SimGNN: A Neural Network Approach to Fast Graph Similarity Computation

WSDM 2019

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- The Proposed Approach
- Experiment

Background

Overview of image search / classification

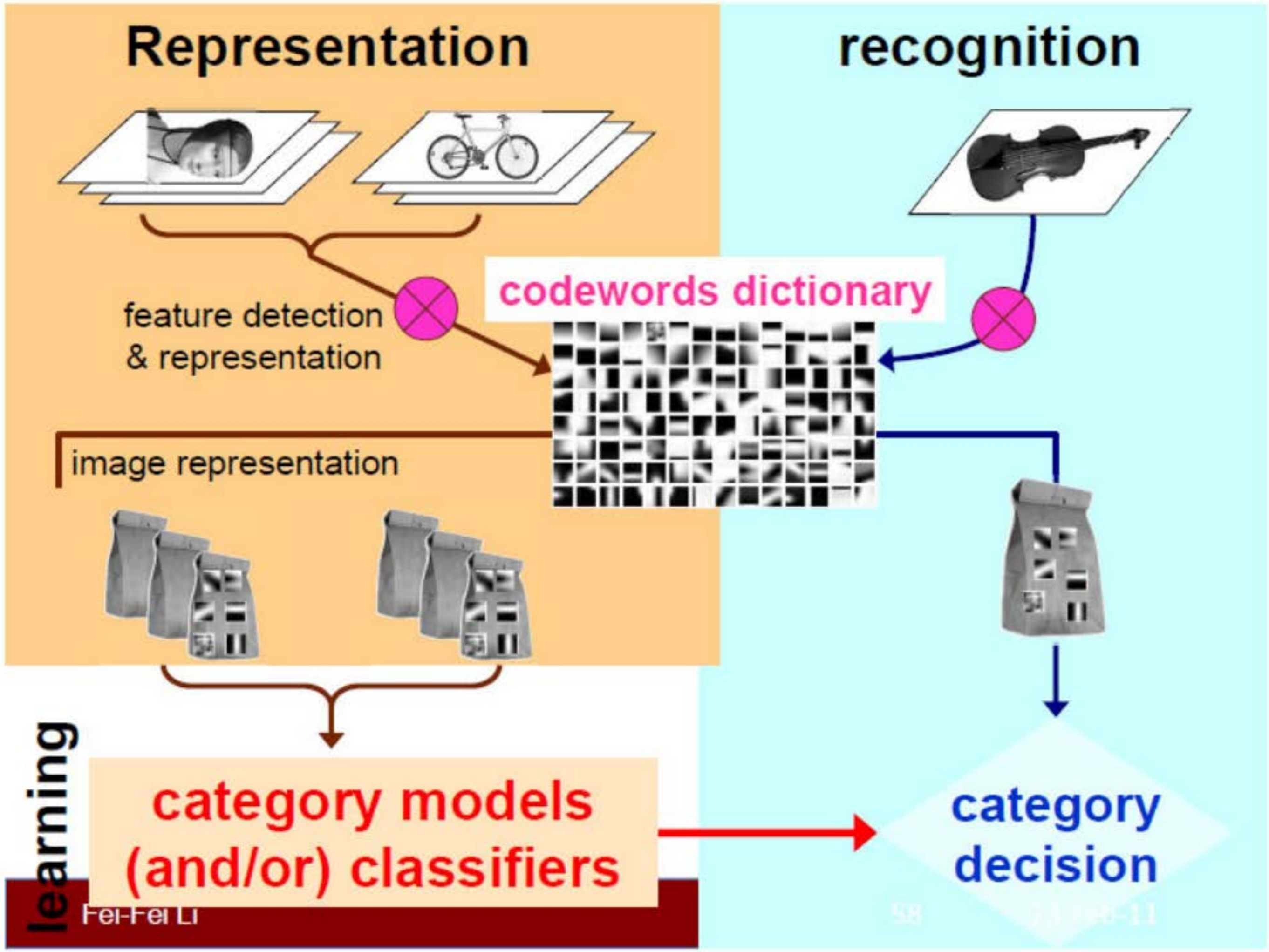
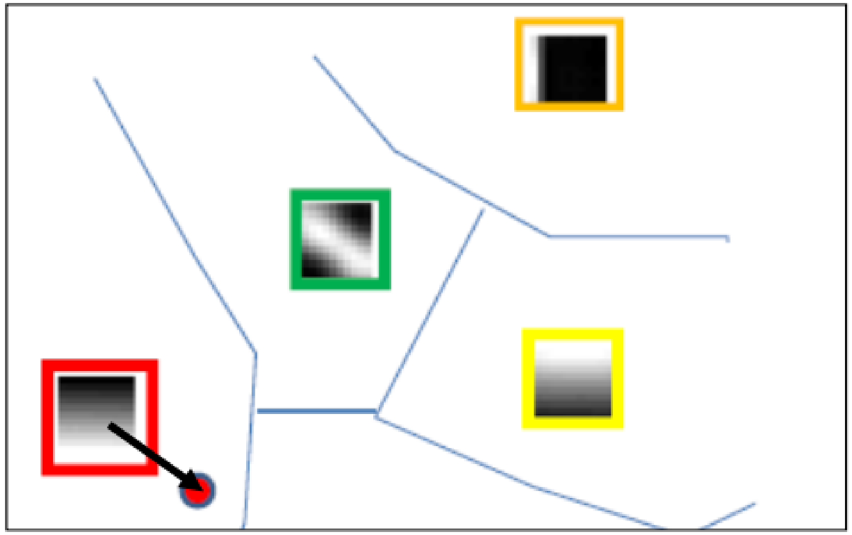


Image representation / Comparison

- **BoW**
  - **Count the number of SIFTs assigned to each cluster**
- **VLAD**
  - **Compute the difference between a feature and its cluster center**

$$v_{i,j} = \sum_{x \text{ such that } \mathrm{NN}(x)=c_i} x_j - c_{i,j}$$

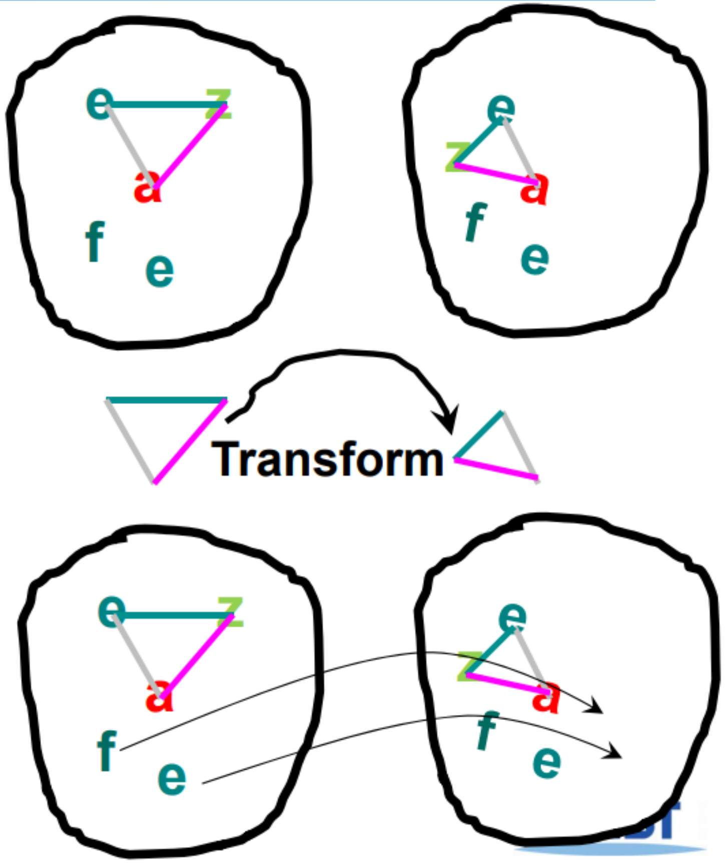


Consider the spatial relationship

Geometric Verification using RANSAC

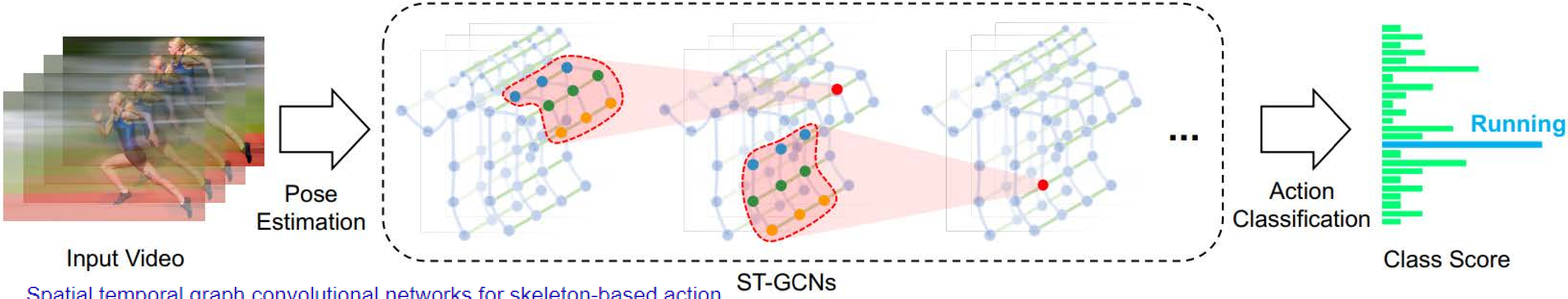
Repeat N times:

- Randomly choose 4 matching pairs
- Estimate transformation
  - Assume a particular transformation (Homography)
- Predict remaining points and count "inliers"



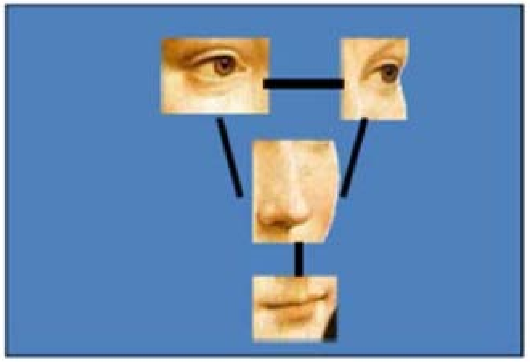
Ack.: Derek Hoiem (UIUC)

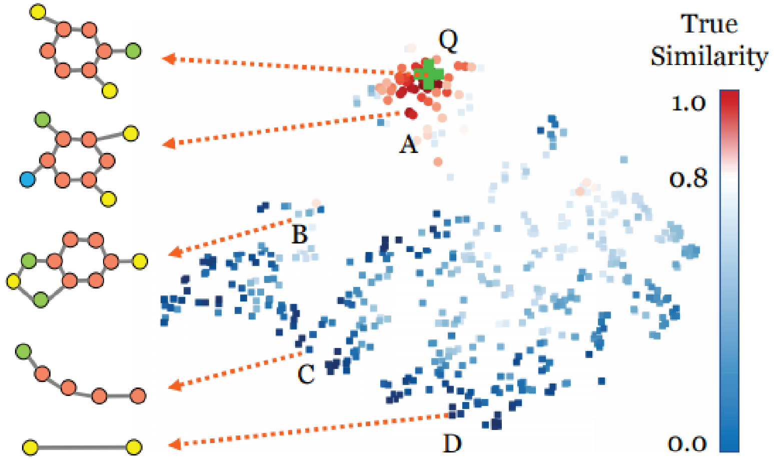
Image as Graph



Spatial temporal graph convolutional networks for skeleton-based action recognition

Graph Similarity



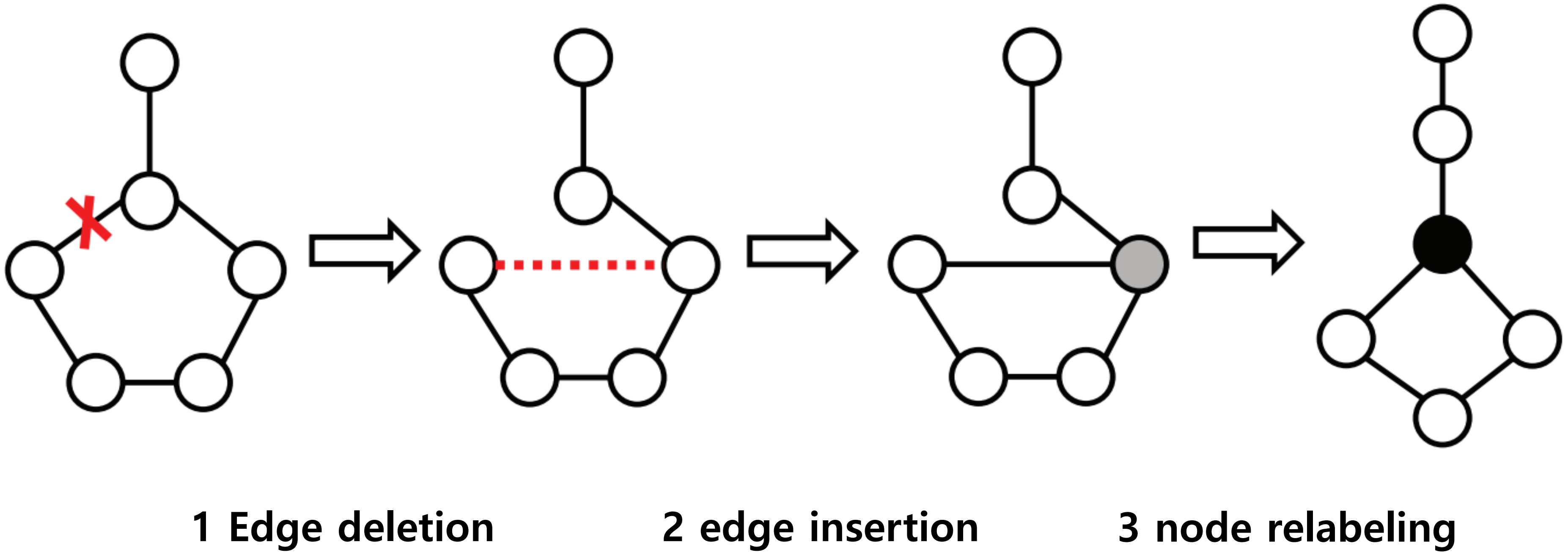


The proposed Approach

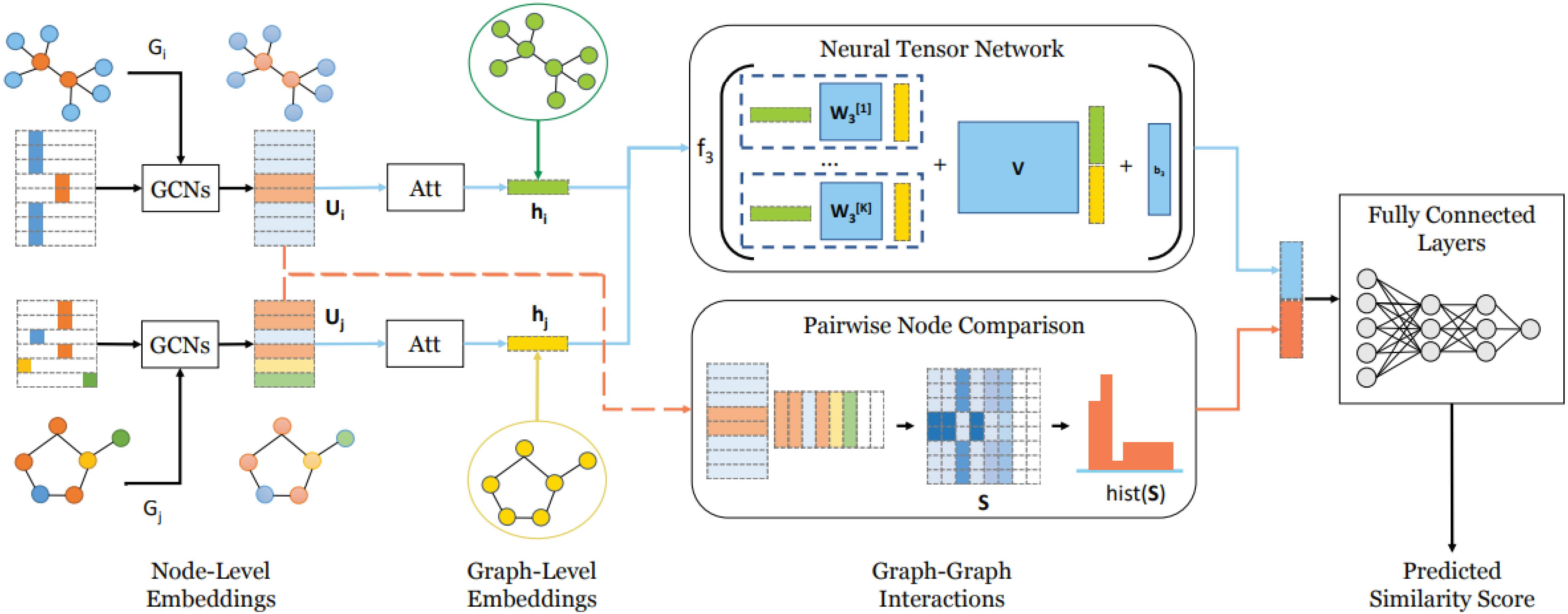
A similarity metric: Graph Edit Distance (GED)

GED (G1, G2) is the number of edit operations in the <u>optimal alignments</u> that transform G1 to G2.

3 kinds of edit operations in total

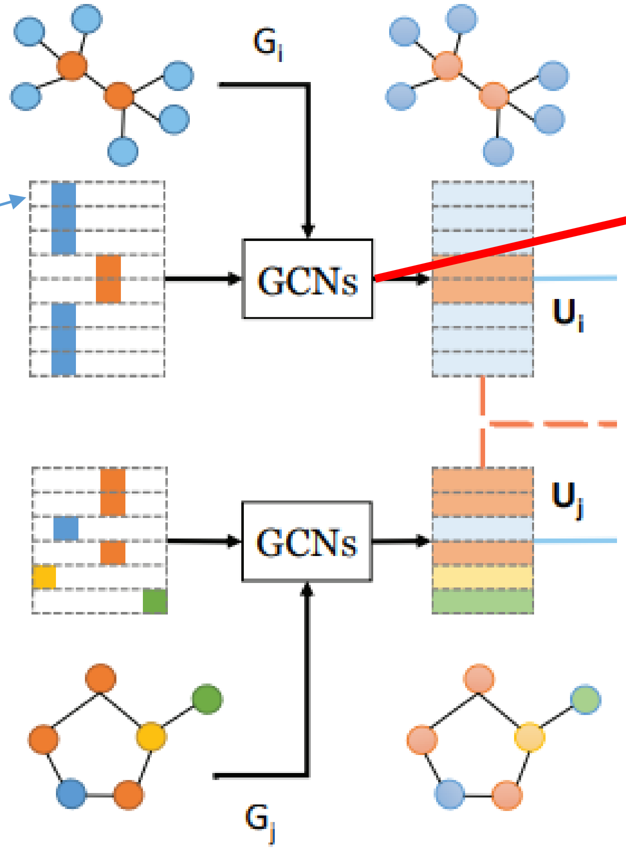


Overview of the framework



Node-level embeddings

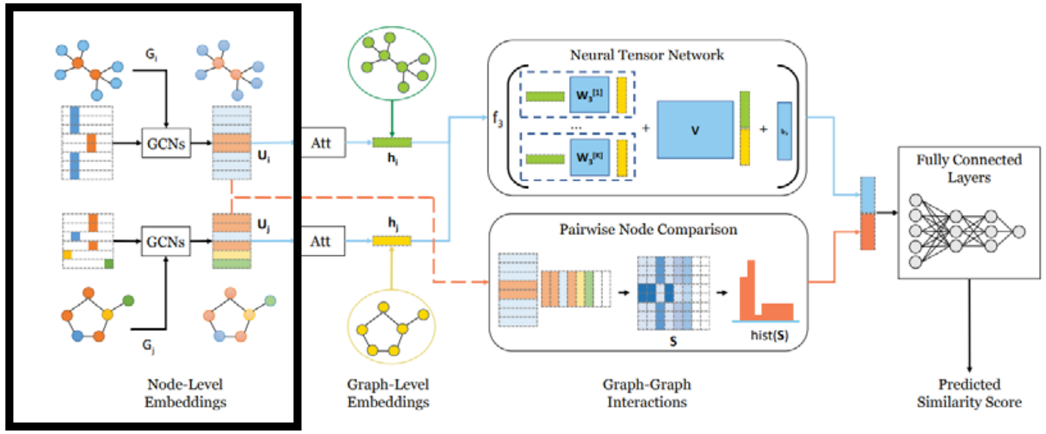
One-hot
embedding



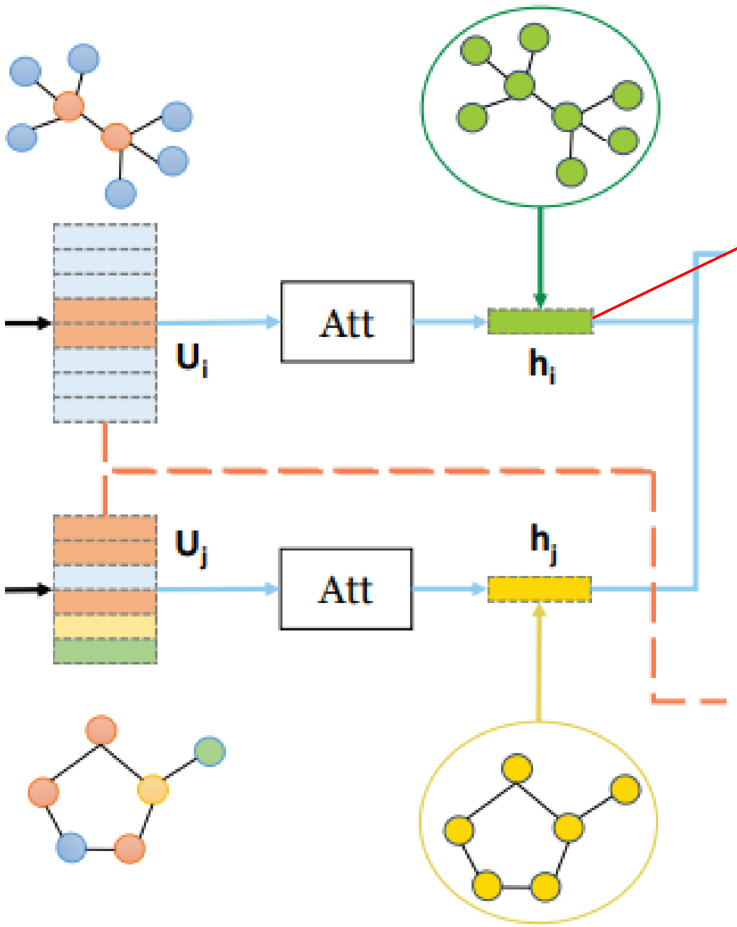
Node-Level
Embeddings

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v) \cup v} \frac{\mathbf{h}_u^{k-1}}{\sqrt{|N(u)||N(v)|}}\right)$$

instead of simple average,
normalization varies acros
s neighbors



Graph-level embeddings

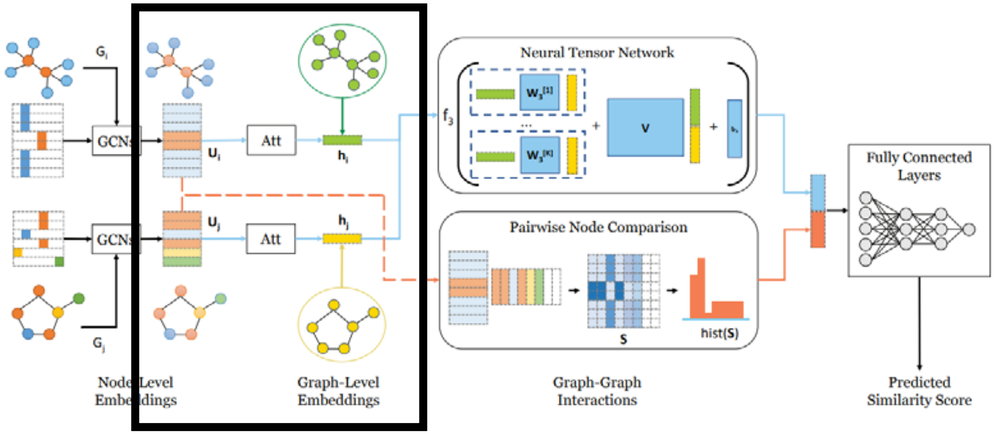


The weight of each node

$$\boxed{\boldsymbol{h}} = \sum_{n=1}^{N} \boxed{f_2(\boldsymbol{u}_n^T \boldsymbol{c})} \boldsymbol{u}_n$$

The context c

$$= \sum_{n=1}^{N} f_2(\boldsymbol{u}_n^T \boxed{\tanh((\frac{1}{N} \sum_{m=1}^{N} \boldsymbol{u}_m) \boldsymbol{W}_2)}) \boldsymbol{u}_n$$



Neural Tensor Network

Similarity $\begin{cases} \textit{Dot product} \\ \\ \textit{MLP} \end{cases}$

Use k dot products to represent the similarity

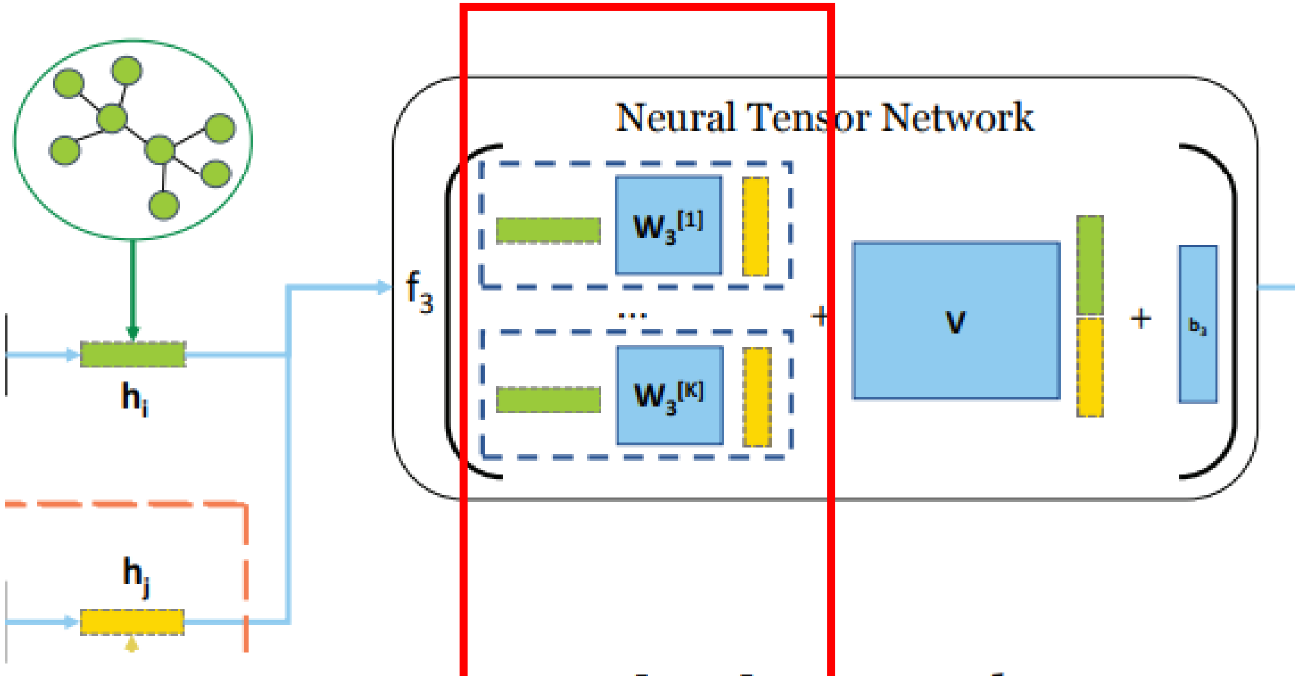
For each dot product:

$$h_i^T W^1 h_j$$

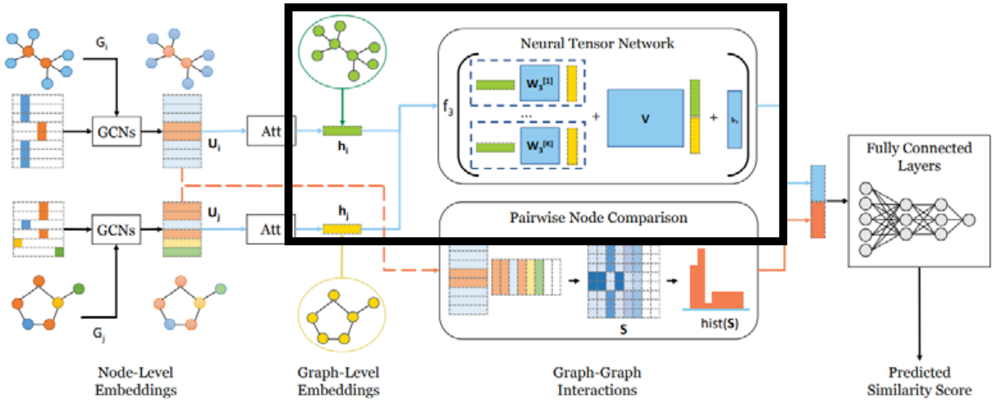
[1*D], [D*D], [D*1] → [1*1]

Could we Improve it?

$$h_i^T W_1^1 W_2^1 W_3^1 h_j$$



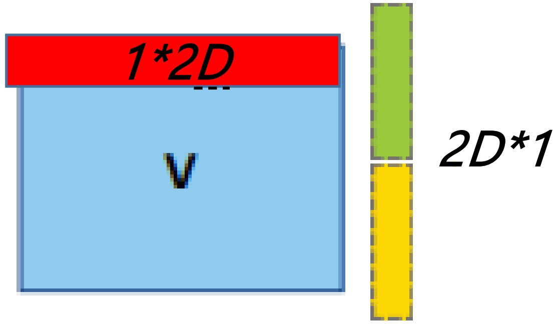
$$g(h_i, h_j) = f_3\left(h_i^T W_3^{[1:K]} h_j + V \begin{bmatrix} h_i \\ h_j \end{bmatrix} + b_3\right)$$



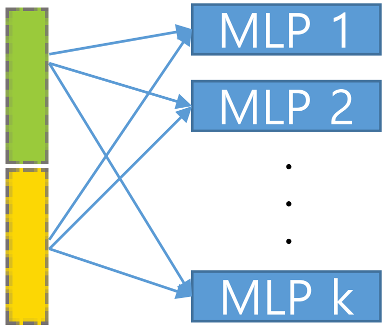
Neural Tensor Network

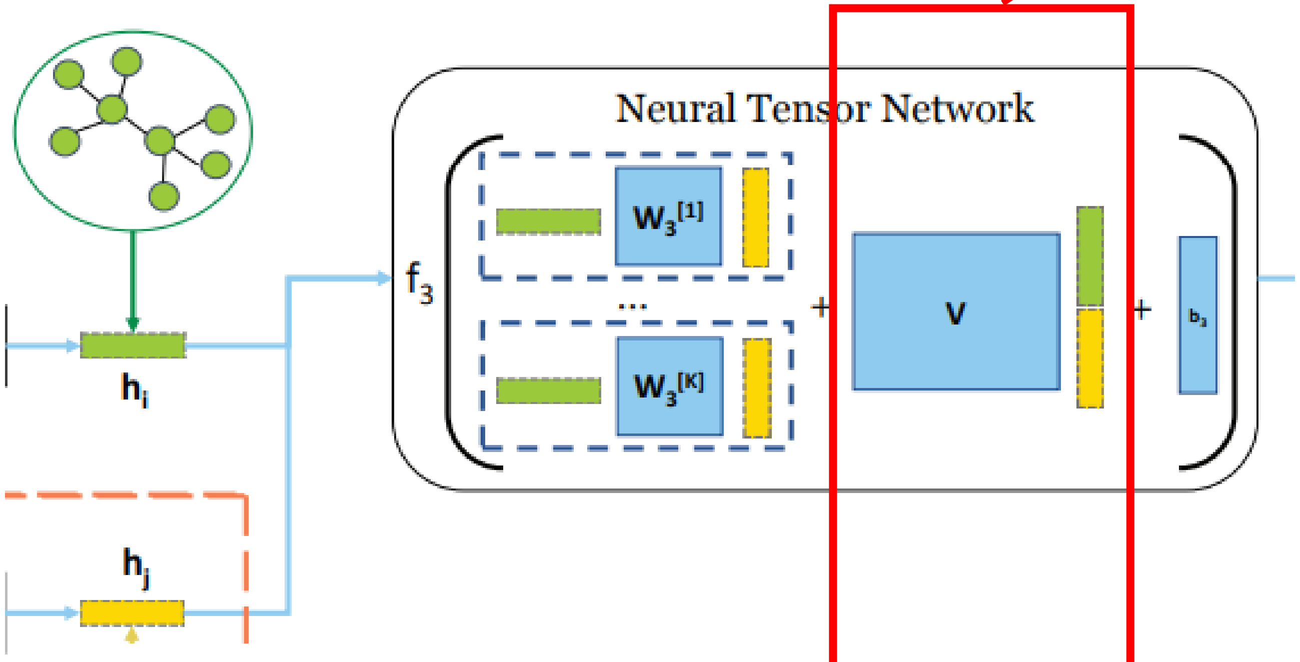
Similarity
- *Dot product*
- *MLP*

$$V \in \mathbb{R}^{K \times 2D}$$

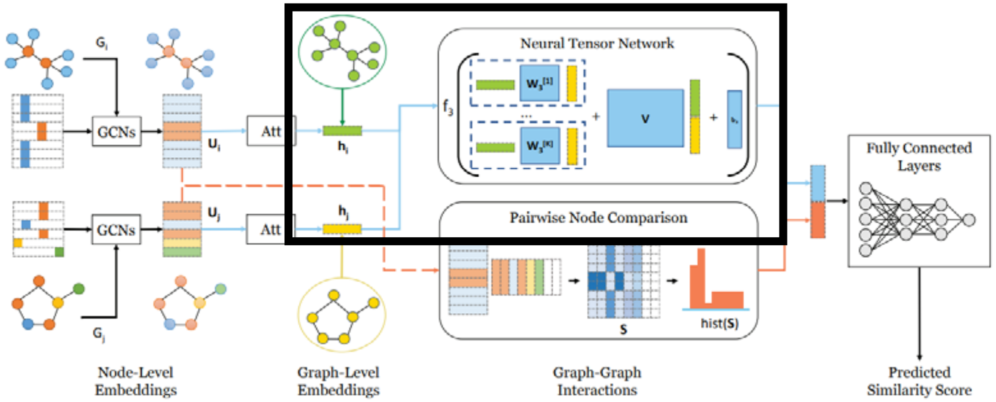


Could we Improve it?

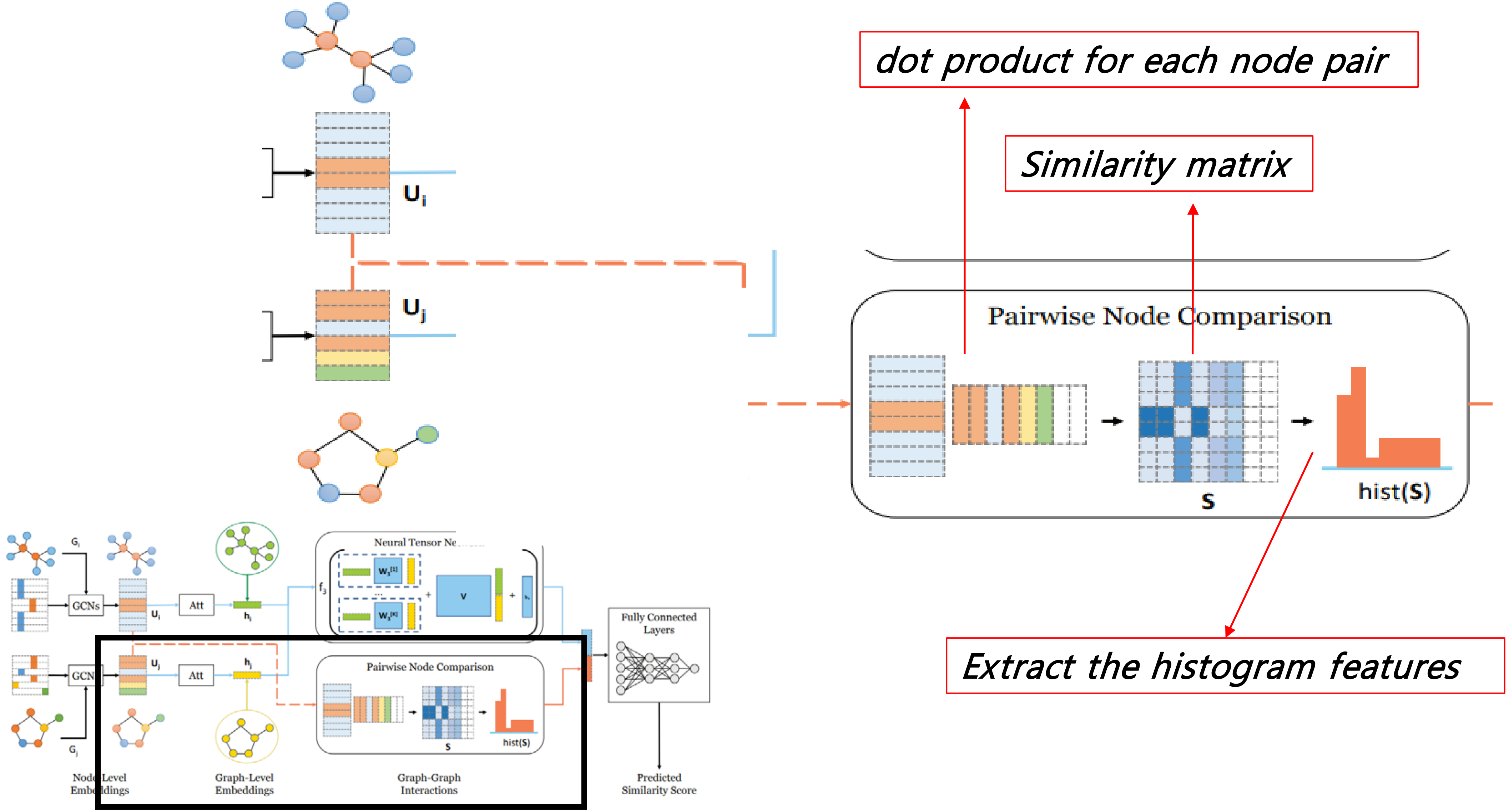




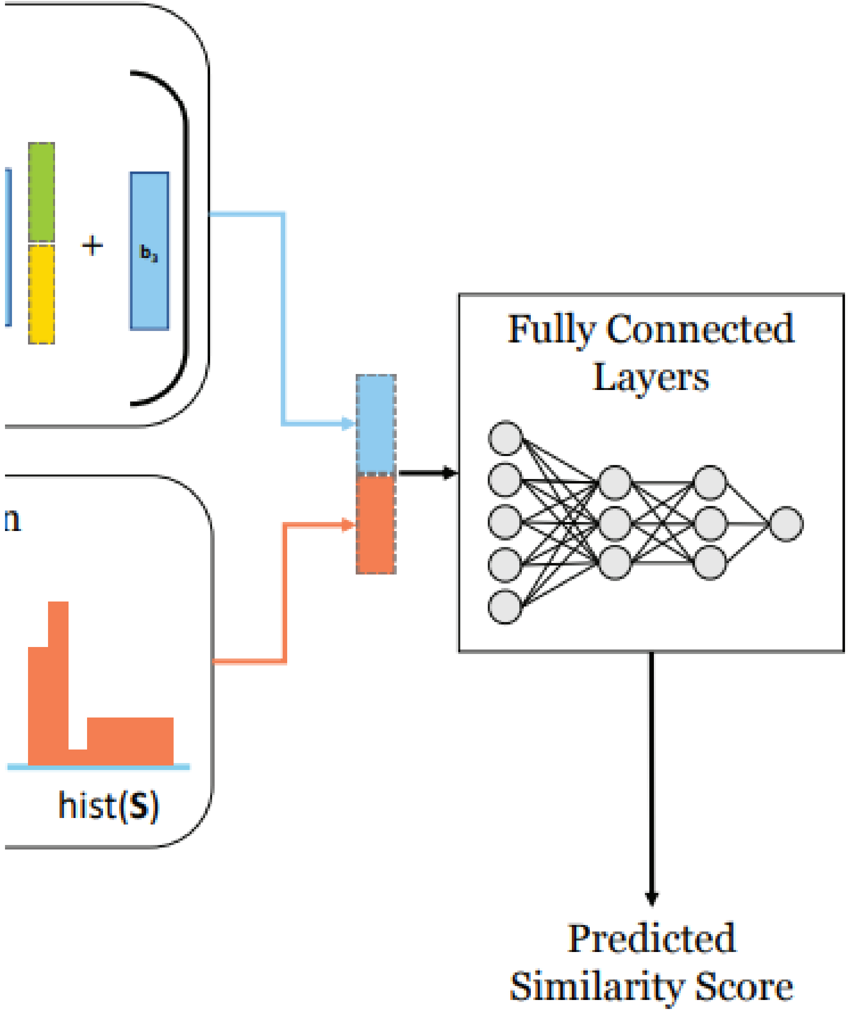
$$g(\boldsymbol{h_i}, \boldsymbol{h_j}) = f_3(\boldsymbol{h}_i^T \boldsymbol{W}_3^{[1:K]} \boldsymbol{h_j} + \boldsymbol{V} \begin{bmatrix} \boldsymbol{h_i} \\ \boldsymbol{h_j} \end{bmatrix} + \boldsymbol{b}_3)$$



Pairwise Node Comparison

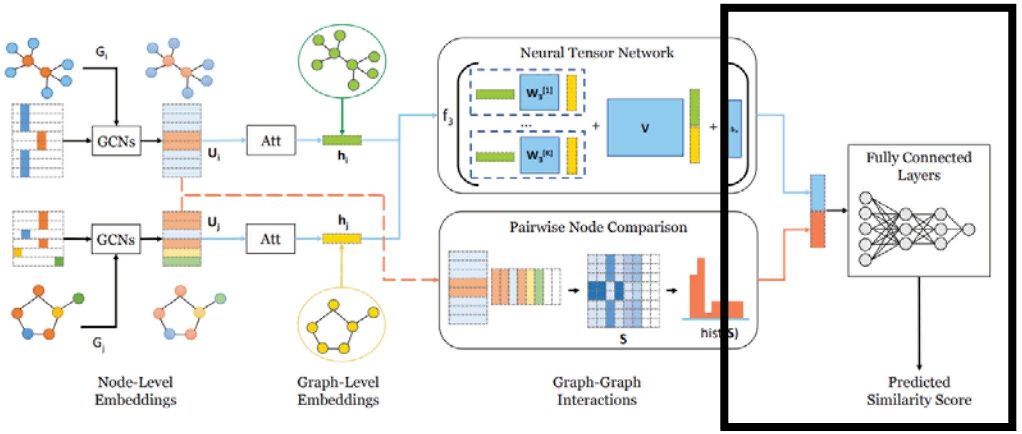


Predicted Similarity Score



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

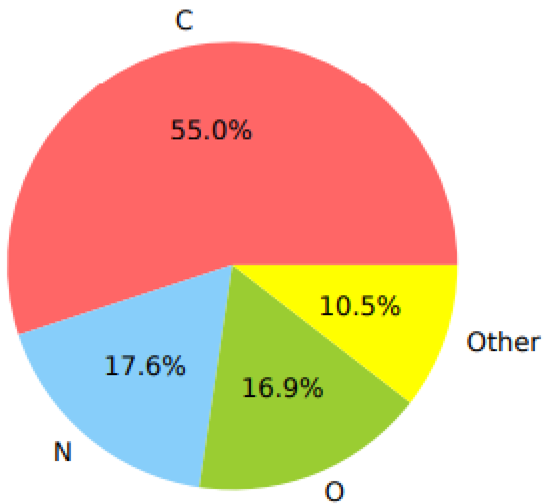
GED (G1, G2)



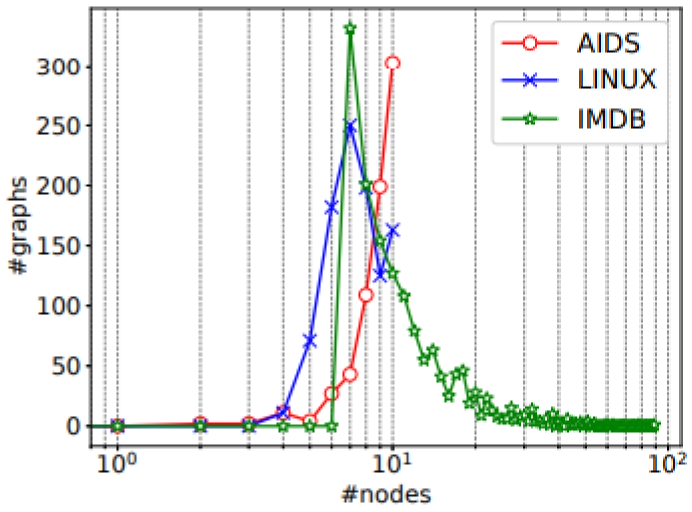
Experiment

Datasets

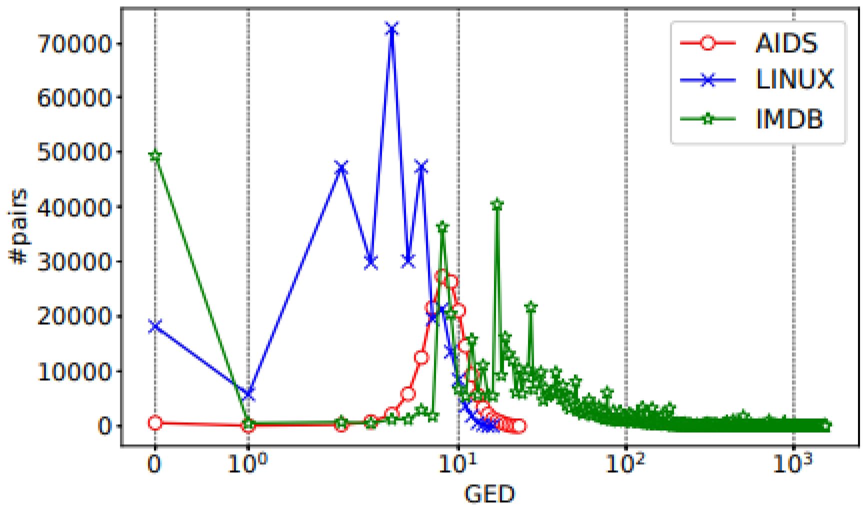
- AIDS
  - Chemical compound structures
- LINUX
  - Program Dependence Graphs (PDG)
- IMDB
  - Networks of movie actors/actresses



(a) Node label distribution of AIDS.



(b) Distribution of graph sizes.



(c) Distribution of GEDs of the training pairs.

Speed and Accuracy

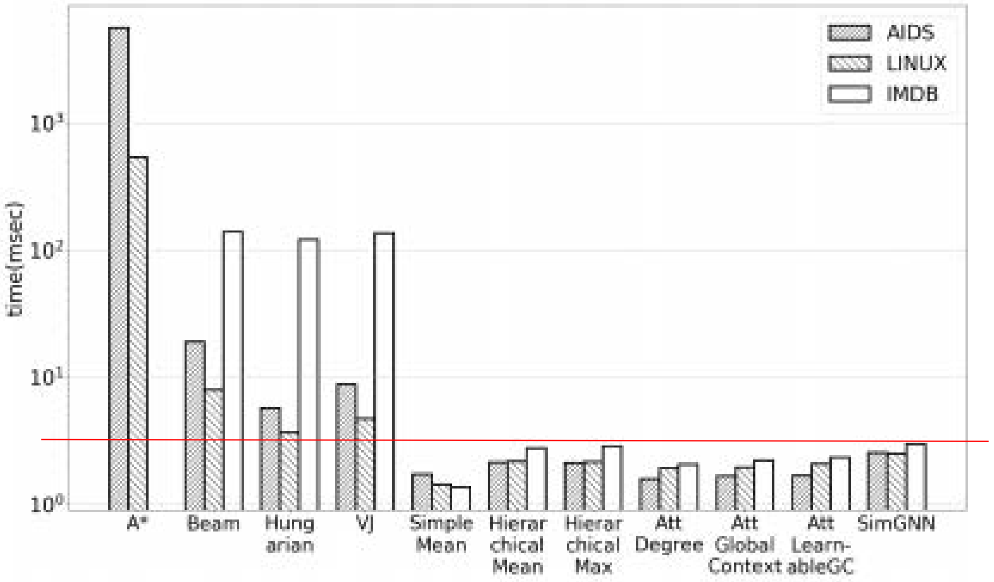


Figure 6: Runtime comparison.

Table 2: Results on AIDS.

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**

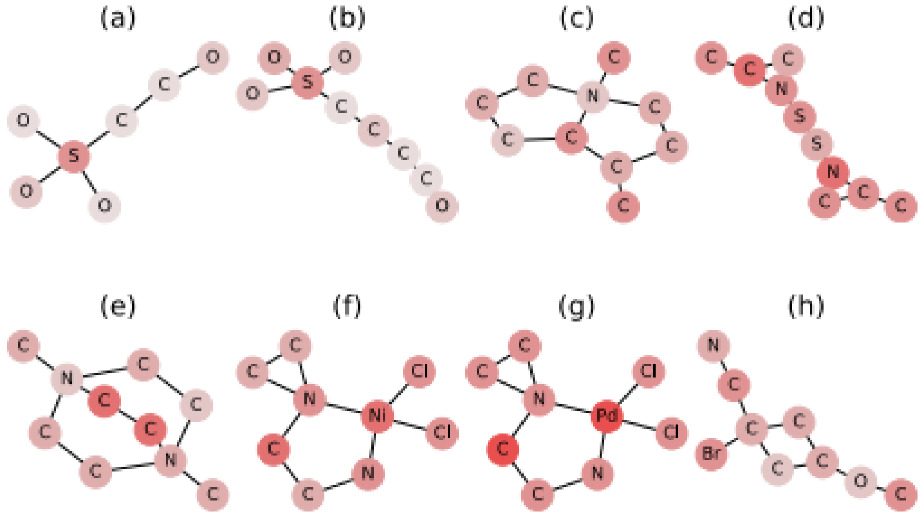
Table 3: Results on LINUX.

Method	mse(10^{-3})	ρ	τ	p@10	p@20
Beam	9.268	0.827	0.714	**0.973**	0.924
Hungarian	29.805	0.638	0.517	0.913	0.836
VJ	63.863	0.581	0.450	0.287	0.251
SimpleMean	16.950	0.020	0.016	0.432	0.465
HierarchicalMean	6.431	0.430	0.525	0.750	0.618
HierarchicalMax	6.575	0.879	0.740	0.551	0.575
AttDegree	8.064	0.742	0.609	0.427	0.460
AttGlobalContext	3.125	0.904	0.781	0.874	0.864
AttLearnableGC	2.055	0.916	0.804	0.903	0.887
SimGNN	**1.509**	**0.939**	**0.830**	0.942	**0.933**

Table 4: Results on IMDB. Beam, Hungarian, and VJ together are used to determine the ground-truth results.

Method	mse(10^{-3})	ρ	τ	p@10	p@20
SimpleMean	3.749	0.774	0.644	0.547	0.588
HierarchicalMean	5.019	0.456	0.378	0.567	0.553
HierarchicalMax	6.993	0.455	0.354	0.572	0.570
AttDegree	2.144	0.828	0.695	0.700	0.695
AttGlobalContext	3.555	0.684	0.553	0.657	0.656
AttLearnableGC	1.455	0.835	0.700	0.732	0.742
SimGNN	**1.264**	**0.878**	**0.770**	**0.759**	**0.777**

Case study



- Attention

Ground truth

Search result

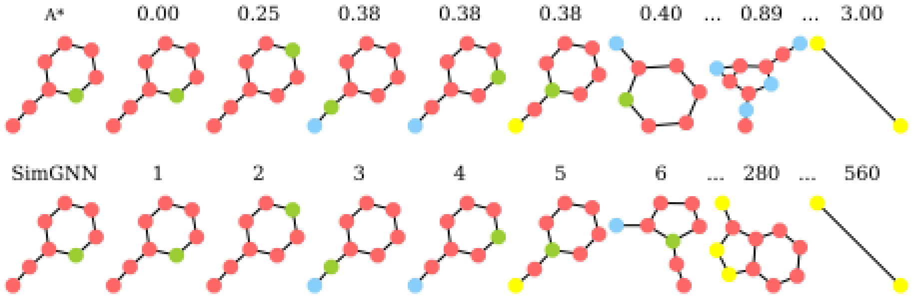


Figure 8: A query case study on AIDS. Meanings of the colors can be found in Fig. 4a.

Ground truth

Search result

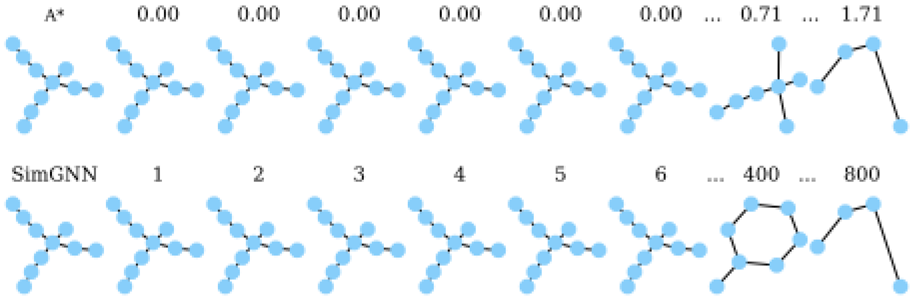


Figure 9: A query case study on LINUX.

Ground truth

Search result

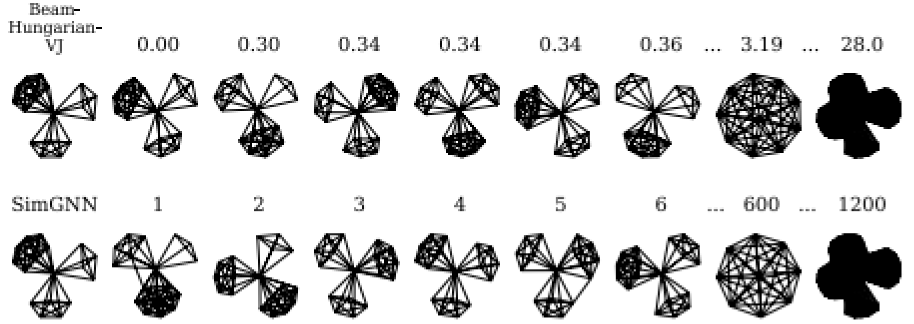


Figure 10: A query case study on IMDB.