cite{12, 14, 17, 18, 19, 20} all adopt the filter-and-verify schema, that is, first filtering graphs to obtain a candidate set and then verifying those candidate graphs. In the verification phase, most of the existing methods adopt A*-GED as their verifiers. As discussed above, BSS_GED greatly outperforms A*-GED, hence it can be also used as a standard verifier to accelerate those graph similarity search query methods.

IX. CONCLUSIONS AND FUTURE WORK

In this paper, we present a novel vertex-based mapping method for the GED computation. First, we reduce the number of invalid and redundant mappings involved in the GED computation and then create a small search space. Then, we utilize beam-stack search to efficiently traverse the search space to compute GED, achieving a flexible trade-off between available memory and expensive backtracking. In addition, we also give two efficient heuristics to prune the search space. However, it is still very hard to compute GED of large graphs within a reasonable time. Thus, the approximate algorithm that fast suboptimally compute GED is left as a future work.

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Fig. 9: Performance comparison with CSI_GED and GSimJoin.

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