Speeding Up GED Verification for Graph Similarity Search

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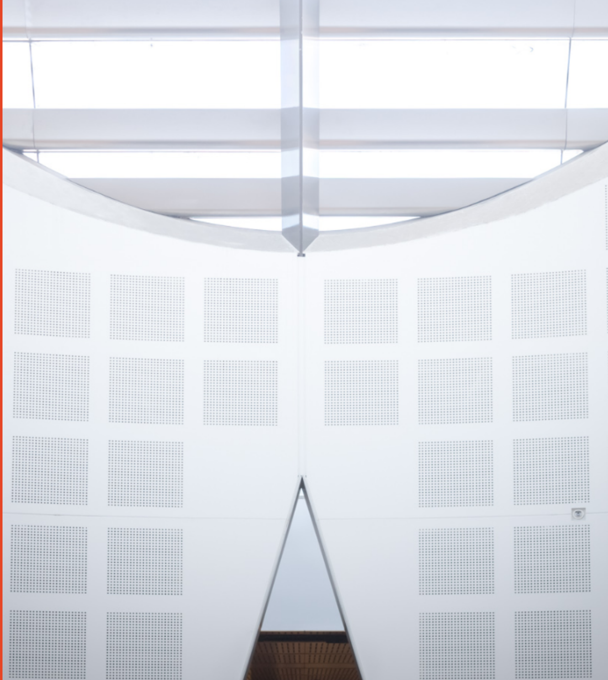
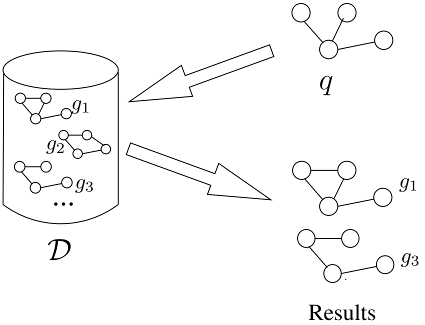


Graph Similarity Search

- Given a database $\mathcal{D} = \{g_1, g_2, g_3, \ldots\}$ consisting of a set of vertex and/or edge labeled graphs, graph similarity search aims to find all graphs in $\mathcal{D}$ that are similar to a user-given query graph q.
  - Here, inexact/similarity search is used
  - Because exact graph search may find no or very few results due to erroneous data entry, data noise or nature of the application



Graph Edit Distance

- Graph edit distance (GED) is a widely used distance/similarity measure in graph similarity search studies.[1234]
  - GED is a metric
    - Applicable to all types of graphs
    - Captures the structural difference between graphs
  - ged(q, g): minimum number of edit operations needed to transform q into g
    - Vertex/Edge relabeling
    - Edge insertion/deletion
    - (Isolated) vertex insertion/deletion

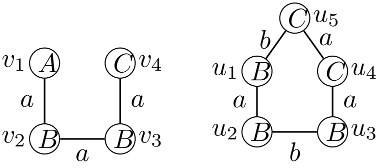
[1] Xiang Zhao et al. "A Partition-Based Approach to Structure Similarity Search". In: *PVLDB* 7.3 (2013).

[2] Yongjiang Liang and Peixiang Zhao. "Similarity Search in Graph Databases: A Multi-Layered Indexing Approach". In: *Proc. of ICDE'17*. 2017.

[3] Xiang Zhao et al. "Efficient structure similarity searches: a partition-based approach". In: *VLDB J.* 27.1 (2018).

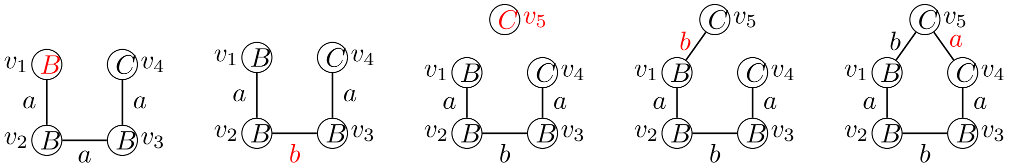
[4] Jongik Kim, Dong-Hoon Choi, and Chen Li. "Inves: Incremental Partitioning-Based Verification for Graph Similarity Search". In: *Proc. of EDBT'19*. 2019.

Graph Edit Distance



Graph q Graph g

- $\text{ged}(q, g) = 5$
  - The following is a sequence of 5 edit operations that transform q into g



(1) Relabel v_1 to 'B' (2) Relabel (v_2, v_3) to 'b' (3) Add v_5 with label 'C' (4) Add (v_1, v_5) with label 'b' (5) Add (v_4, v_5) with label 'a'

Filtering-and-Verification

- Formally, the graph similarity search problem is to compute $\{g \in \mathcal{D} \mid \text{ged}(q, g) \leq \tau\}$ for user-specified q and τ
  - A naive approach is checking, for every $g \in \mathcal{D}$, whether $\text{ged}(q, g) \leq \tau$
  - This is expensive as deciding whether $\text{ged}(q, g) \leq \tau$ is NP-complete

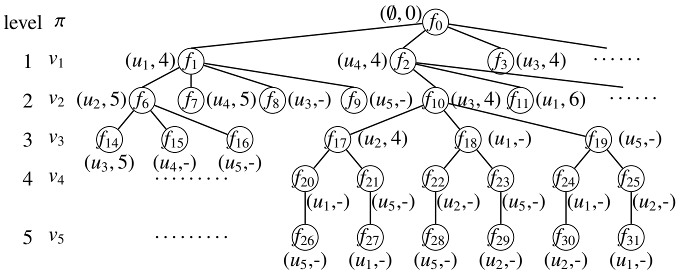
- Filtering-and-verification paradigm.
  1. Candidate generation: cand $\subseteq \mathcal{D}$
     - $\text{ged}(q, g) > \tau$ for every $g \in \mathcal{D} \backslash \text{cand}$
     - Filter out unpromising data graphs (possibly by probing an offline-constructed index)
     - Based on pigeonhole principle: if there are $\tau + 1$ disjoint substructures (*e.g.*, path, tree, subgraph) of q not appearing in g, then $\text{ged}(q, g) > \tau$
  2. Candidate verification
     - Verify whether $\text{ged}(q, g) \leq \tau$, for every $g \in$ cand

Our Contribution: Speeding Up GED Verification

- The existing studies focus on generating a small candidate set (by designing different index structures), while using an outdated algorithm A^*GED for GED verification
- We propose an efficient algorithm AStar$^+$-LSa to speed up GED verification, which is orthogonal to the existing indexing/filtering techniques
- Our experimental results show that
  - The existing indexing/filtering techniques either have very limited filtering power or take a very long filtering time (*e.g.*, may even longer than directly verifying all data graphs by AStar$^+$-LSa)
  - Thus, the existing indexing/filtering techniques become obsolete given our efficient GED verification algorithm AStar$^+$-LSa

GED Computation Via Vertex Mapping

- ged(q, g) can be computed by enumerating vertex mappings from q to g.
  - Vertex insertion can be encoded by mapping a dummy vertex to $V(g)$
  - Vertex deletion can be encoded by mapping $V(q)$ to a dummy vertex



A search tree $\mathcal{T}$ compactly represents all vertex mappings from $V(q)$ to $V(g)$: f_i is a partial mapping, and beside f at level j is a pair (u, lb_f) where $u \in V(g)$ is the vertex to which v_j maps and lb_f is a lower bound of f

Our GED Verification Algorithm AStar$^+$-LSa

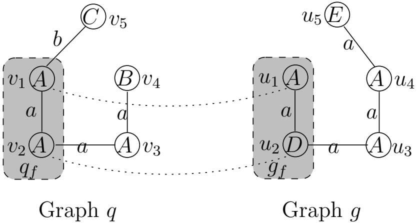
- AStar$^+$-LSa conducts a best-first search of the search tree $\mathcal{T}$, based on lower bounds lb_f of partial mappings f
  - AStar$^+$-LSa uses a fixed matching order of $V(q)$

- The efficiency of AStar$^+$-LSa is achieved by three ingredients
  1. Don't need to add dummy vertices to q or g
  2. Tighter lower bound estimation
  3. Efficient lower bound computation

Ingredient 1: Don't Add Dummy Vertices

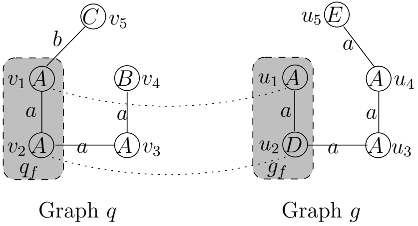
- We prove that if $|V(q)| \leq |V(g)|$, then there is no vertex deletion in the optimal sequence of edit operations that transform q into g
- W.l.o.g., we assume that $|V(q)| = |V(g)|$
  - If $|V(q)| < |V(g)|$, then we can add $|V(g)| - |V(q)|$ dummy vertices to q
  - Thus, we don't need to consider vertex insertion/deletion
  - In implementation, we don't add dummy vertices to q even if $|V(q)| < |V(g)|$
- Advantages of not considering vertex insertion/deletion
  - Reduces the number of full mappings from $\approx (|V(g)| + 1)^{|V(q)|+|V(g)|}$ to $|V(g)|^{|V(q)|}$
  - Simplies algorithm implementation

Ingredient 2: Tighter Lower Bound Estimation



- Consider the partial mapping $f = \{v_1 \mapsto u_1, v_2 \mapsto u_2\}$
- The existing algorithms use label set-based lower bound $\mathsf{lb}_f^{\mathrm{LS}}$
  - mc_f: the number of edit operations required to transform q_f into g_f by obeying f
  - The vertex (resp. edge) label difference between the unmapped parts $q_{\bar{f}}$ and $g_{\bar{f}}$
  - $\mathsf{lb}_f^{\mathrm{LS}} = \mathsf{mc}_f + \Upsilon\left(L_V(q_{\bar{f}}), L_V(g_{\bar{f}})\right) + \Upsilon\left(L_E(q_{\bar{f}}), L_E(g_{\bar{f}})\right) =$
    $1 + \Upsilon(\{A, B, C\}, \{A, A, E\}) + \Upsilon(\{a, a, b\}, \{a, a, a\}) = 4$

Ingredient 2: Tighter Lower Bound Estimation



- We propose anchor-aware label set-based lower bound $\mathsf{lb}_f^{\mathtt{LSa}}$ by seperating the cross edges from the unmapped parts: $\mathsf{lb}_f^{\mathtt{LSa}} = \mathsf{mc}_f +$
  - $\Upsilon(L_{E_C}(v_1), L_{E_C}(u_1))+$: $\Upsilon(\{b\}, \{\}) = 1$
  - $\Upsilon(L_{E_C}(v_2), L_{E_C}(u_2))+$: $\Upsilon(\{a\}, \{a\}) = 0$
  - $\Upsilon(L_{E_I}(q_{\bar{f}}), L_{E_I}(g_{\bar{f}}))+$: $\Upsilon(\{a\}, \{a, a\}) = 1$
  - $\Upsilon(L_V(q_{\bar{f}}), L_V(g_{\bar{f}}))$: $\Upsilon(\{A, B, C\}, \{A, A, E\}) = 2$
  - $\mathsf{lb}_f^{\mathtt{LSa}} = 5 > \mathsf{lb}_f^{\mathtt{LS}} = 4$
- We prove that $\mathsf{lb}_f^{\mathtt{LSa}} \geq \mathsf{lb}_f^{\mathtt{LS}}$ holds for any mapping f

Ingredient 3: Efficient Lower Bound Computation

- In the best-first search, for a partial mapping f, we need to **compute the lower bound for all children h (i.e., one-vertex extension) of f**

- The existing works compute the lower bound for each child h independently
  - Total time complexity of $\mathcal{O}(|V(g)| \times (|E(q)| + |E(g)|))$

- We propose an algorithm with total time complexity of $\mathcal{O}(|E(q)| + |E(g)|)$, by online constructing a data structure and conducting computation incrementally

Experimental Setting

- Datasets
  - AIDS: an antivirus screen chemical compound dataset published by the Developmental Therapeutics Program at NCI/NIH [5]
  - PubChem: a chemical compound dataset [6]

Database $\mathcal{D}$	$\lvert\mathcal{D}\rvert$	Avg $\lvert V\rvert$	Avg $\lvert E\rvert$	Max $\lvert V\rvert$	Max $\lvert E\rvert$	#vlabels	#elabels
AIDS	42,689	25.6	27.5	222	247	66	3
PubChem	23,903	48.3	50.8	88	92	10	3

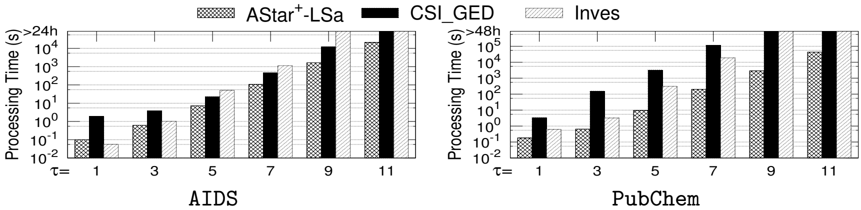
- All algorithms are run in main memory, and run as single-thread algorithms

[5] https://cactus.nci.nih.gov/download/nci/AID2DA99.sdz

[6] http://pubchem.ncbi.nlm.nih.gov: Compound_000975001_001000000.sdf

Index-free Graph Similarity Search

- Algorithms
  - AStar^{+}-LSa: our algorithm
  - CSI_GED[7]: depth-first search + edge mapping
  - Inves[8]: online graph partitioning-based filtering
- To verify ged$(q, g) \leq \tau$, all the three algorithms first run LabelF for filtering
  - That is, if the label-set based lower bound is larger than τ, then g is pruned



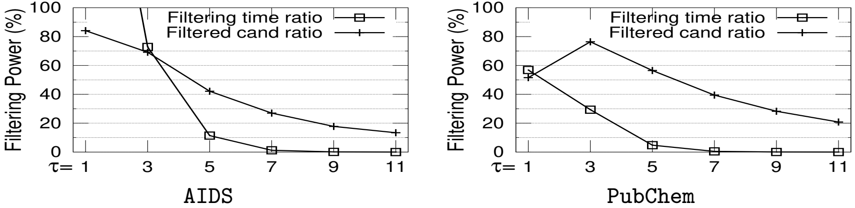
Processing time for 100 random queries

[7] Karam Gouda and Mosab Hassaan. "CSI_GED: An efficient approach for graph edit similarity computation". In: *Proc. of ICDE'16*. 2016.

[8] Jongik Kim, Dong-Hoon Choi, and Chen Li. "Inves: Incremental Partitioning-Based Verification for Graph Similarity Search". In: *Proc. of EDBT'19*. 2019.

Index-based Filtering for Graph Similarity Search

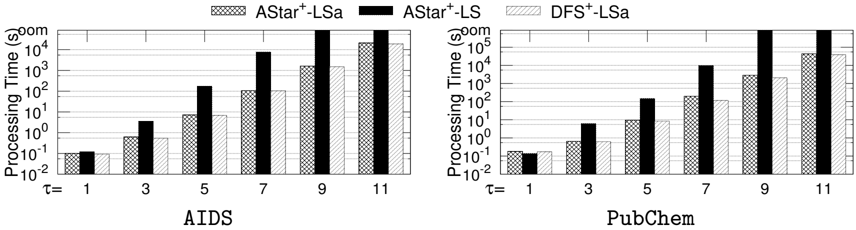
- *Filtering time ratio* of Pars[9]: $\frac{\text{filtering time of Pars}}{\text{total running time of AStar}^{+}\text{-LSa}}$
- *Filtered candidate ratio* of Pars: $\frac{\text{number of candidates filtered by Pars}}{\text{total number of candidates generated by LabelF}}$



Filtering effectiveness of Pars

[9] Xiang Zhao et al. "Efficient structure similarity searches: a partition-based approach". In: *VLDB J.* 27.1 (2018).

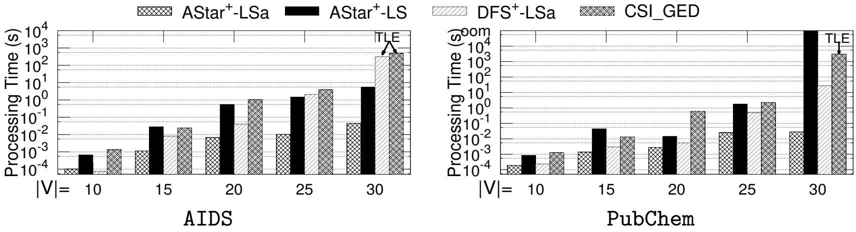
Our Algorithms for Graph Similarity Search



Processing time of our algorithms for 100 random queries

- AStar$^+$-LSa and DFS$^+$-LSa perform similarly
  - For graph similarity search, most of the pairs (q, g) are dissimilar pairs
  - We show in the paper that for dissimilar pairs, best-first search and depth-first search have the same search space and thus similar running time

GED Computation



Processing time for GED computation (ged $= 9$)

Conclusion

- We proposed an efficient algorithm AStar$^+$-`LSa` to speed up GED verification, which is achieved by three ingredients
  - Don't need to add dummy vertices to q or g
  - Tighter lower bound estimation
  - Efficient lower bound computation
- The existing indexing/filtering techniques become obsolete given our efficient GED verification algorithm AStar$^+$-`LSa`
- The source code of our algorithms will be available at https://github.com/LijunChang/Graph_Edit_Distance.