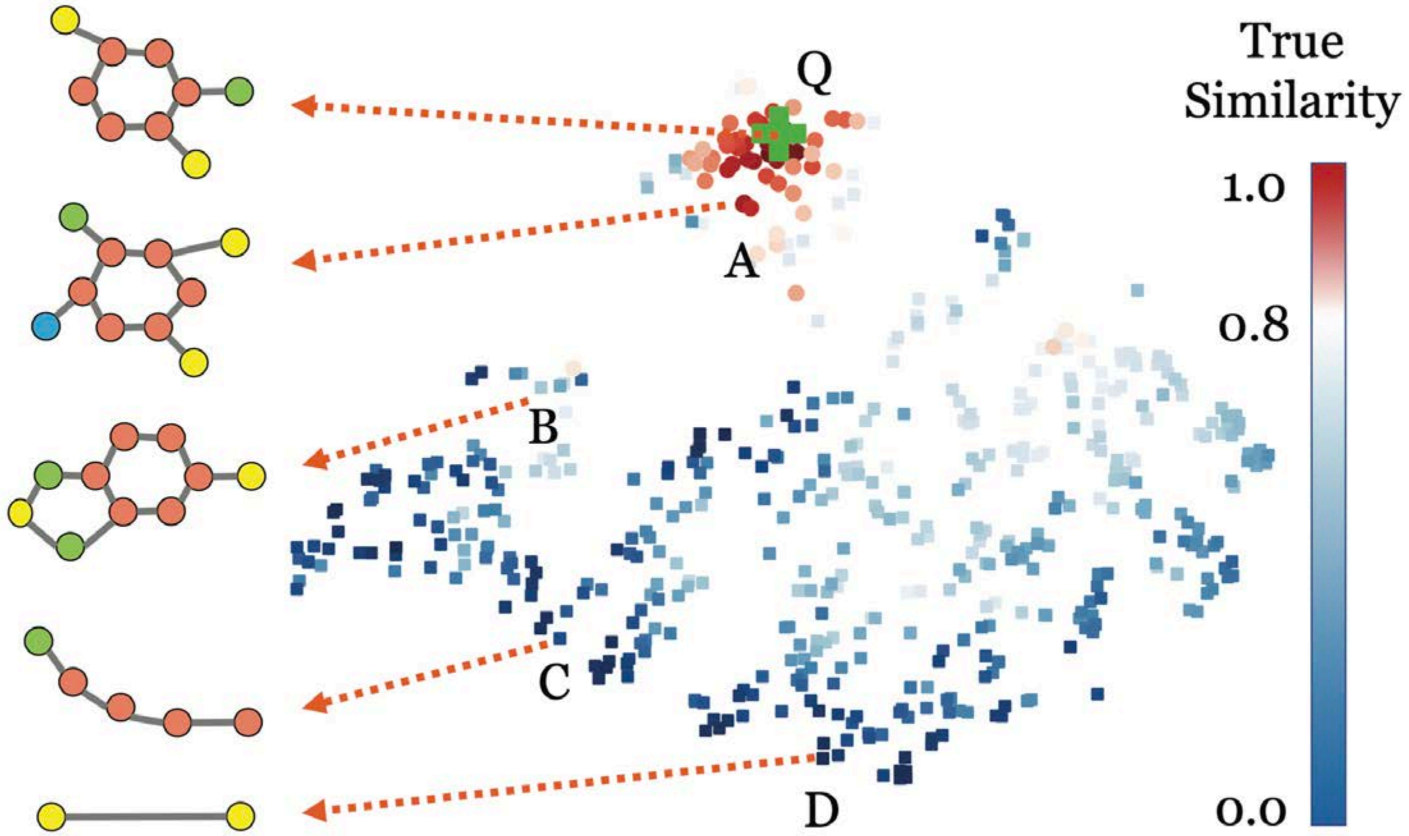
Paper Analysis related to Graph Similarity Search

SimGNN: A Neural Network Approach to Fast Graph Similarity Computation



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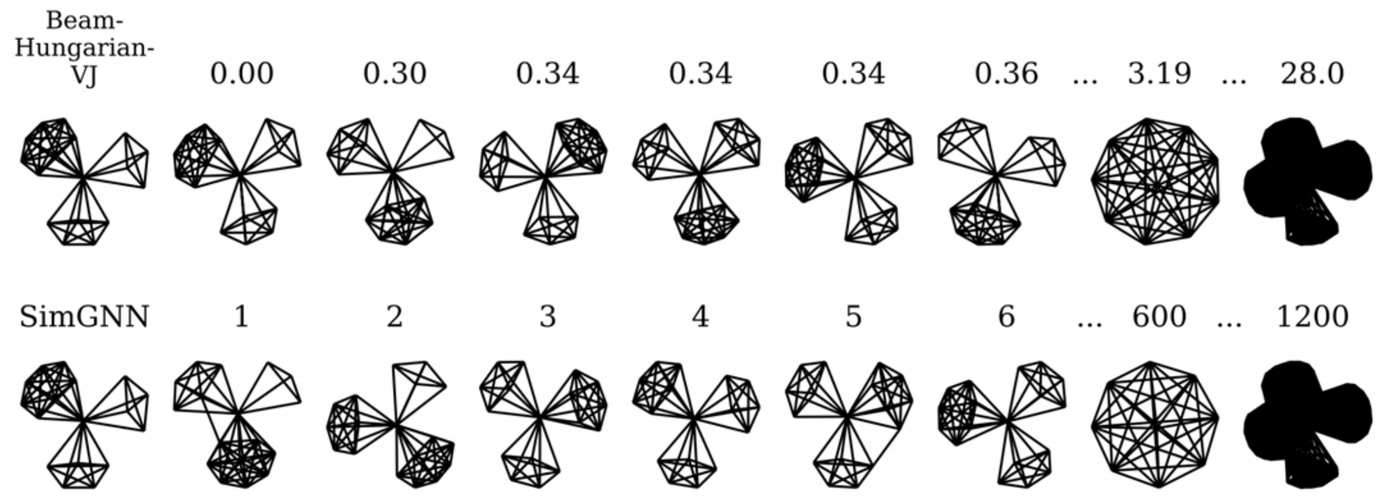

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- **SimGNN: A Neural Network Approach to Fast Graph Similarity Computation**
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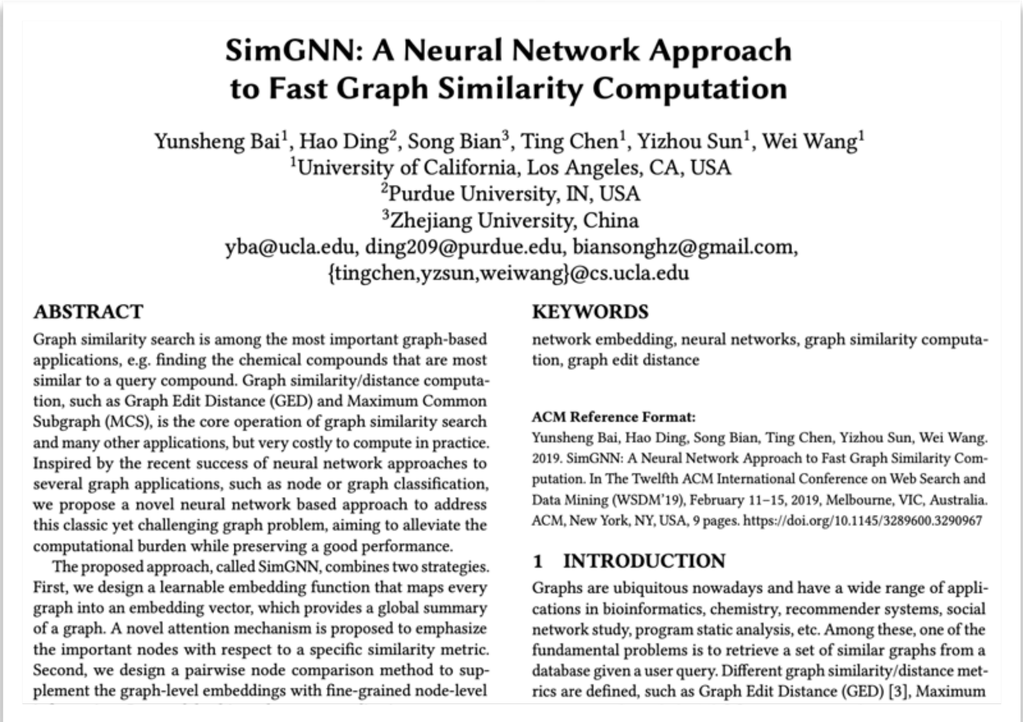

SimGNN: A Neural Network Approach to Fast Graph Similarity Computation

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ABSTRACT

Graph similarity search is among the most important graph-based applications, e.g. finding the chemical compounds that are most similar to a query compound. Graph similarity/distance computation, such as Graph Edit Distance (GED) and Maximum Common Subgraph (MCS), is the core operation of graph similarity search and many other applications, but very costly to compute in practice. Inspired by the recent success of neural network approaches to several graph applications, such as node or graph classification, we propose a novel neural network based approach to address this classic yet challenging graph problem, aiming to alleviate the computational burden while preserving a good performance.

The proposed approach, called SimGNN, combines two strategies. First, we design a learnable embedding function that maps every graph into an embedding vector, which provides a global summary of a graph. A novel attention mechanism is proposed to emphasize the important nodes with respect to a specific similarity metric. Second, we design a pairwise node comparison method to supplement the graph-level embeddings with fine-grained node-level

KEYWORDS

network embedding, neural networks, graph similarity computation, graph edit distance

ACM Reference Format:
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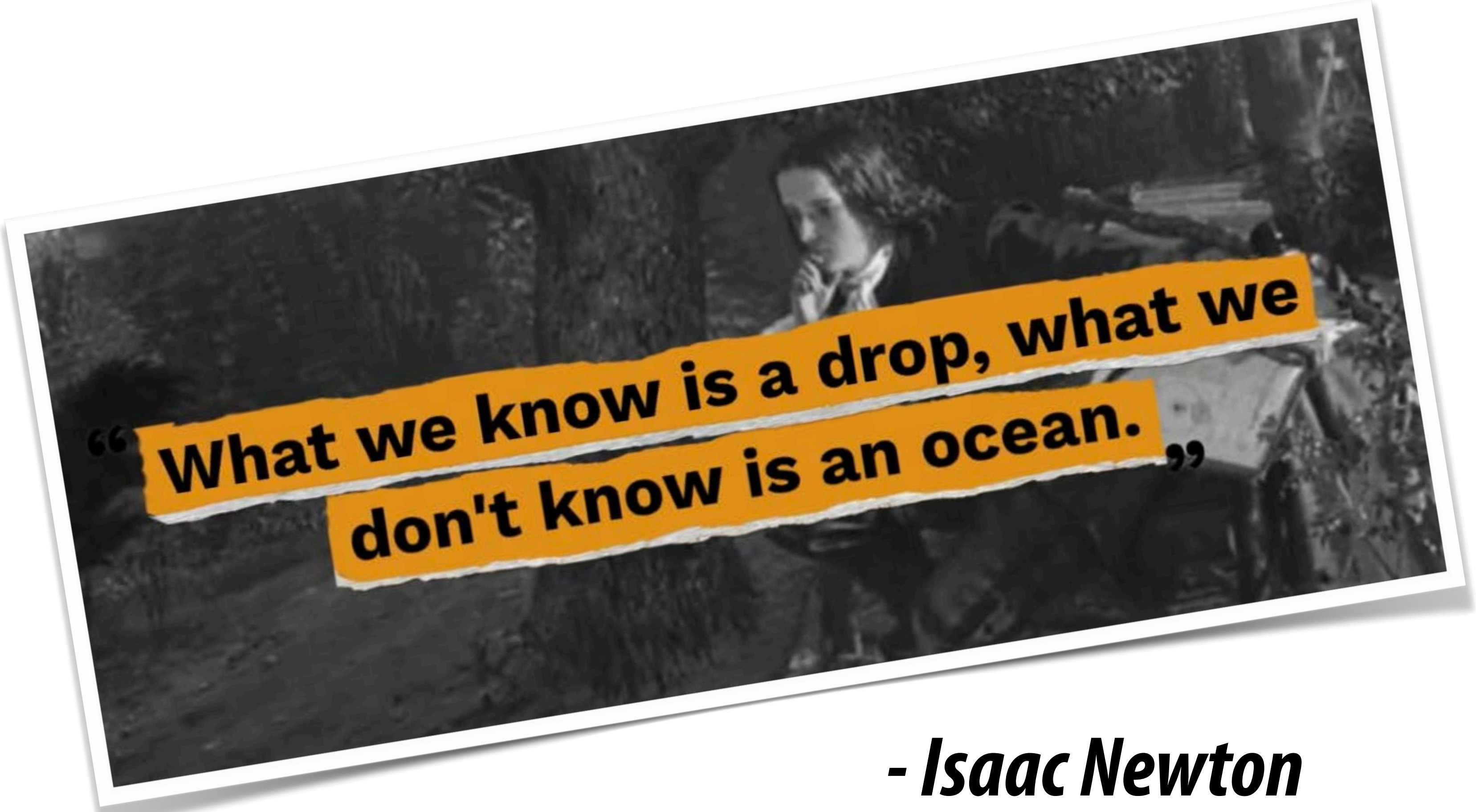
1 INTRODUCTION

Graphs are ubiquitous nowadays and have a wide range of applications in bioinformatics, chemistry, recommender systems, social network study, program static analysis, etc. Among these, one of the fundamental problems is to retrieve a set of similar graphs from a database given a user query. Different graph similarity/distance metrics are defined, such as Graph Edit Distance (GED) [3], Maximum

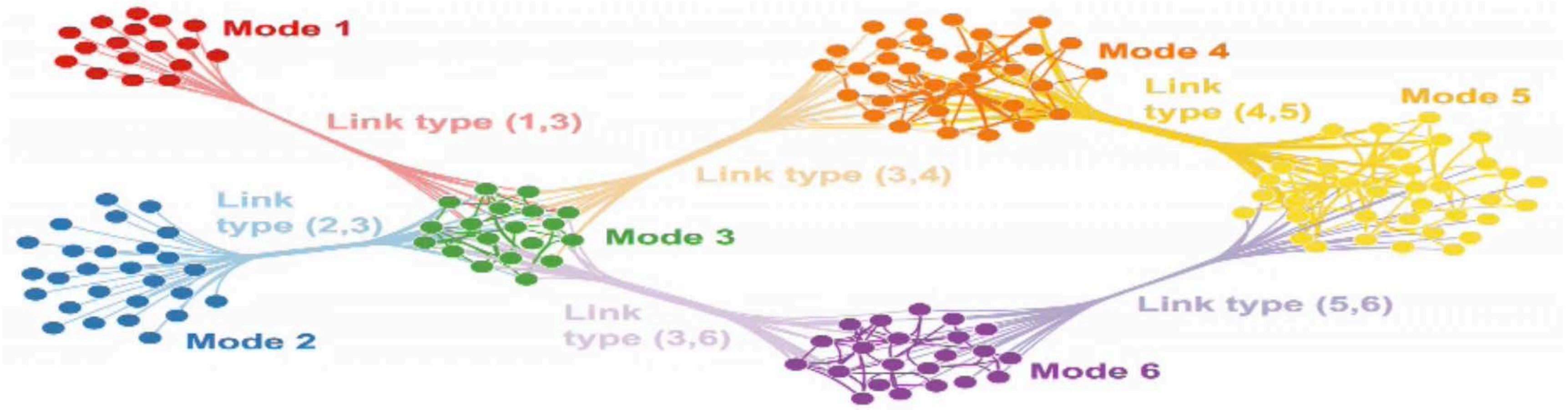
WSDM 2019

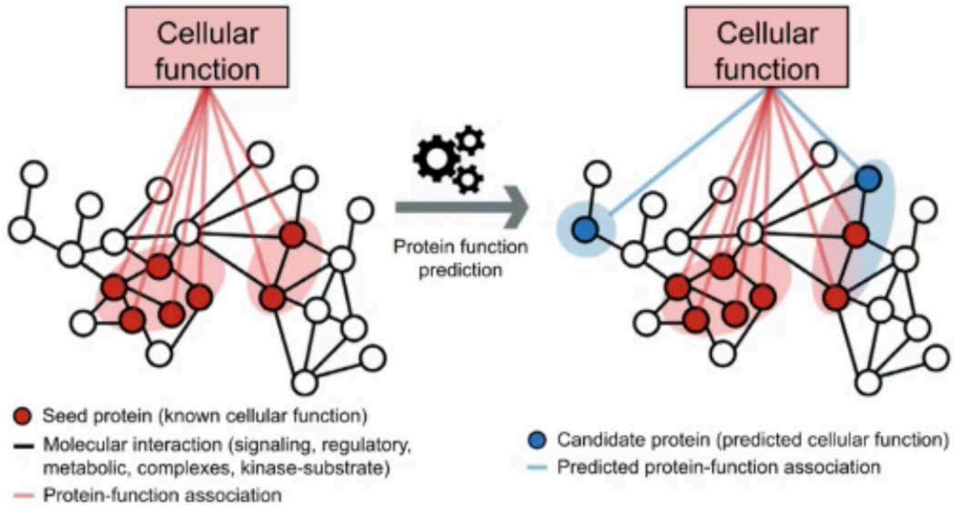


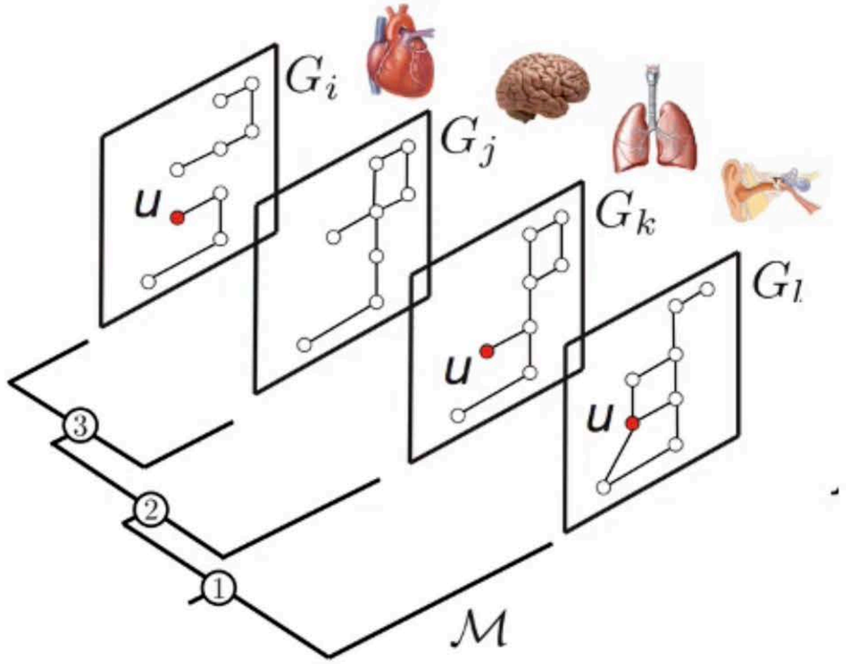
- Isaac Newton

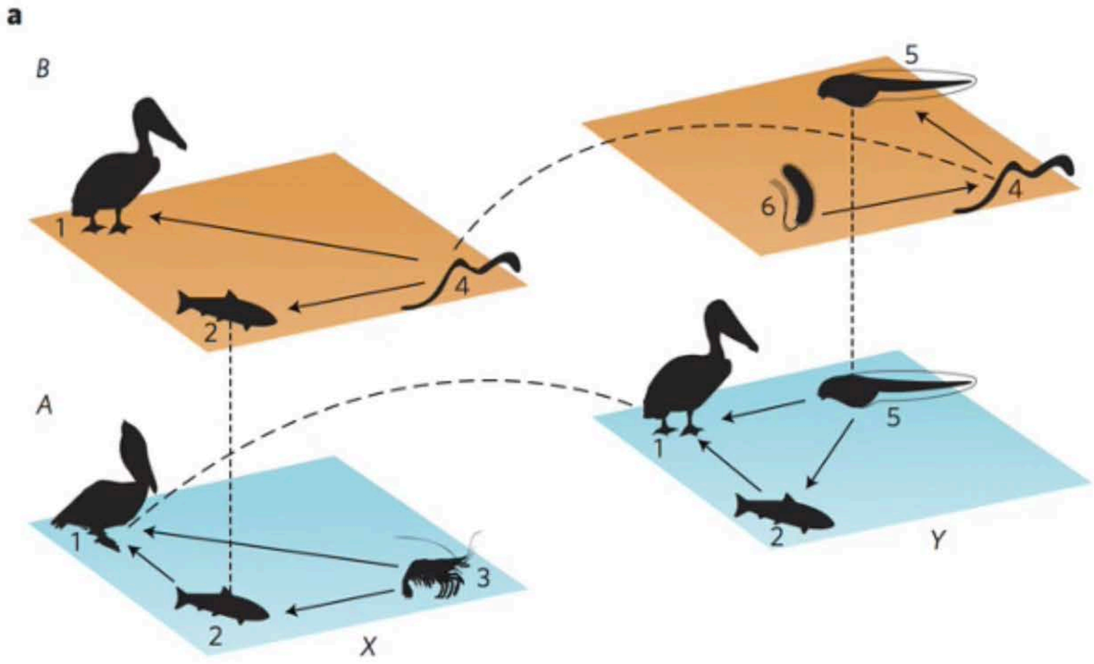
Graph Applications: Biology

- **Biology**
- Chemistry
- Social Network Analysis
- Software Analysis
- Circuit Design









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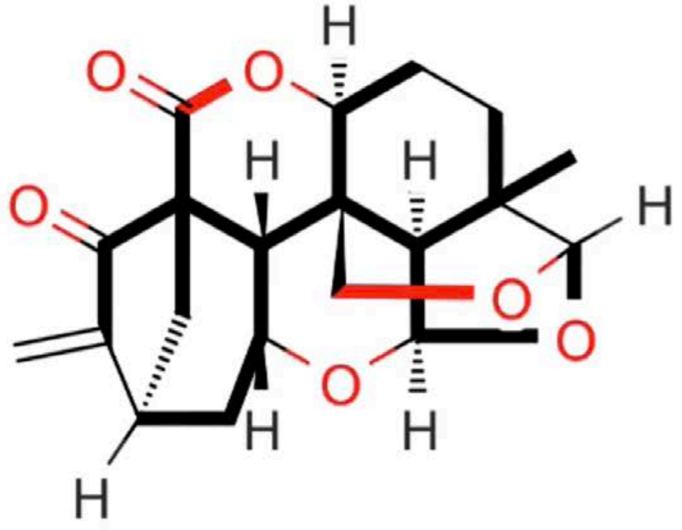
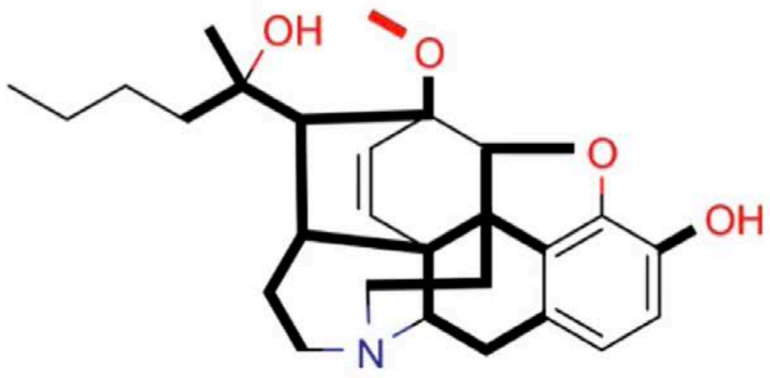
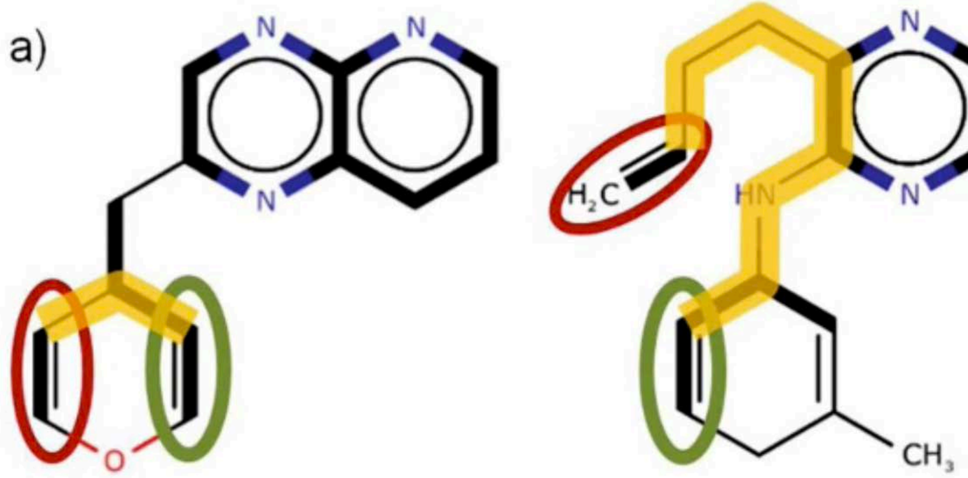
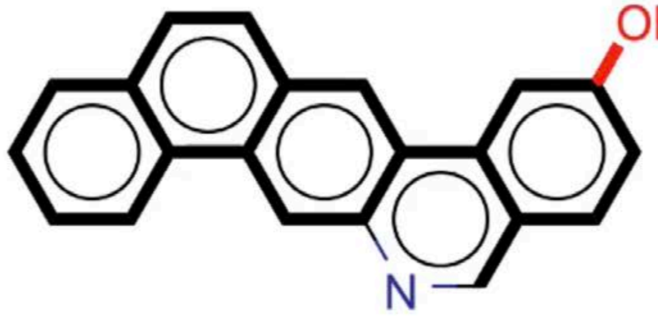
Graph Applications: Chemistry

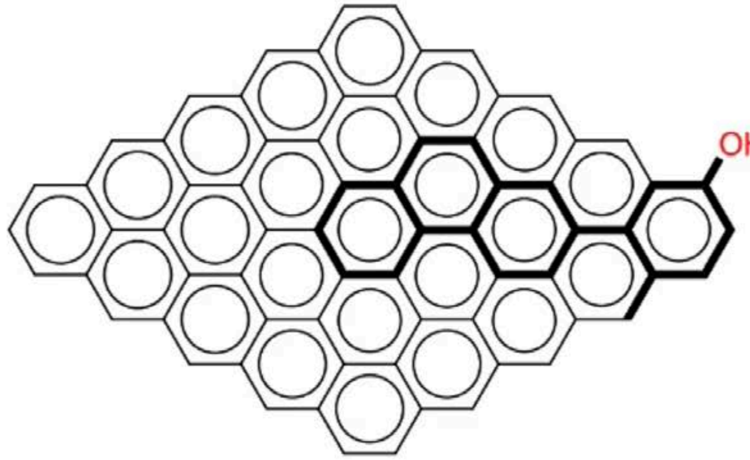
- Biology
- **Chemistry**
- Social Network Analysis
- Software Analysis
- Circuit Design











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Graph Applications: Social Network Analysis

- Biology
- Chemistry
- **Social Network Analysis**
- Software Analysis
- Circuit Design

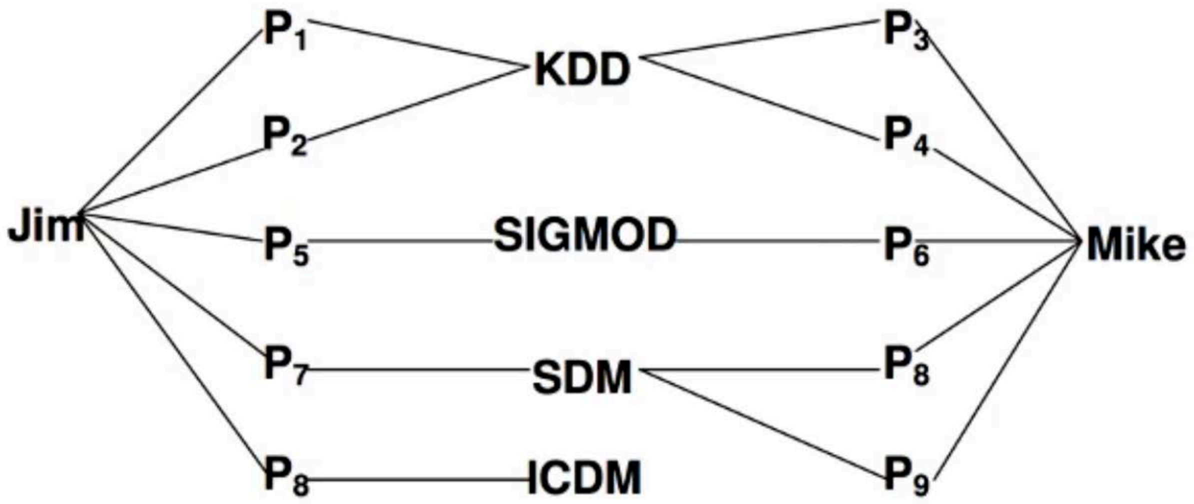
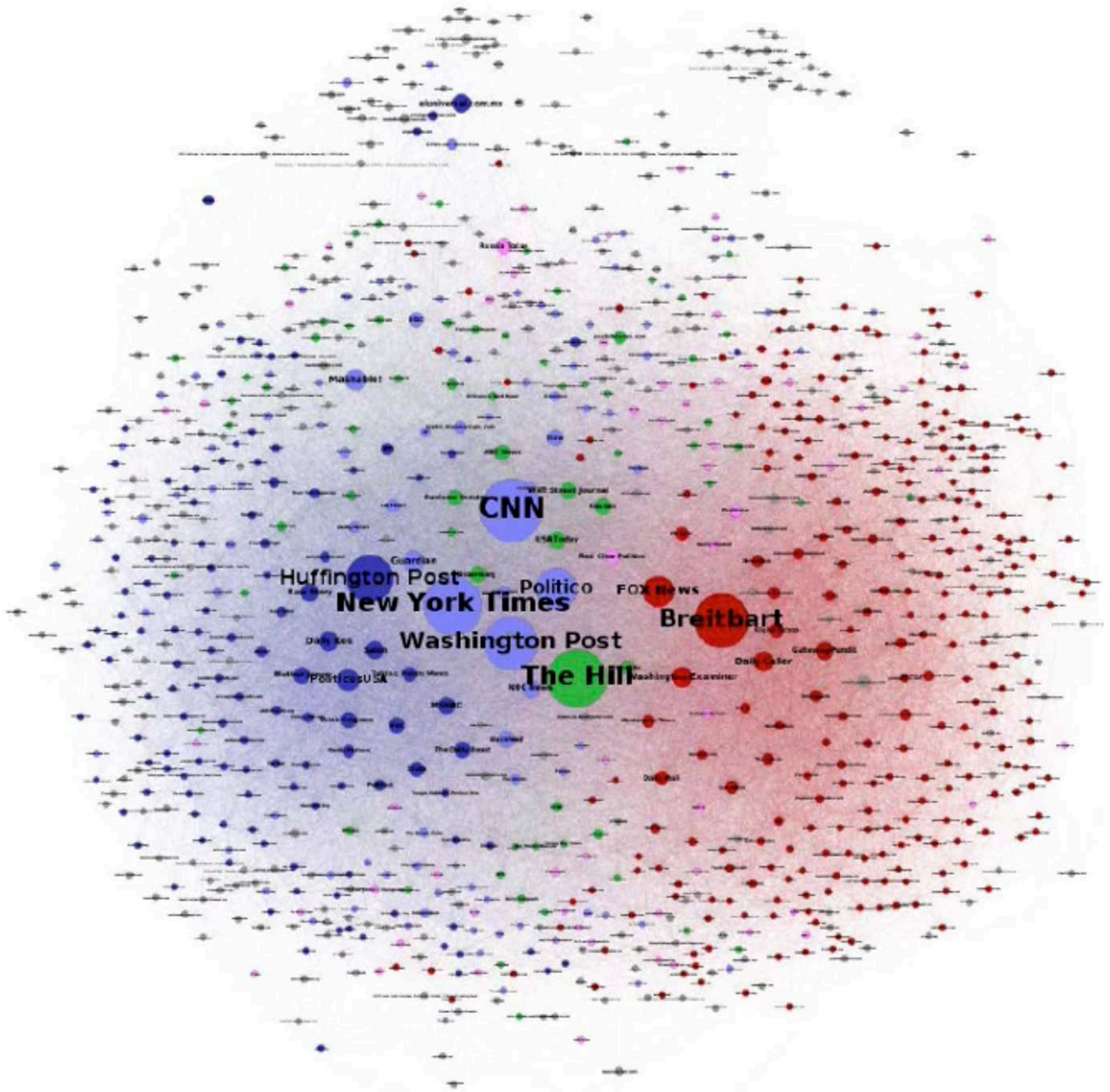


Figure 3. An Example of A-P-V-P-A Paths Between Two Authors



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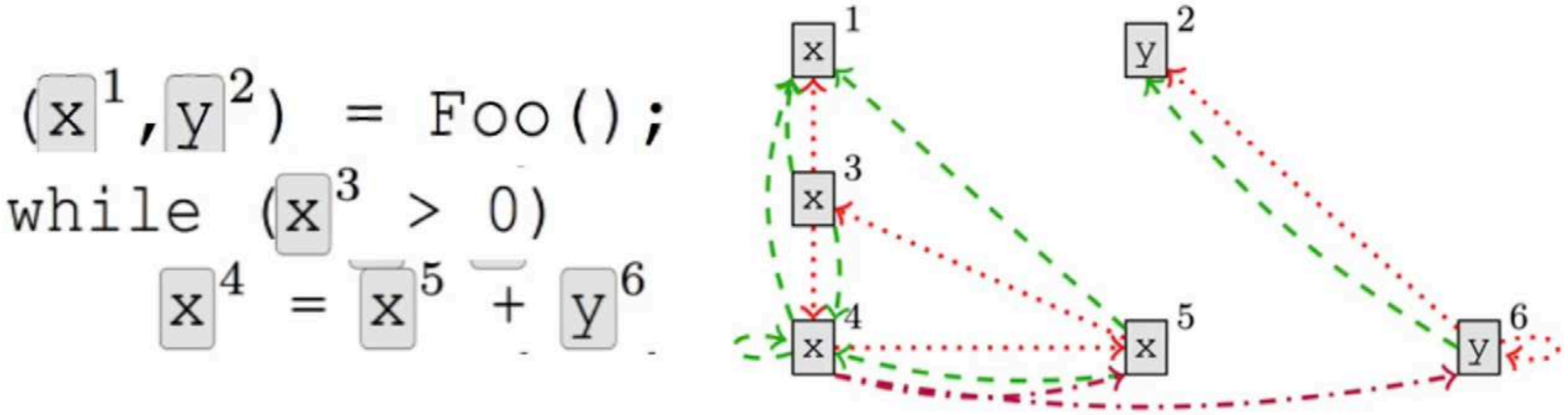
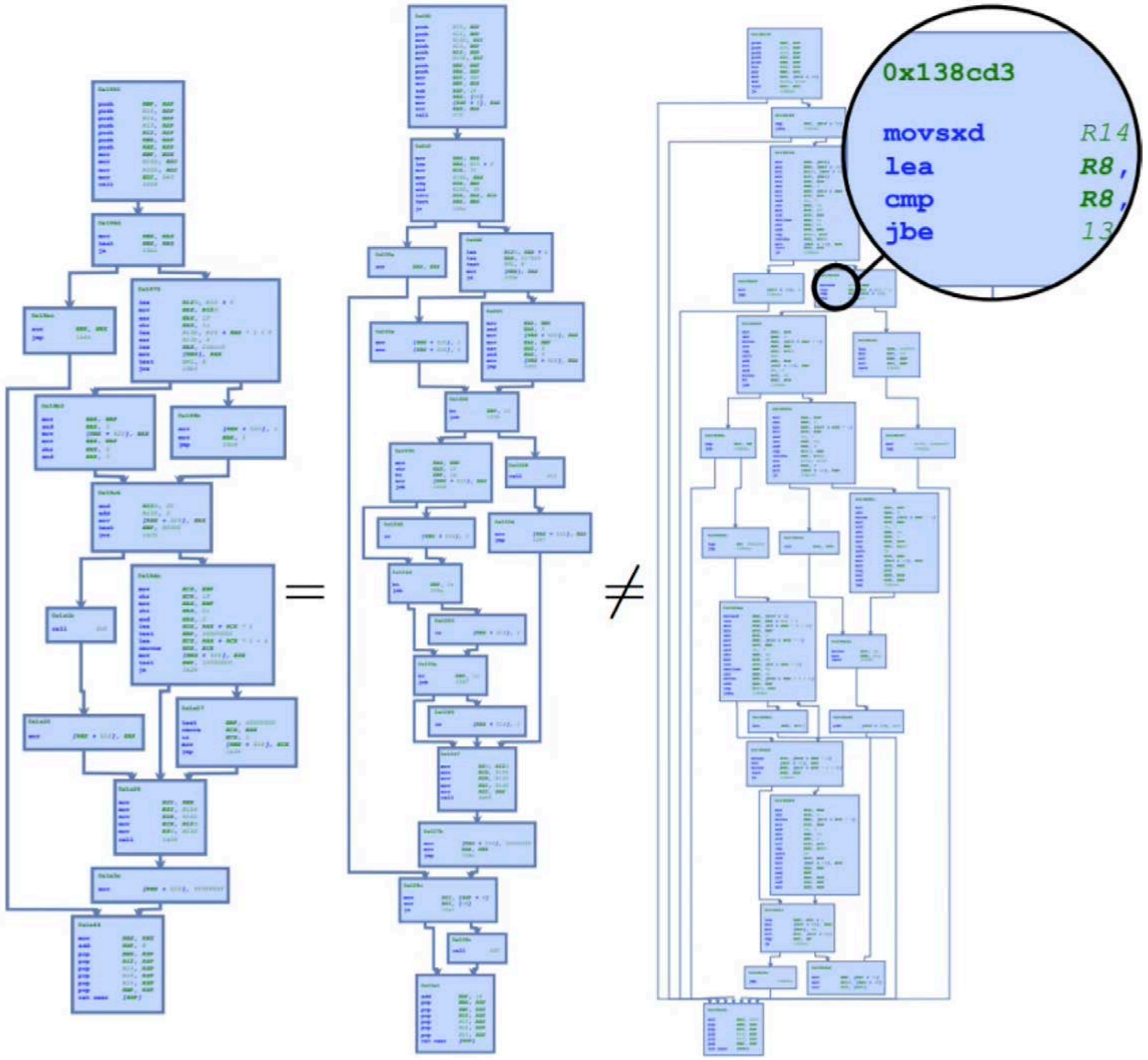
Graph Applications: Software Analysis

- Biology
- Chemistry
- Social Network Analysis
- **Software Analysis**
- Circuit Design





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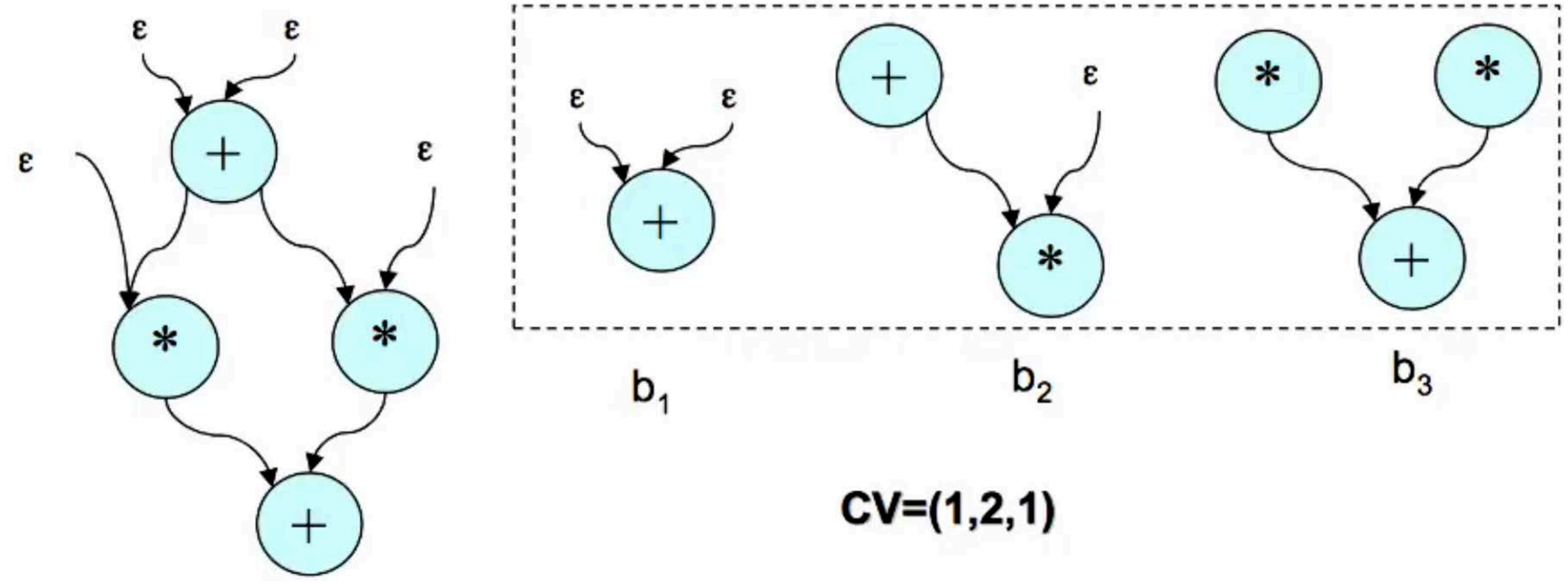
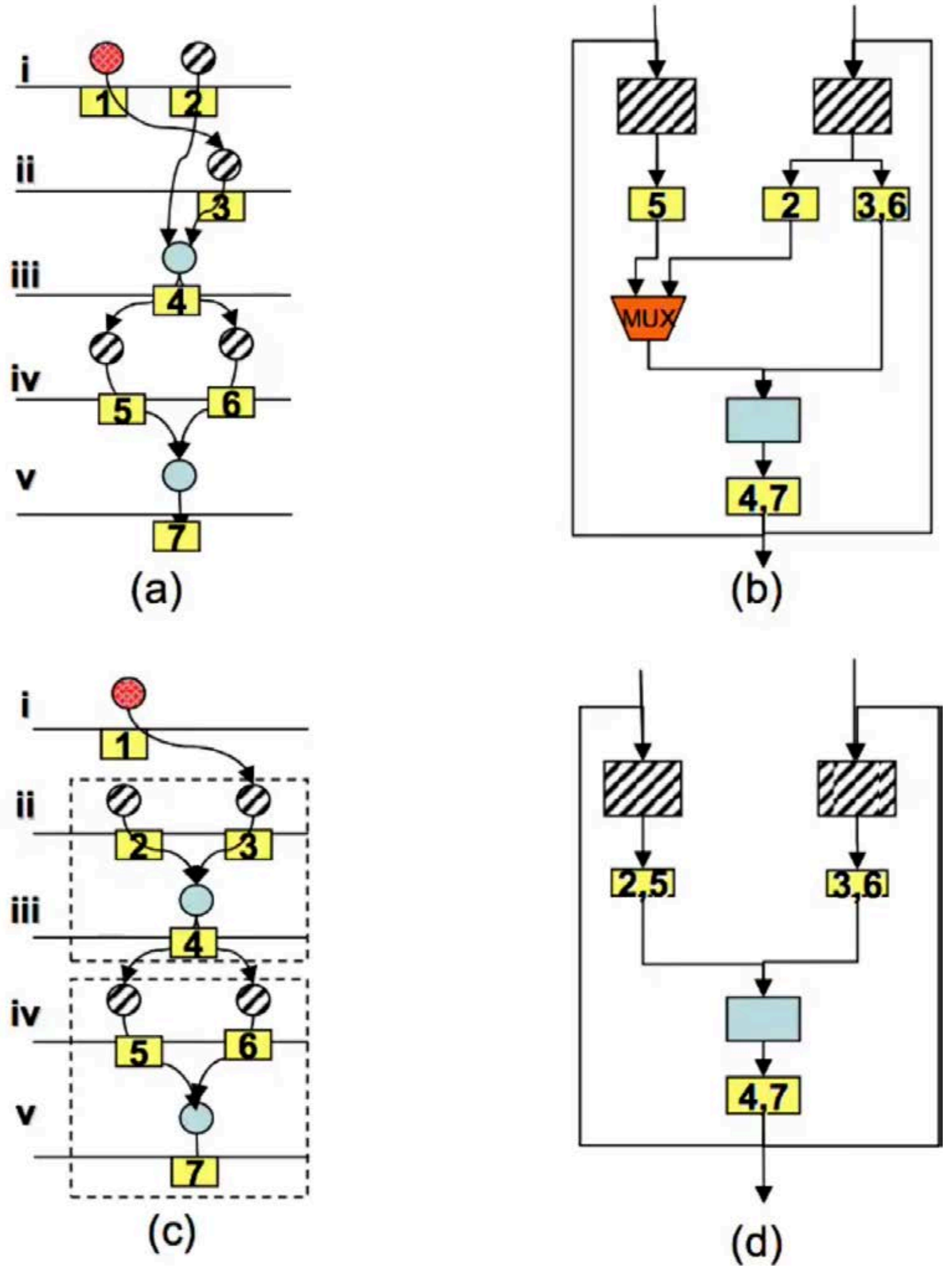
Graph Applications: Circuit Design

- Biology
- Chemistry
- Social Network Analysis
- Software Analysis
- **Circuit Design**





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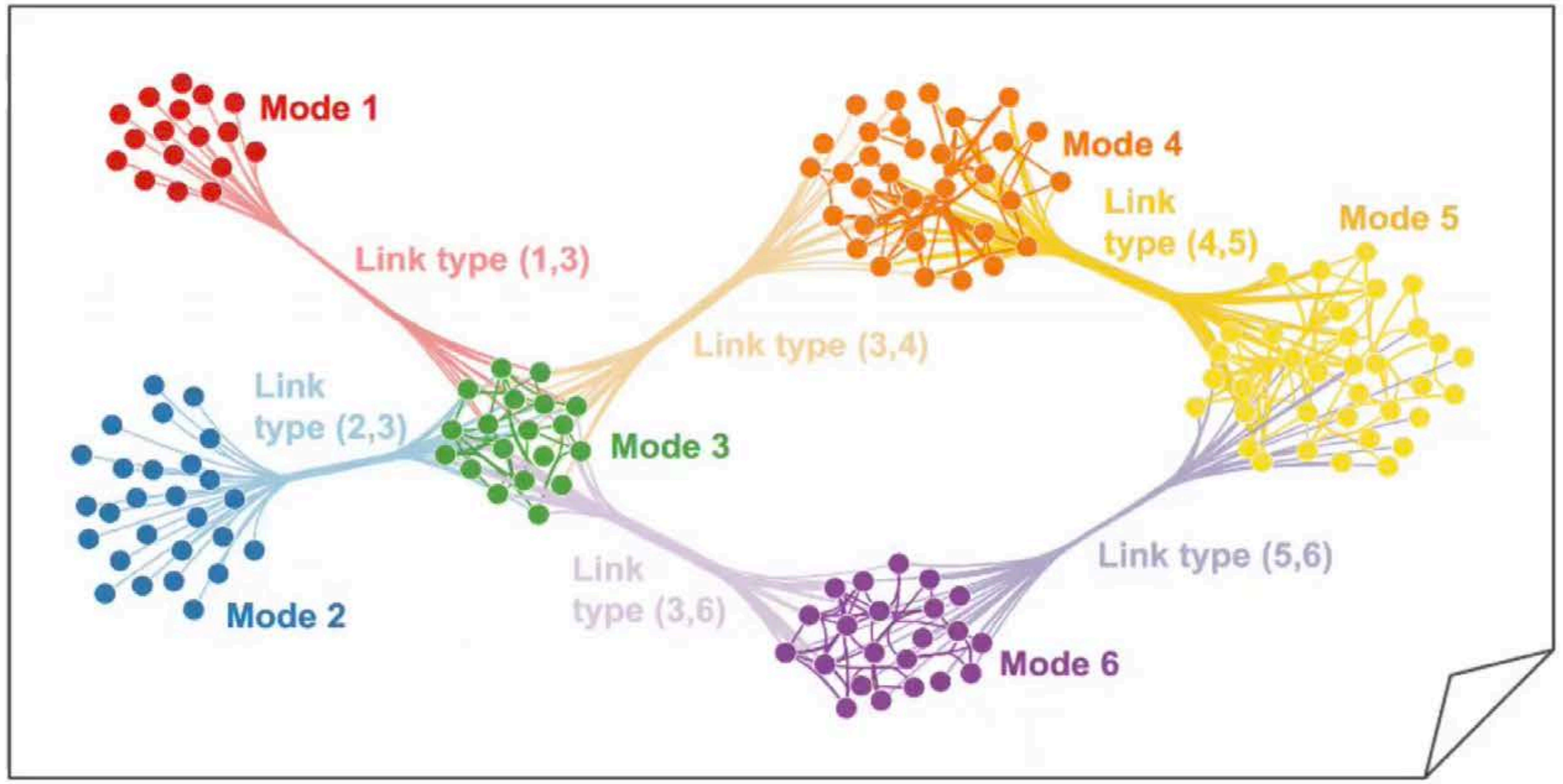
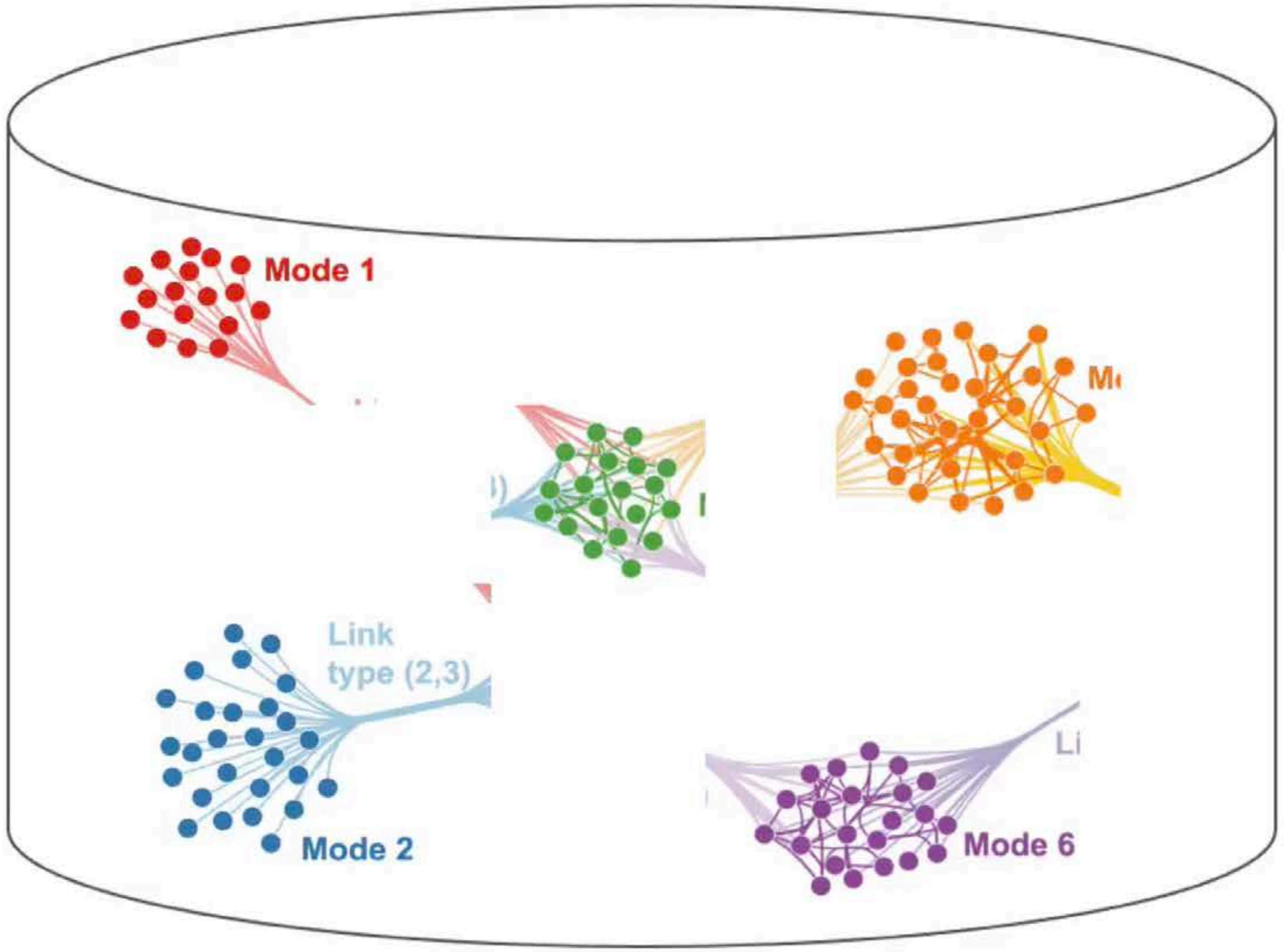
Applications: Node-Level vs. Graph-Level



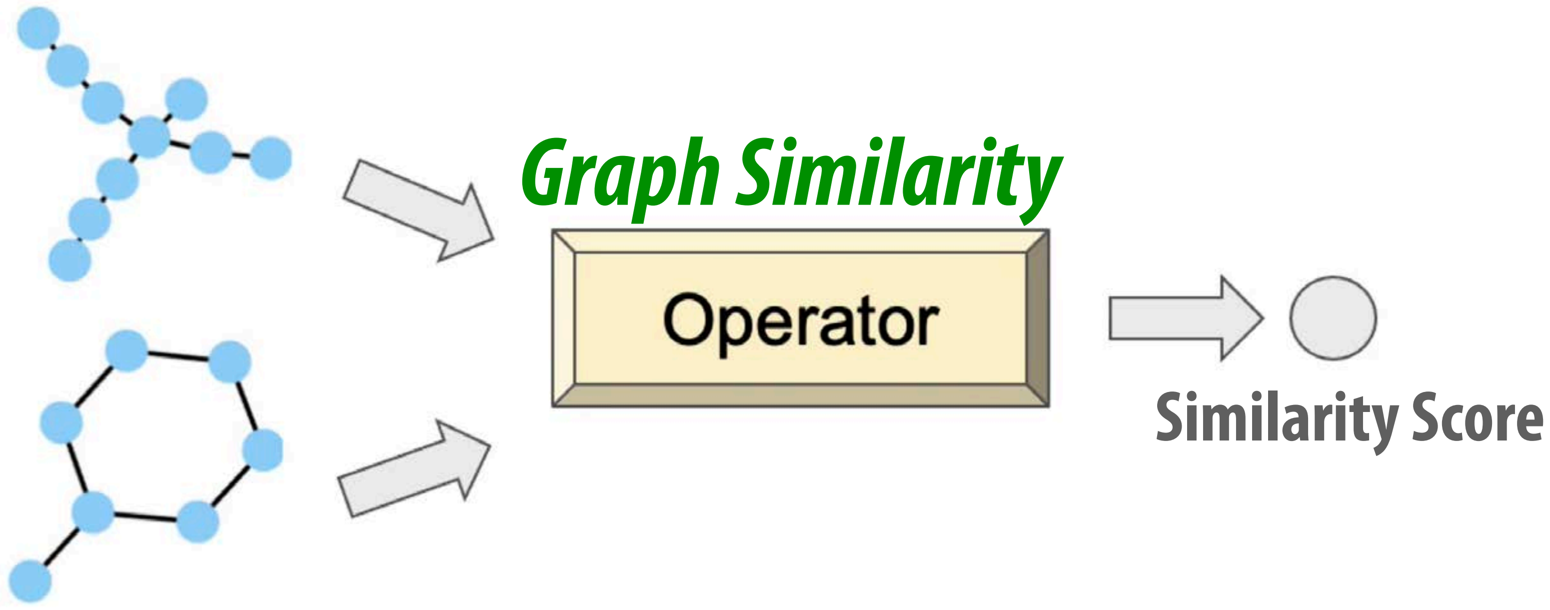
One Single Graph

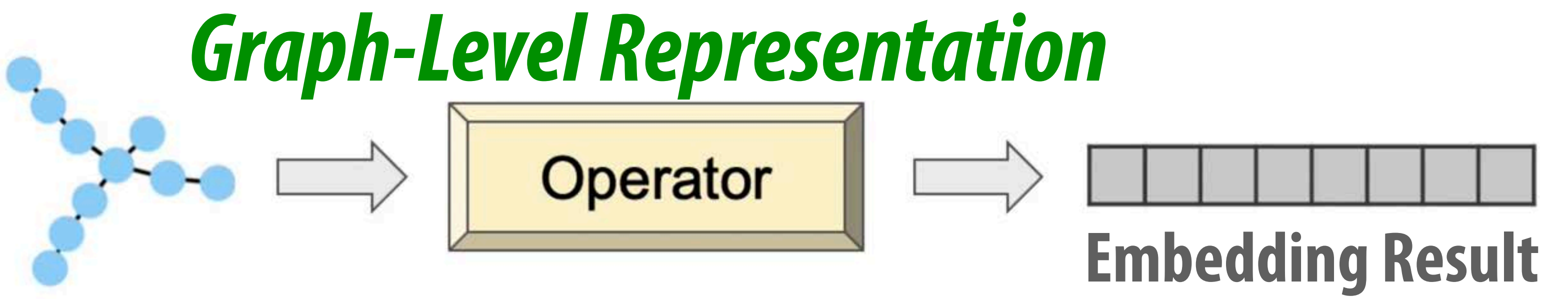


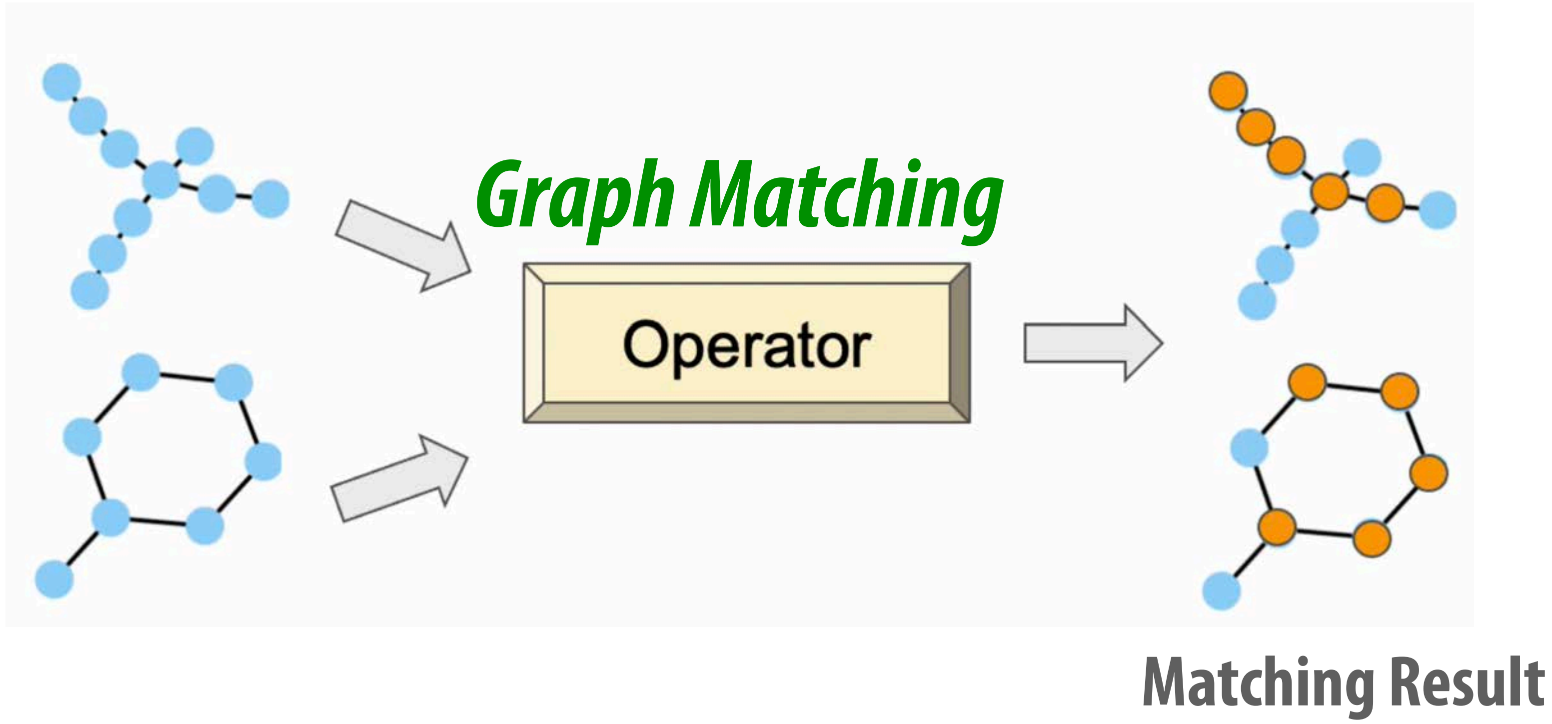
A Collection of Graphs

Graph-Level Operators

- Graph Similarity
- Graph Matching
- Graph-Level Representation
- …

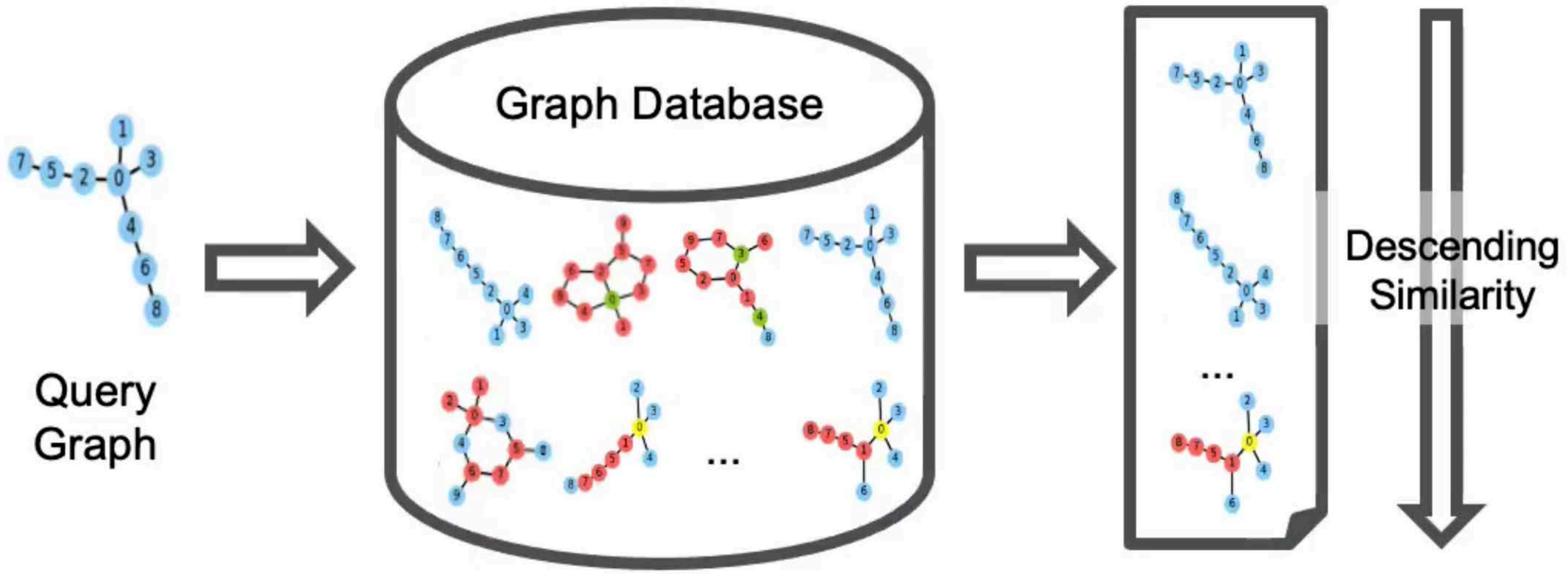




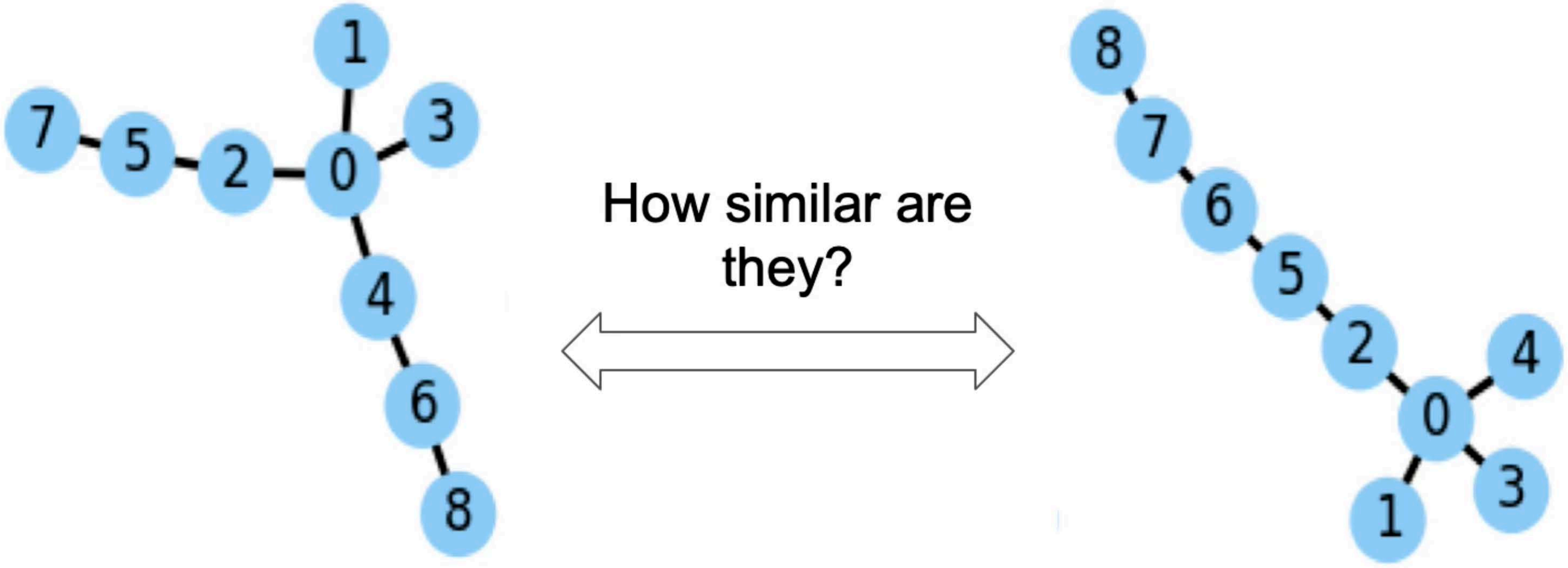


SimGNN: Introduction

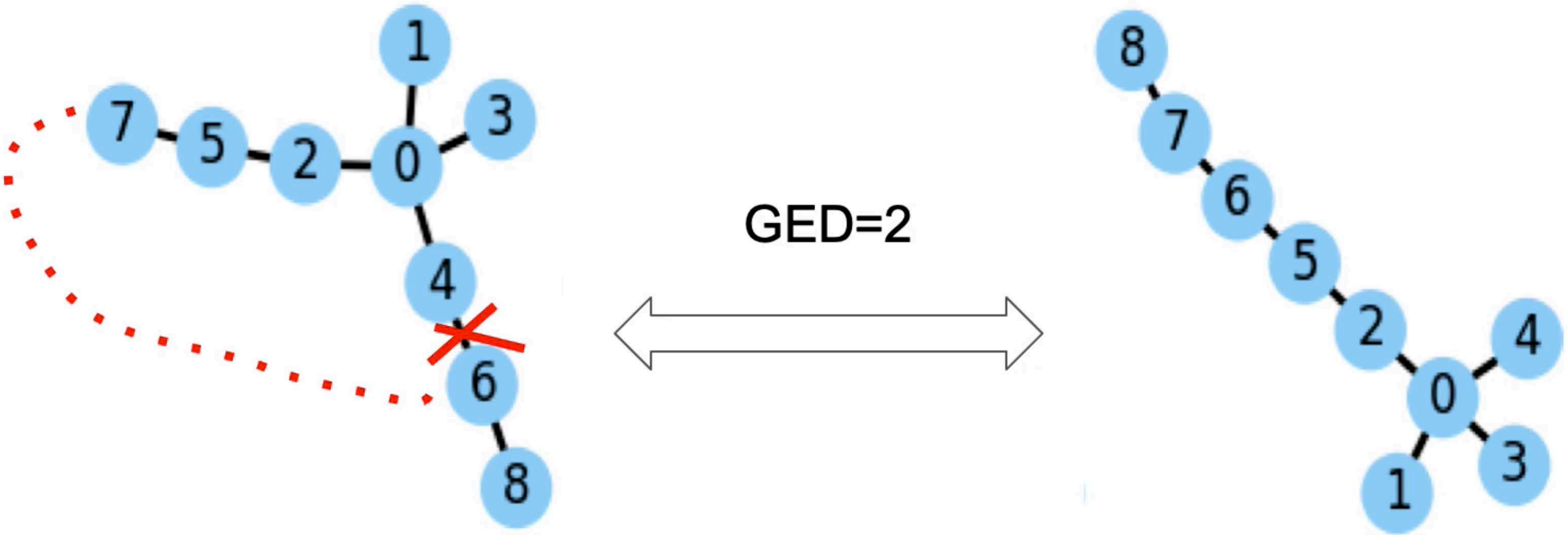
- **Neural Network Based Approach for Graph Analytics**
- **Graph-Graph Similarity**
  - **Applications:**
    - Drug design
    - Computer security
    - Social network analysis
    - Anomaly detection
  - **Challenging (NP-hard)**



Graph Similarity Computation



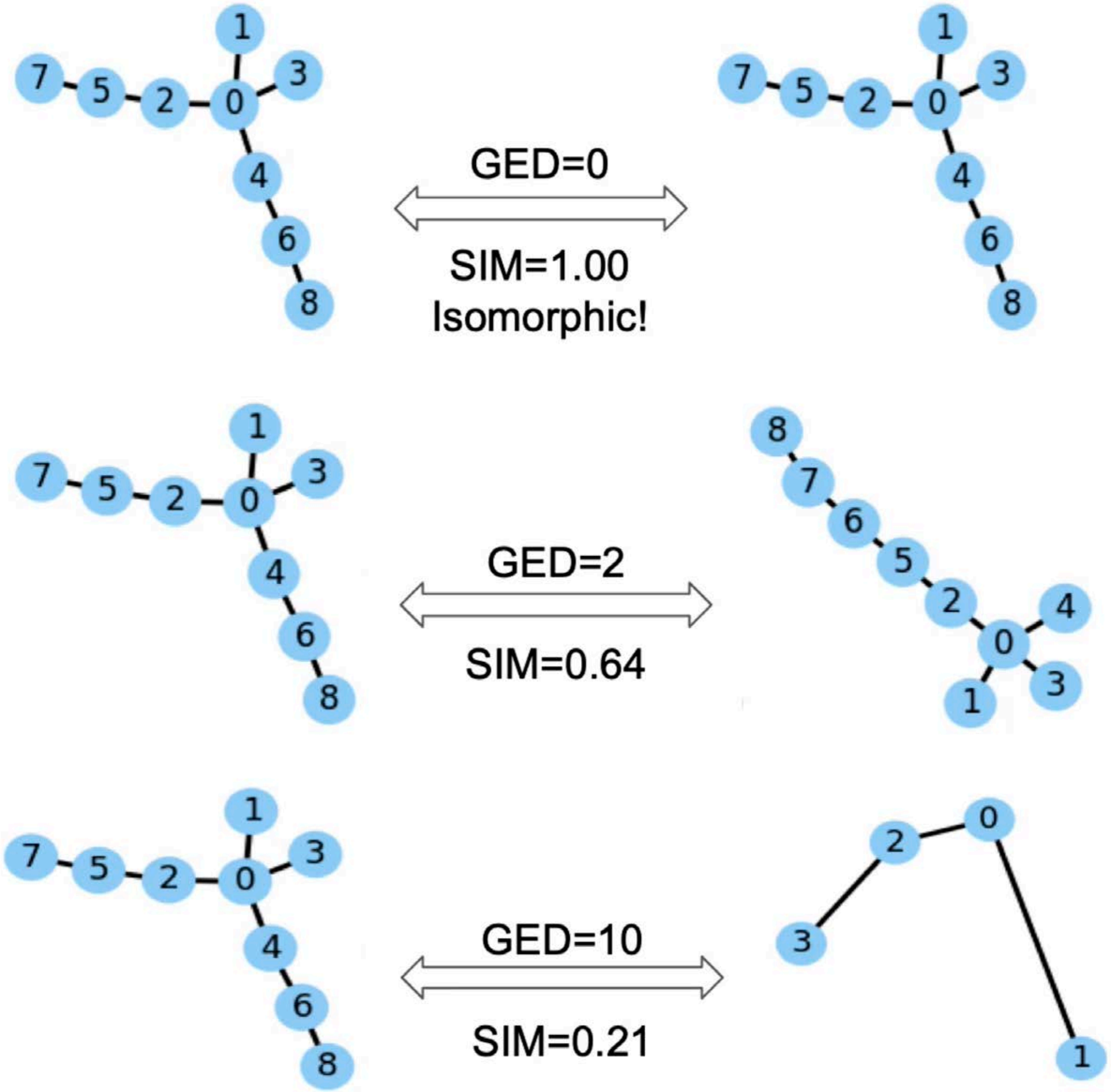
Graph Edit Distance (GED)



Examples of GED-Based Similarity Computation

The GED and similarity can be *transformed* to one another via a ***bijective mapping***:

sim = exp (-GED)

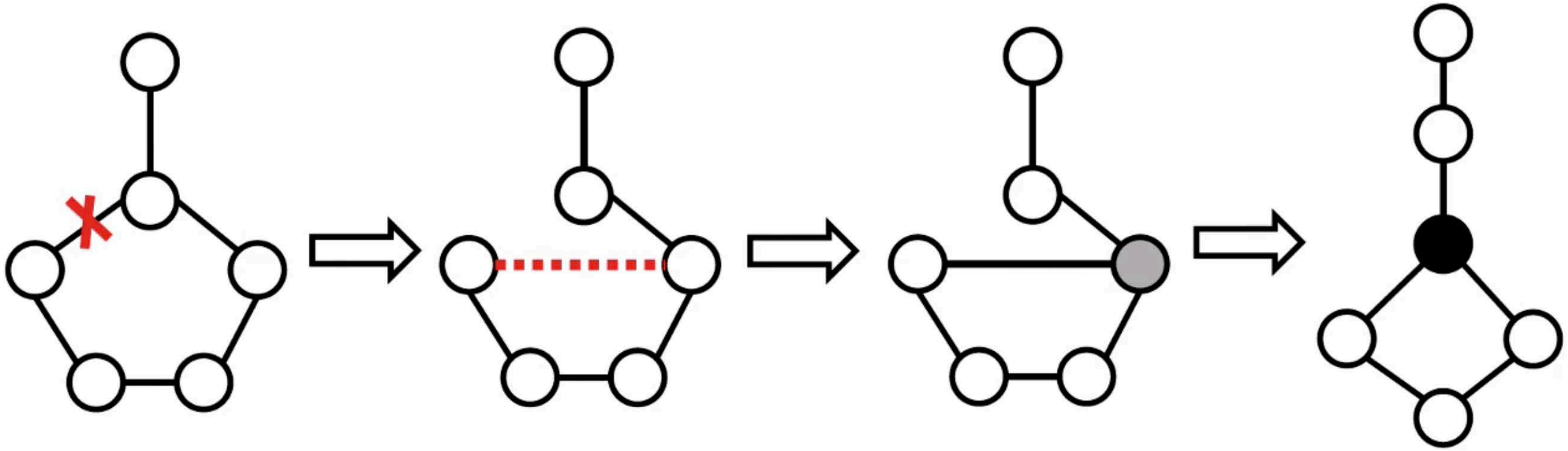


Existing Work on Graph Similarity Computation

- **Computation of exact GED between two graphs: NP-hard!**

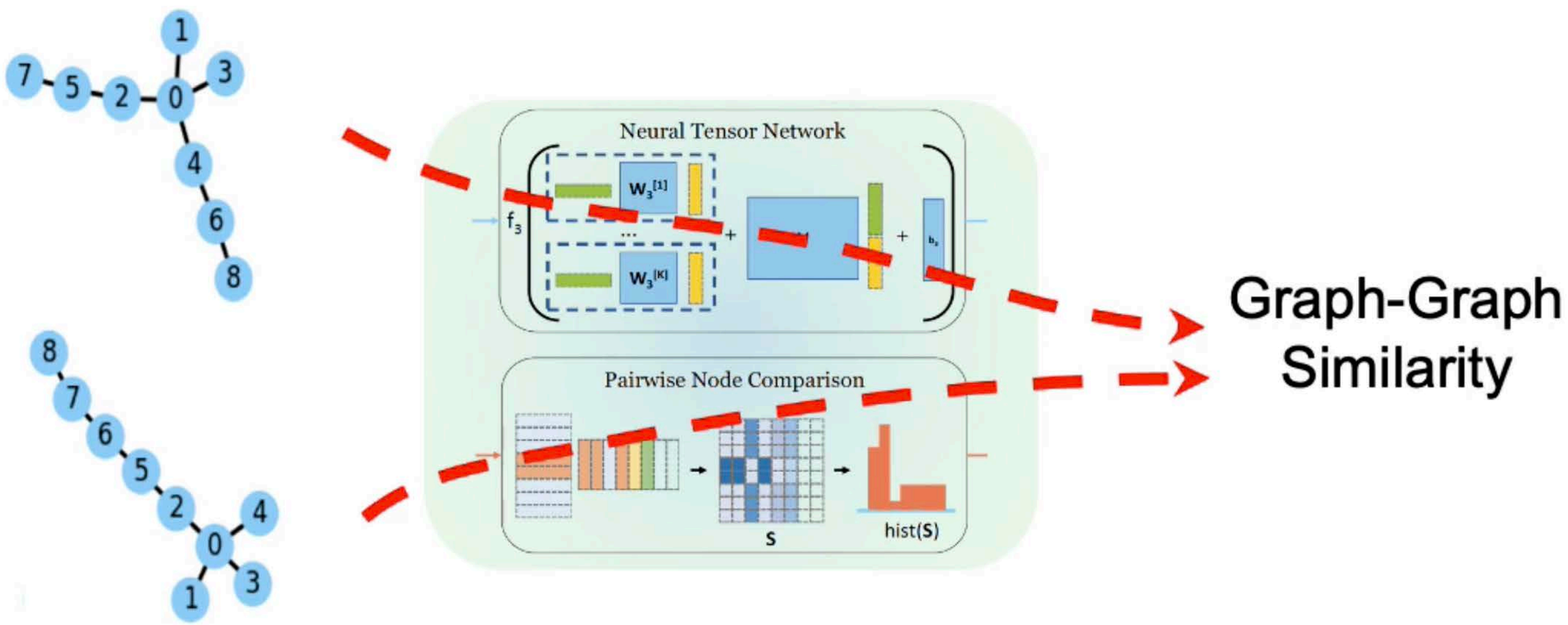
- **Search/Combinatorial optimization approaches:**
  - Domain knowledge and heuristics
  - Difficult to design

Method	Time Complexity
A* [19]	$O(N_1{}^{N_2})$
Beam [11]	subexponential
Hungarian [13]	$O((N_1+N_2)^3)$
VJ [12]	$O((N_1+N_2)^3)$
HED [14]	$O((N_1+N_2)^2)$

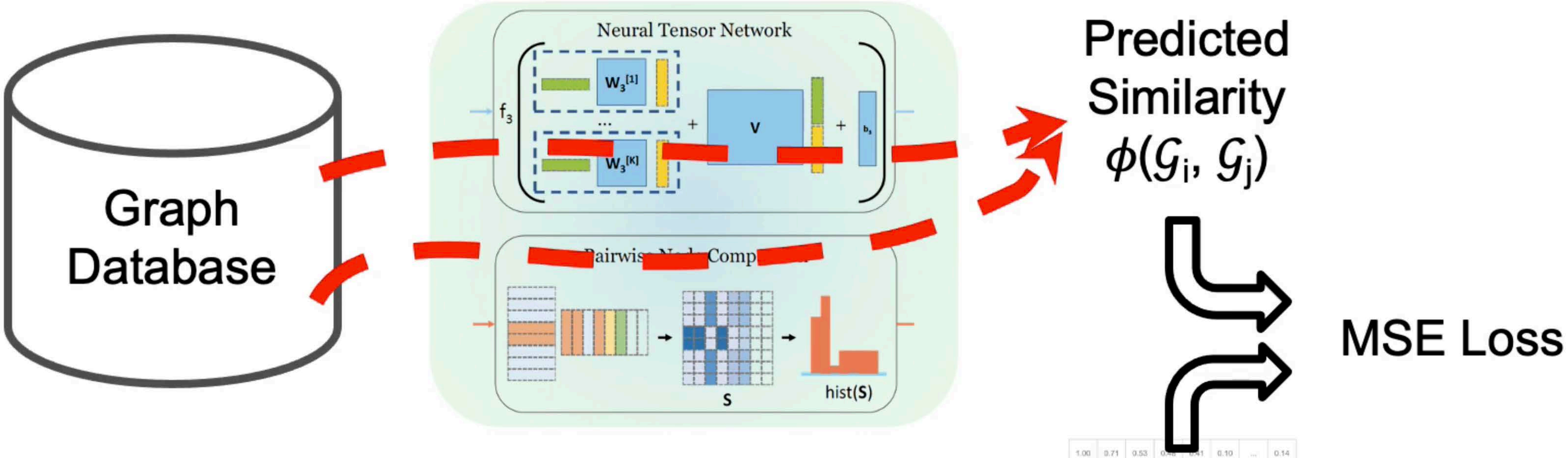


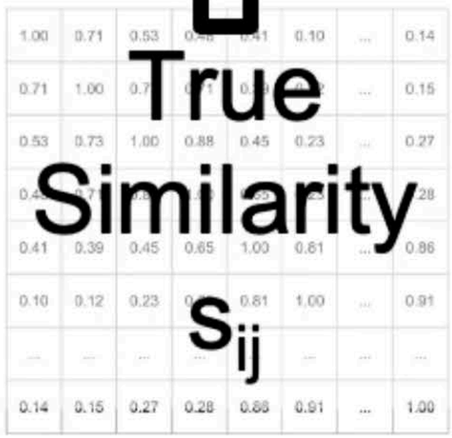
A General Learning Framework for Graph Similarity

- **Goal:** Learn a *neural network*-based similarity function $\phi(G_i, G_j)$
  - **Input:** A pair of graph, G_i and G_j
  - **Output:** The estimated graph-graph similarity
  - **Desired properties of ϕ:**
    - Representation-invarian
    - Inductive
    - Learnable



Training Phase: Minimize $(\phi(G_i, G_j) - s_{ij})^2$

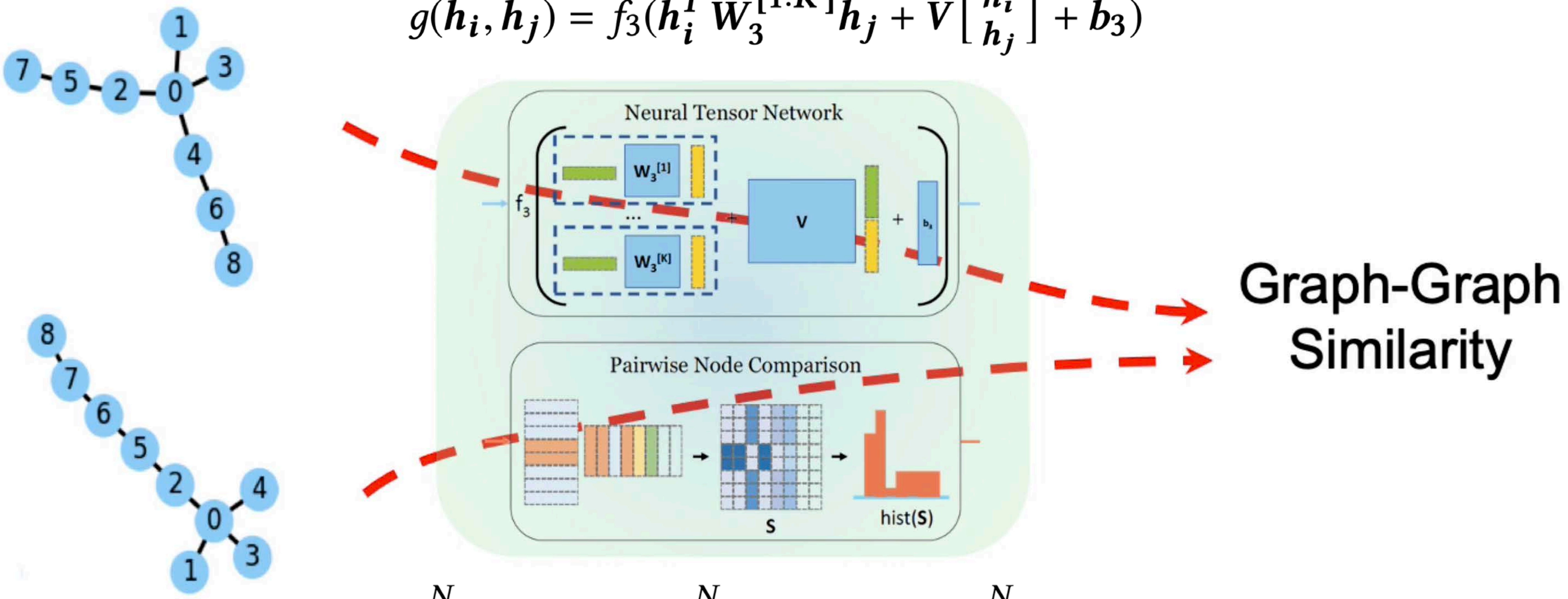




$$\mathcal{L} = \frac{1}{|\mathcal{D}|} \sum_{(i,j) \in \mathcal{D}} (\hat{s_{ij}} - s(\mathcal{G}_i, \mathcal{G}_j))^2$$

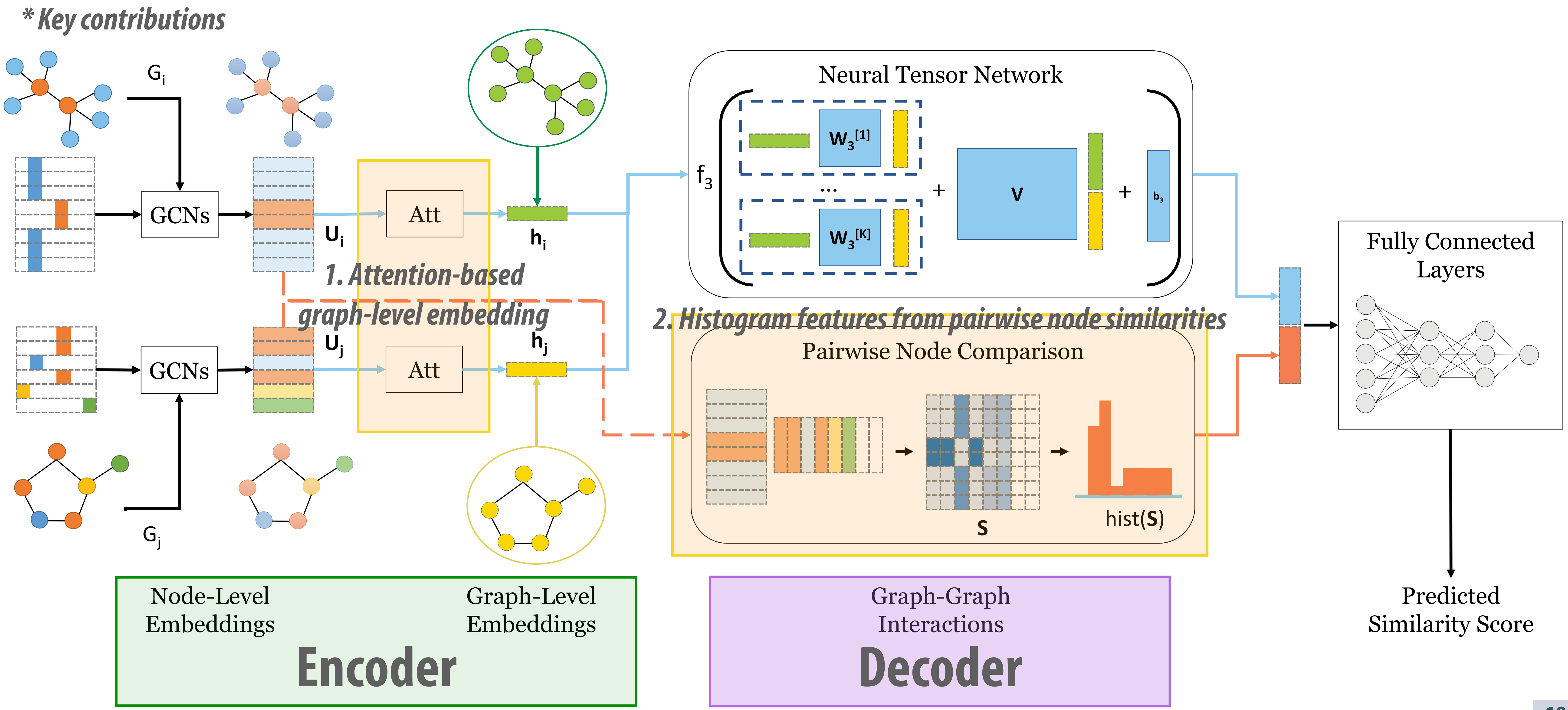
Testing Phase: Graph Similarity Computation

$$g(\boldsymbol{h_i}, \boldsymbol{h_j}) = f_3(\boldsymbol{h_i^T} \boldsymbol{W_3^{[1:K]}} \boldsymbol{h_j} + \boldsymbol{V} \begin{bmatrix} \boldsymbol{h_i} \\ \boldsymbol{h_j} \end{bmatrix} + \boldsymbol{b_3})$$



$$\boldsymbol{h} = \sum_{n=1}^{N} f_2(\boldsymbol{u_n^T} \boldsymbol{c}) \boldsymbol{u_n} = \sum_{n=1}^{N} f_2(\boldsymbol{u_n^T} \tanh((\frac{1}{N} \sum_{m=1}^{N} \boldsymbol{u_m}) \boldsymbol{W_2})) \boldsymbol{u_n}$$

SimGNN: A Novel Framework



Evaluation: Effectiveness

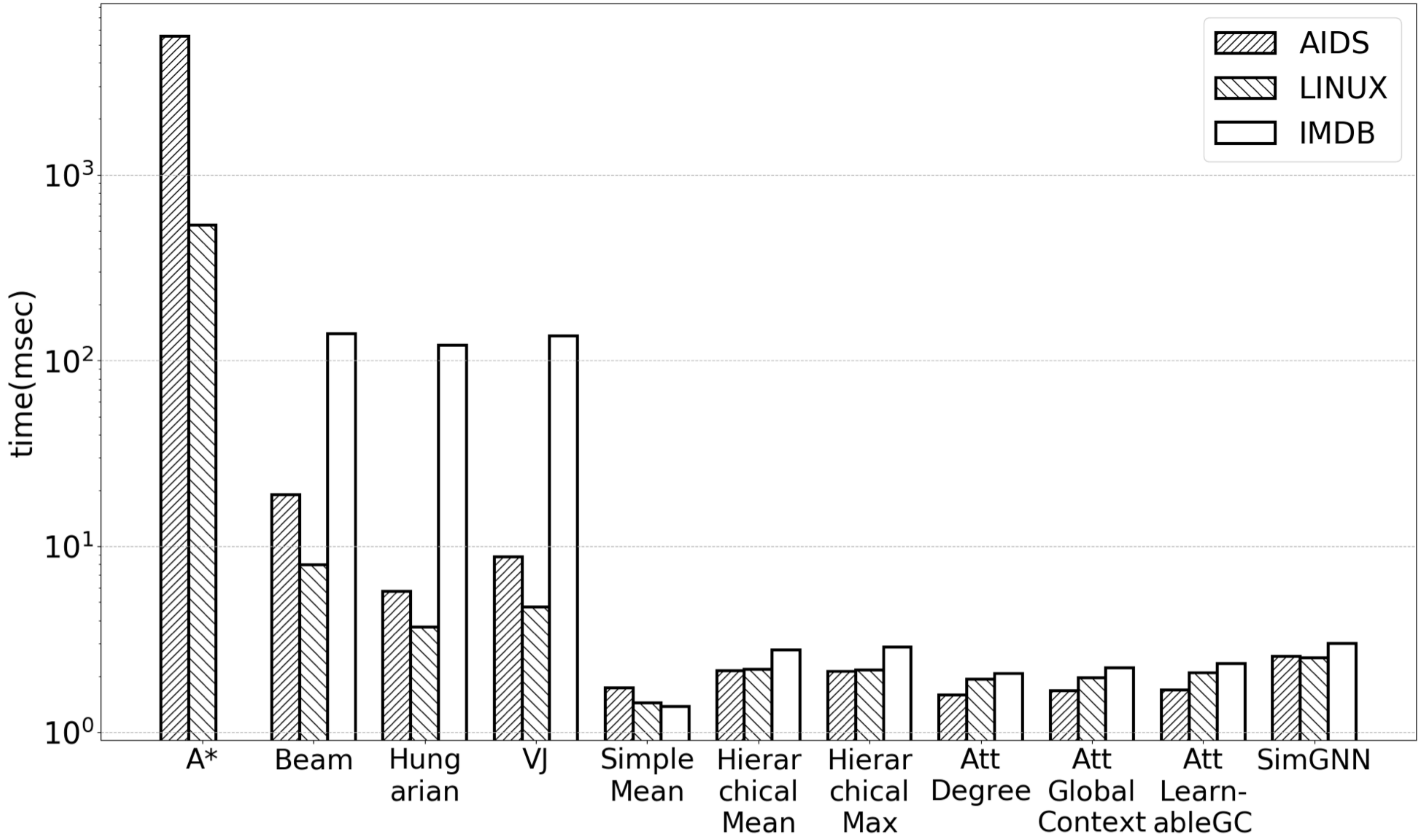
Spearman's Rank Correlation Coefficient (ρ) Kendall's Rank Correlation Coefficient (τ)

Method	mse(10^{-3})	ρ	τ	p@10	p@20
Beam	12.090	0.609	0.463	**0.481**	0.493
Hungarian	25.296	0.510	0.378	0.360	0.392
VJ	29.157	0.517	0.383	0.310	0.345
SimpleMean	3.115	0.633	0.480	0.269	0.279
HierarchicalMean	3.046	0.681	0.629	0.246	0.340
HierarchicalMax	3.396	0.655	0.505	0.222	0.295
AttDegree	3.338	0.628	0.478	0.209	0.279
AttGlobalContext	1.472	0.813	0.653	0.376	0.473
AttLearnableGC	1.340	0.825	0.667	0.400	0.488
SimGNN	**1.189**	**0.843**	**0.690**	**0.421**	**0.514**

More *accurate* than *most* the existing approximate GED algorithms.

Precision at k (**p@k**) is computed by taking the intersection of the predicted top k results and the ground-truth top k results divided by k.

Evaluation: Efficiency

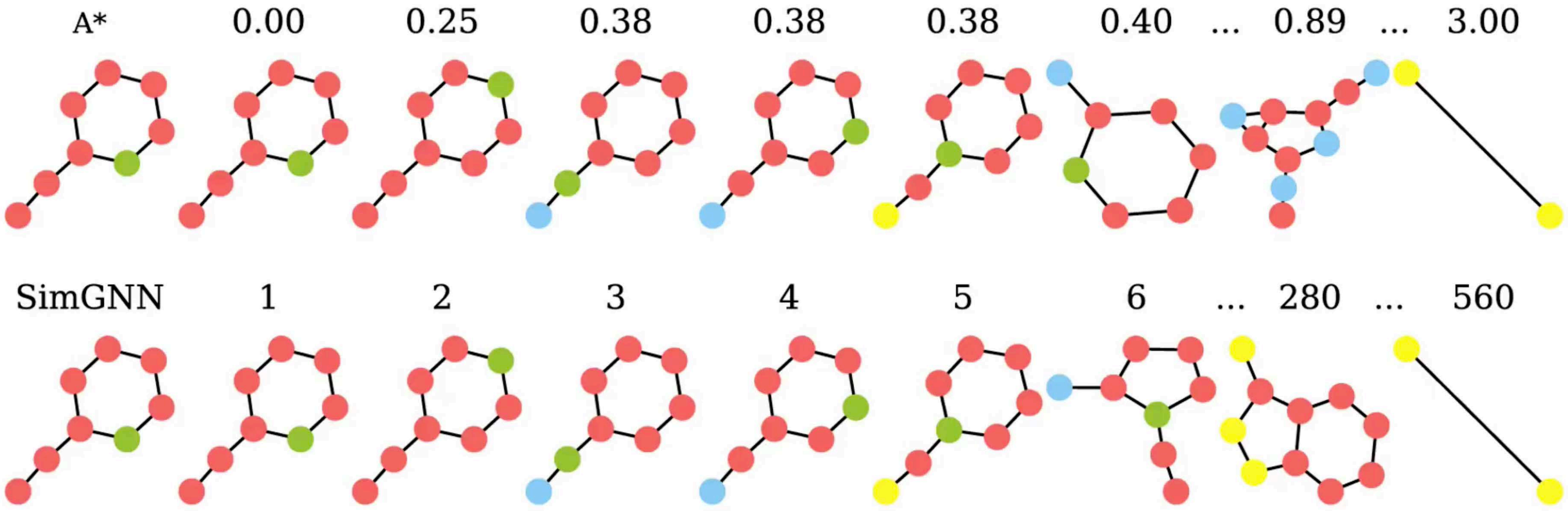


Other NN approaches are *fast* but *less accurate* than SimGNN.

Beam is better, but is *much slower* (log-scale).

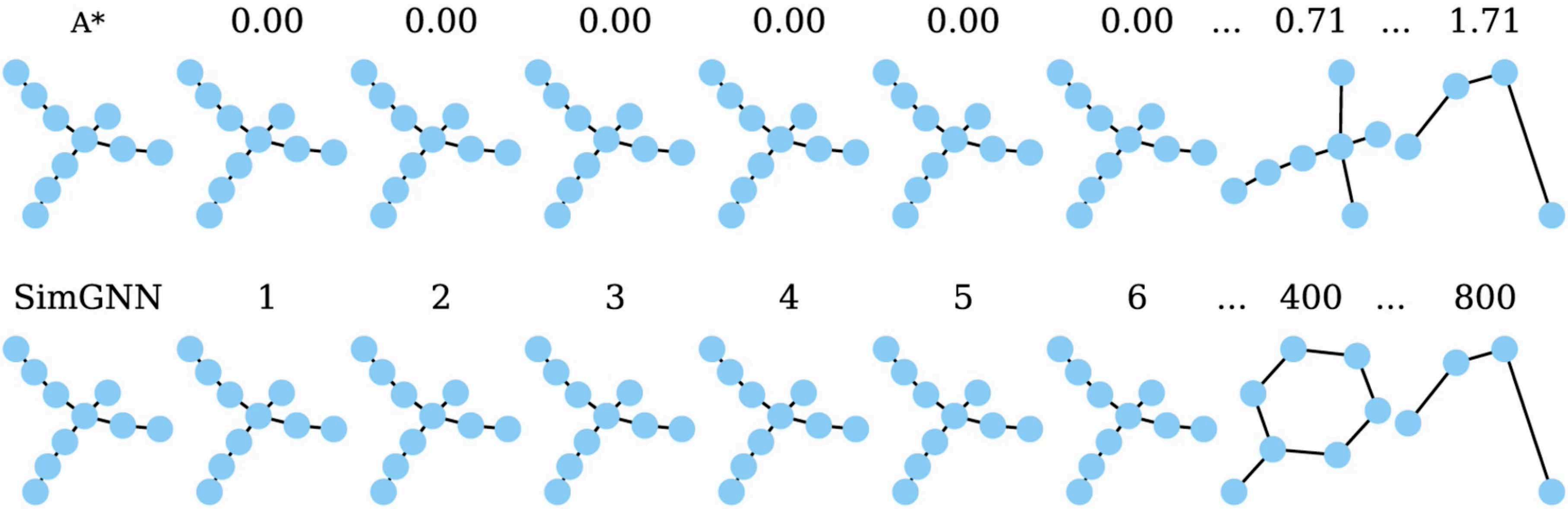
Case Study: AIDS

A*: the *exact* algorithm



Case Study: LINUX

A*: the *exact* algorithm



Key Takeaways

- **SimGNN enjoys the key advantage of *efficiency* due to the nature of neural network computation.**
- **Representation-invariant.** The same graph can be represented by different adjacency matrices by *permuting* the order of nodes. The computed similarity score *should be invariant* to such changes.
- **Inductive.** The similarity computation should *generalize to unseen graphs*, i.e. compute the similarity score for graphs outside the training graph pairs.
- **Learnable.** The model should be adaptive to any similarity metric, by *adjusting its parameters through training*.

Summary

- **The intersection of *graph deep learning* and *graph search* problem**
- **Tackling the core operation of *graph similarity* computation via a novel neural network based approach**
- **Key idea is to learn a *neural network based function* that is *representation-invariant, inductive*, and *adaptive* to the specific similarity metric**
- **SimGNN runs very *fast* compared to existing classic algorithms on approximate Graph Edit Distance computation, and achieves very competitive *accuracy*.**

Thank you