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# PaGE-Link: Path-based Graph Neural Network Explanation for Heterogeneous Link Prediction

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Soji Adeshina<sup>2</sup>, Da Zheng<sup>2</sup>, Christos  
Faloutsos<sup>2,3</sup>, Yizhou Sun<sup>1,2</sup>

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<sup>2</sup>Amazon <sup>3</sup>Carnegie Mellon University

April 2023

# Outline

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- Problem and Motivation
- Existing Work
- Main Idea
- Experiments

# Problem: Model Explainability

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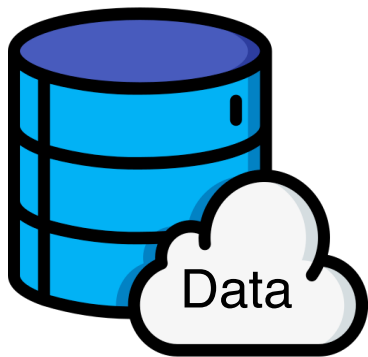
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- Many start-of-the-art AI models are black boxes.

# Problem: Model Explainability

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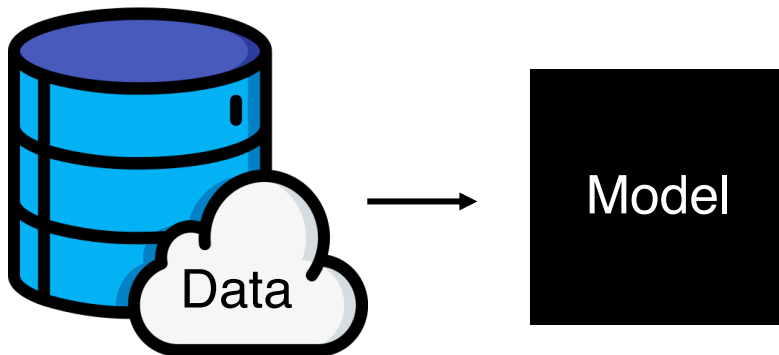
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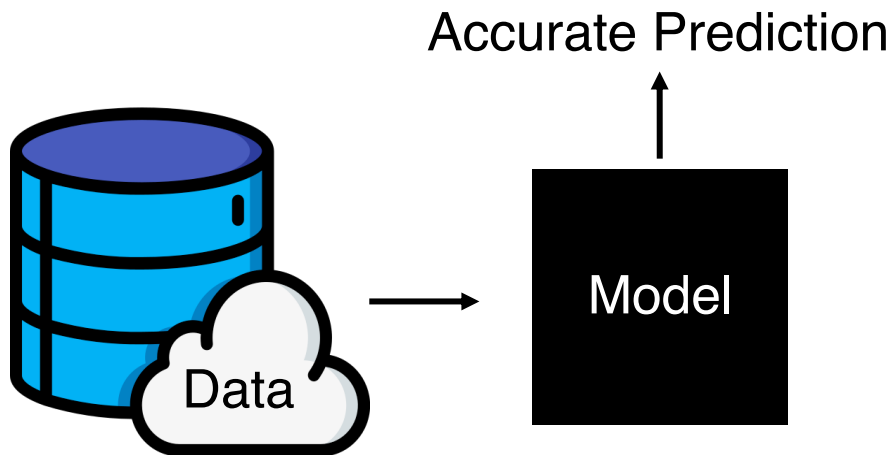
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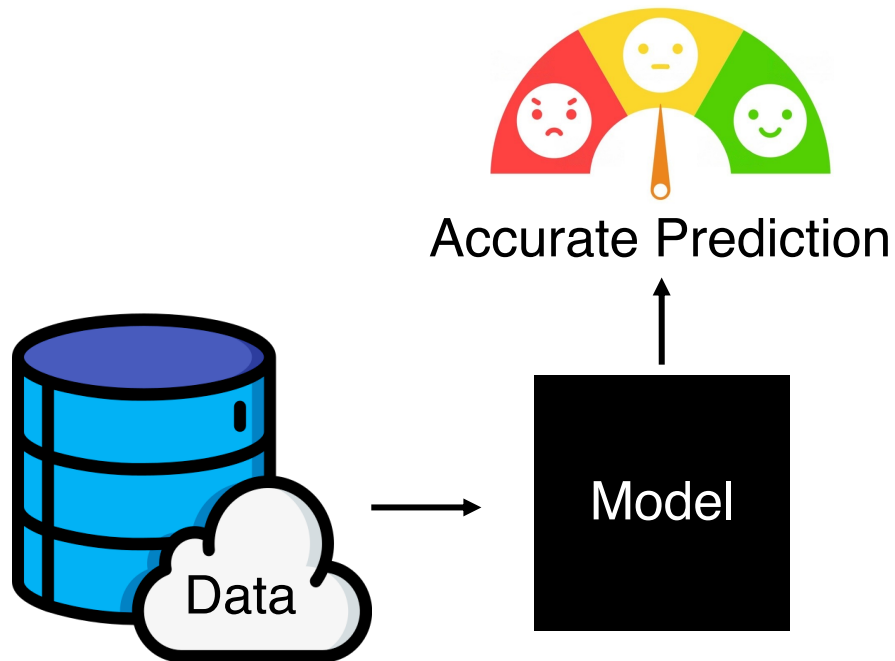
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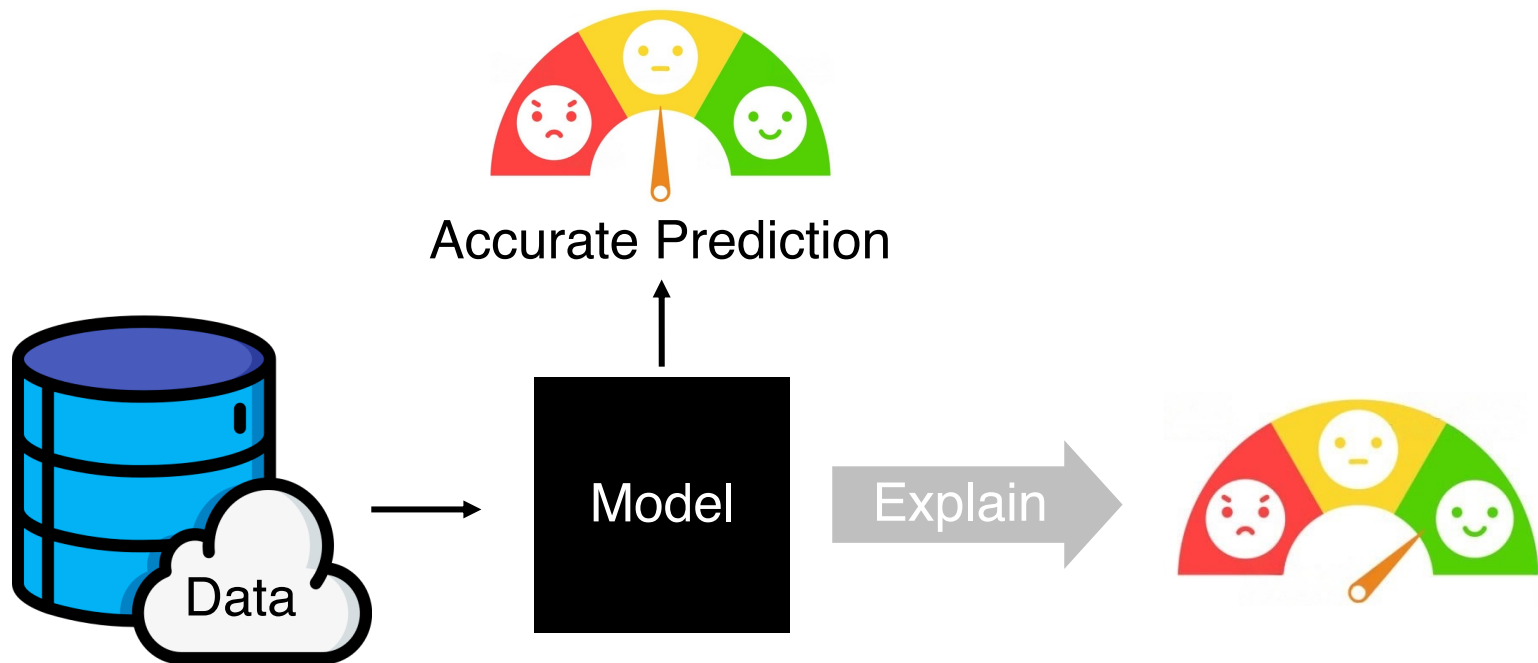
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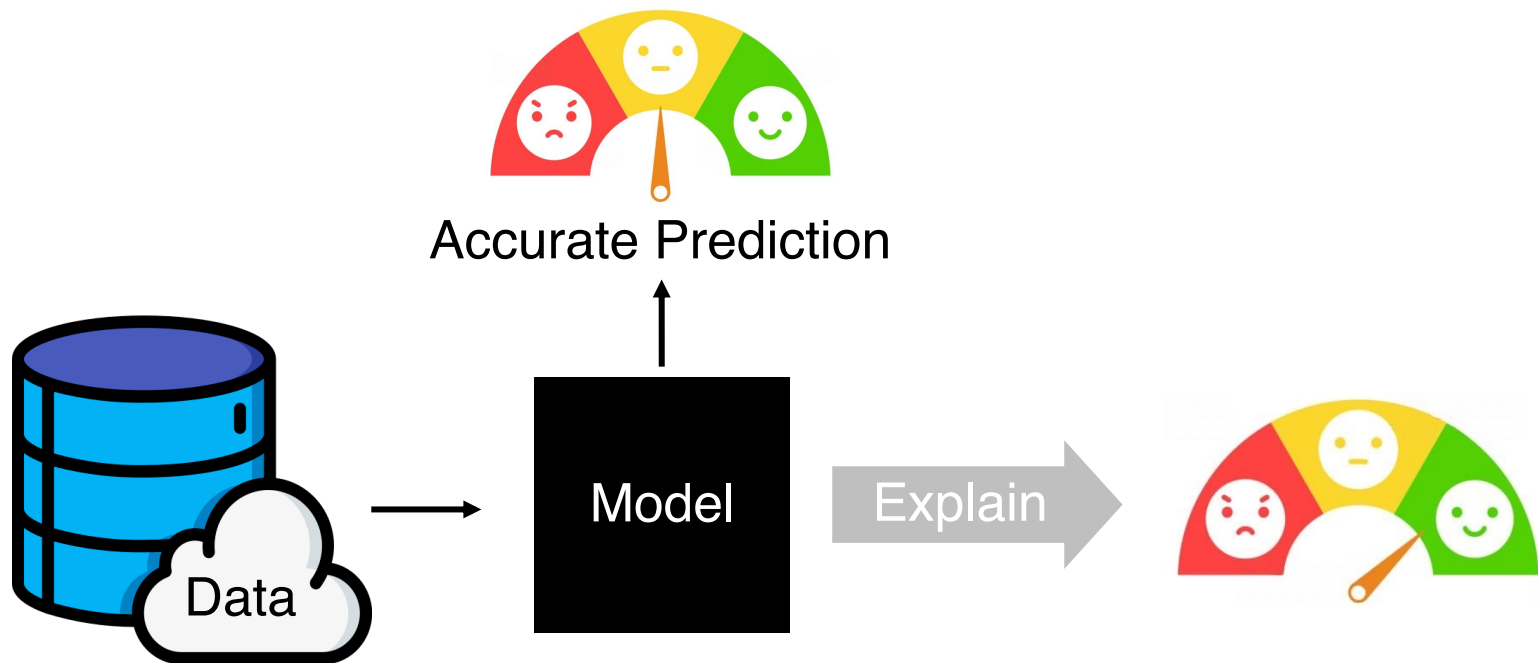
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- Many start-of-the-art AI models are black boxes.
- Explainability helps to increase user satisfaction and improve model design.



# Model Explainability on The Web

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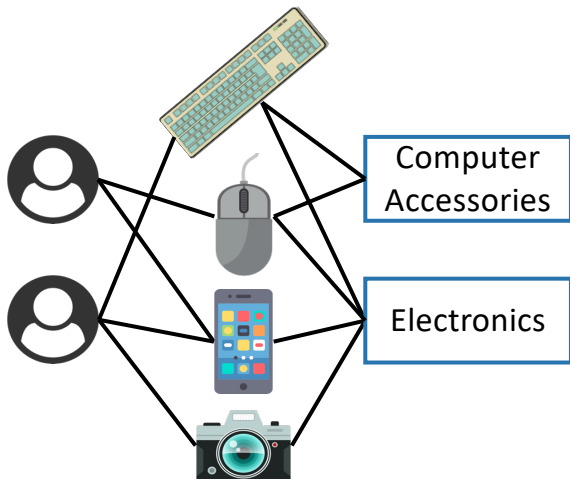
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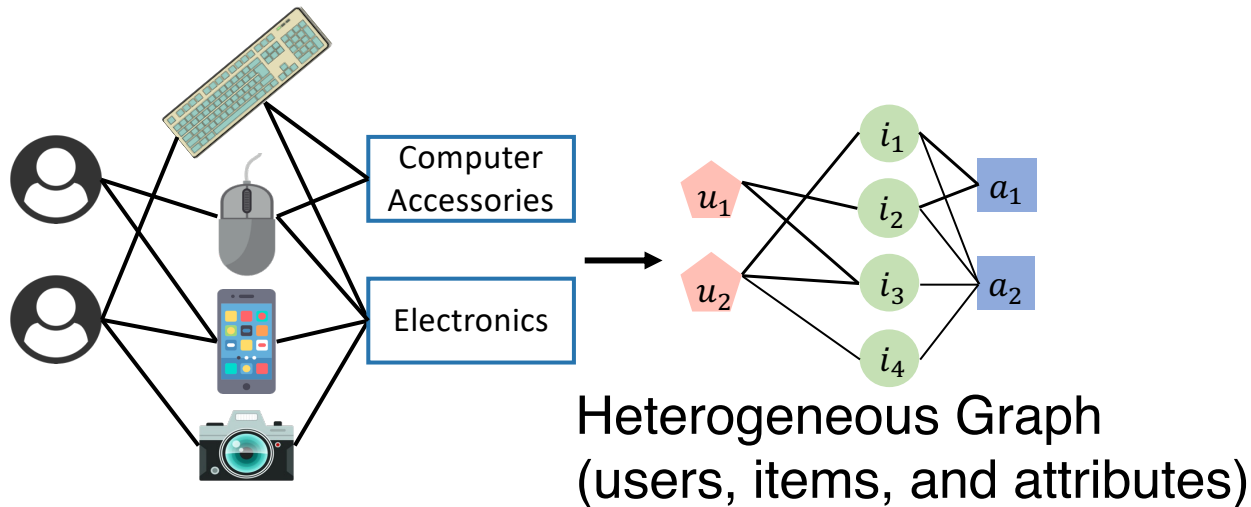
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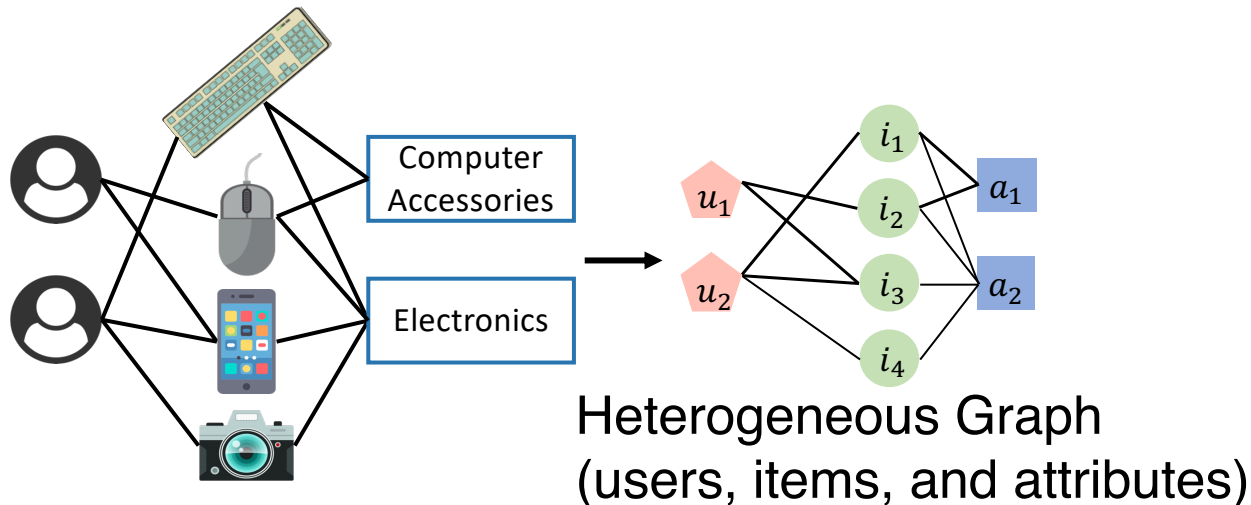
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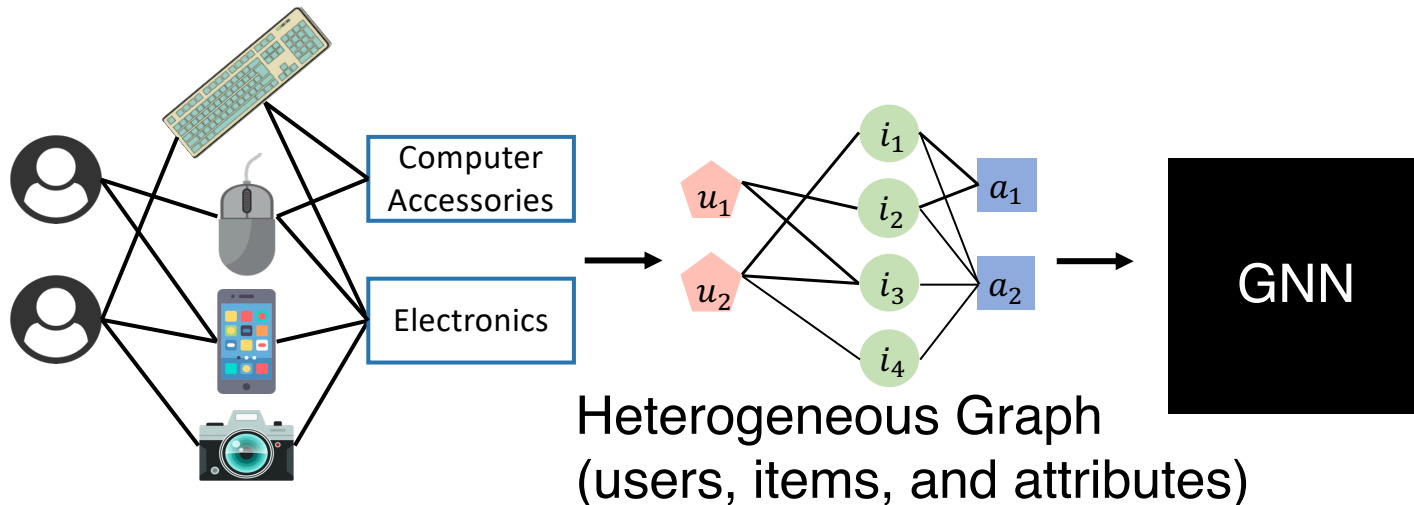
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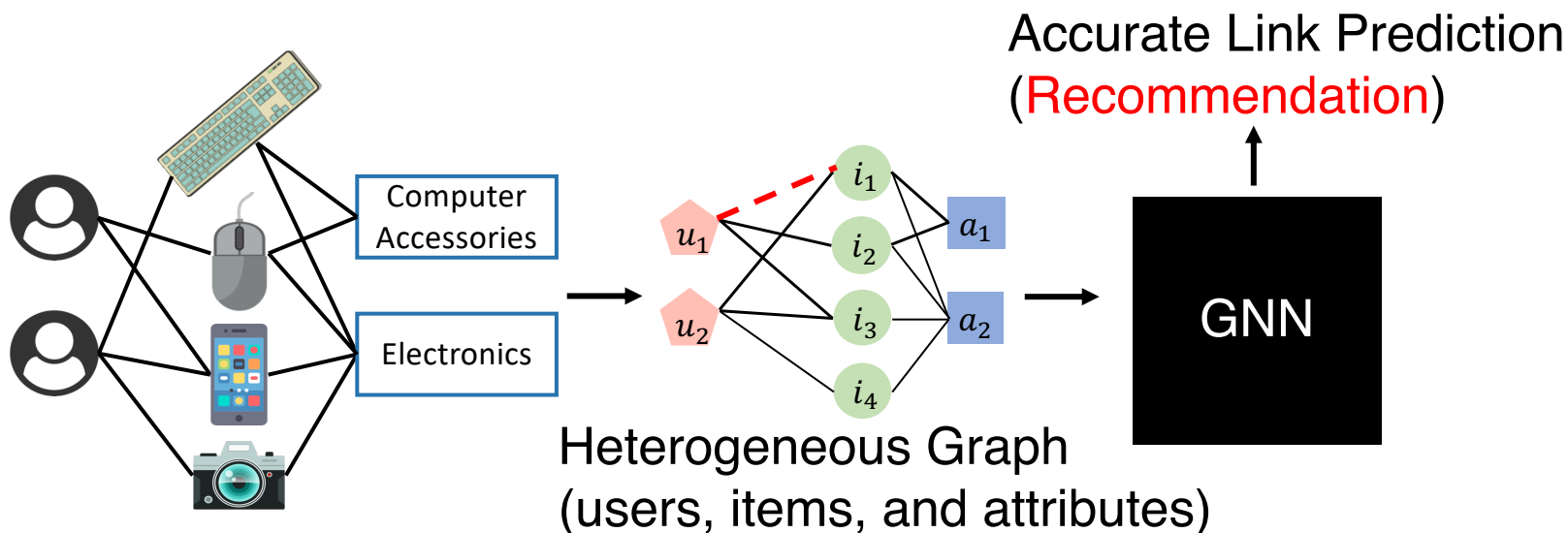
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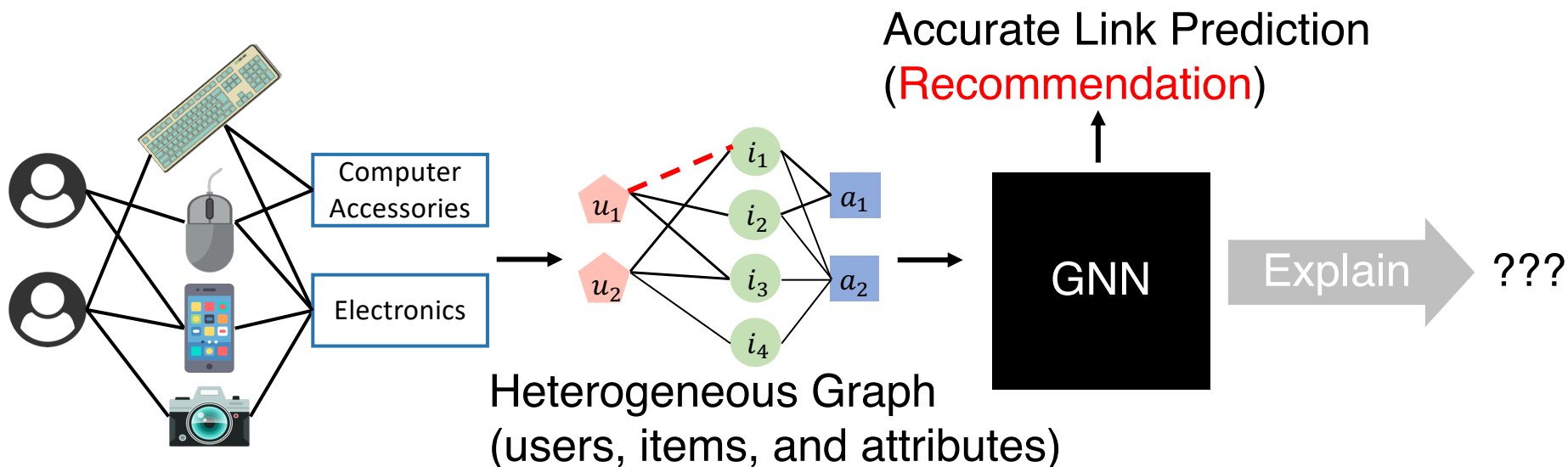
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# Model Explainability on The Web

- Data: often as heterogeneous graphs.
- Model: Graph Neural Networks (GNNs) work well for heterogeneous link prediction.
- Explanation: Why recommend an item to a user? (Why predict a user-item link?)



# Existing Work: GNN Explanation

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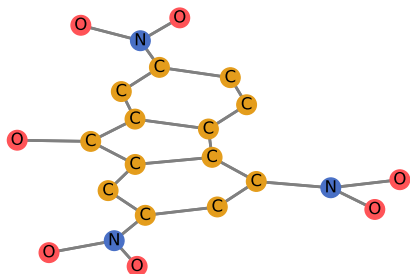
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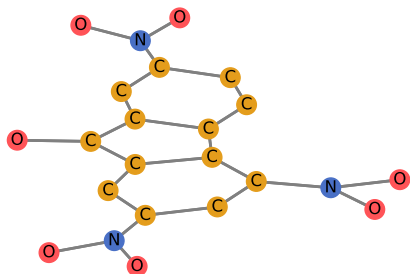
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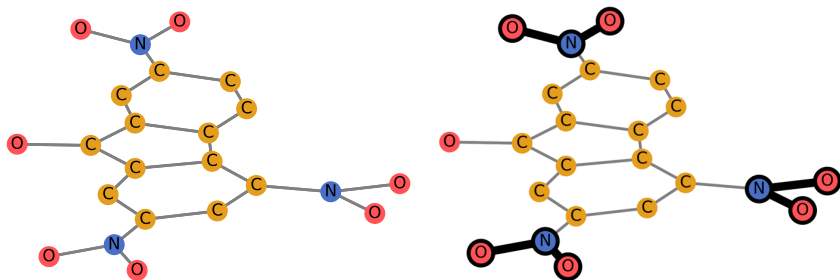
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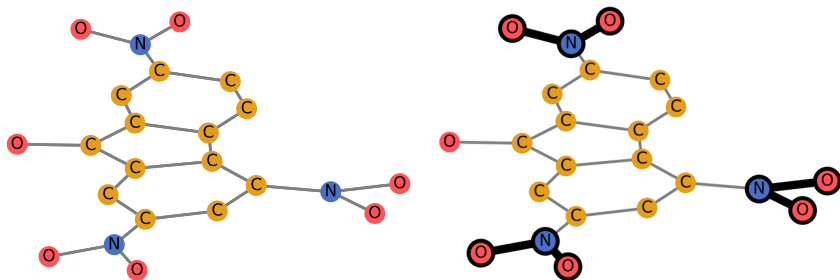
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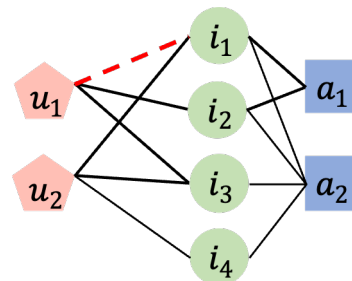
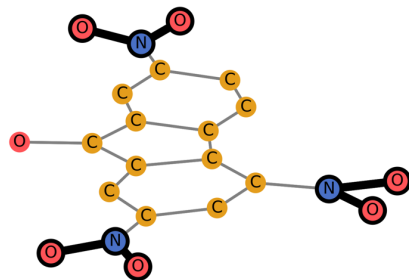
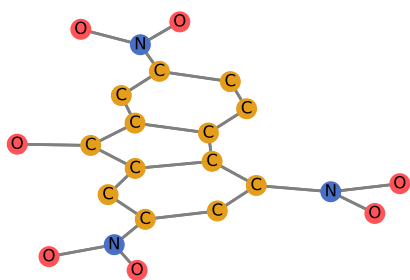


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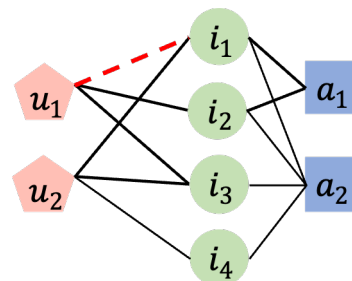
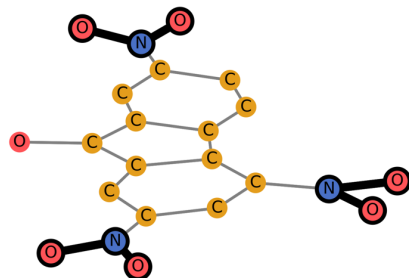
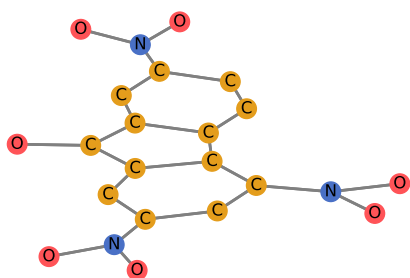
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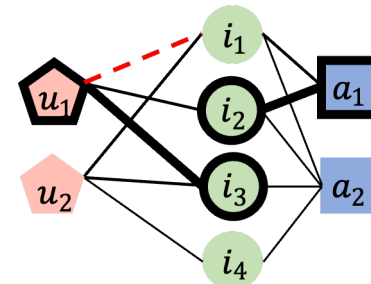
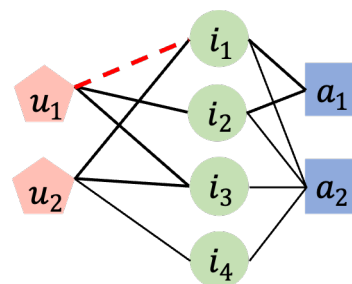
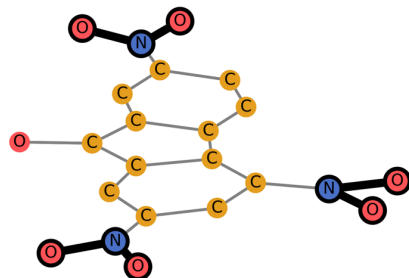
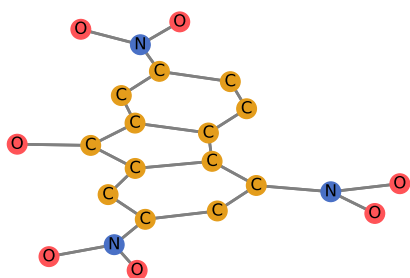


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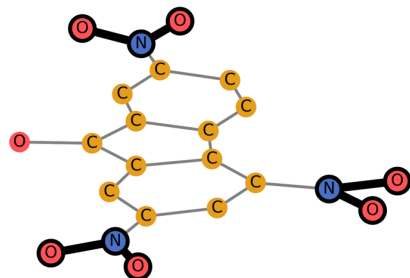
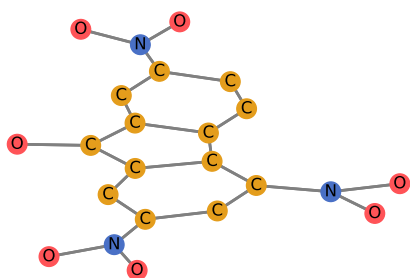


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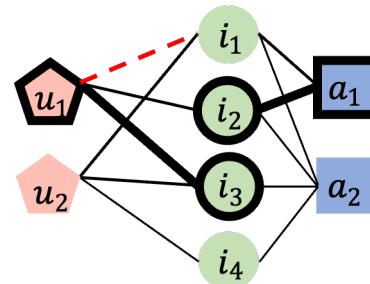
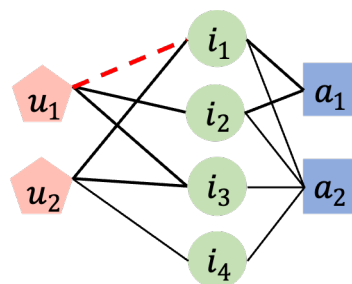
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- Heterogeneous link prediction: recommendation.
  - An ideal explanation should capture the connection between the source and the target.



- Explanation: subgraphs for  $-NO_2$  motif



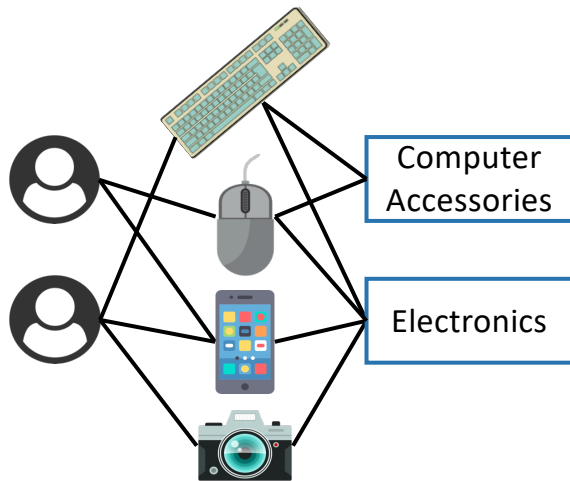
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# Main Idea: Paths As Explanations

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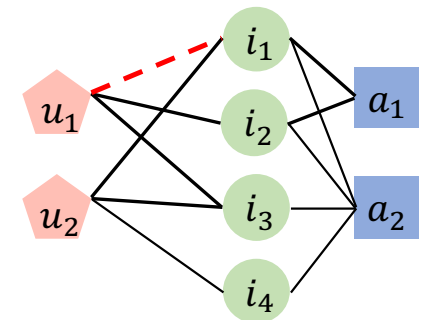
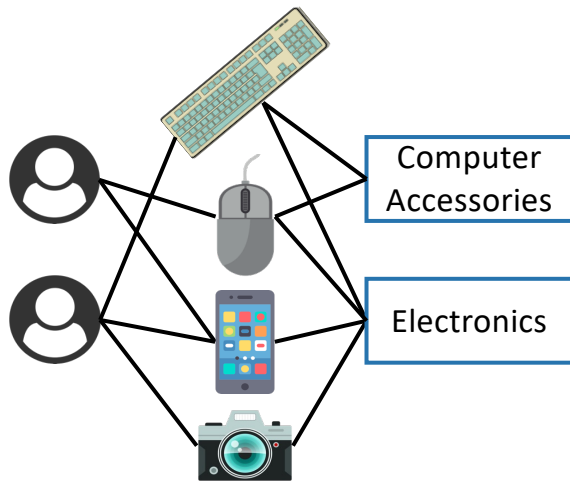
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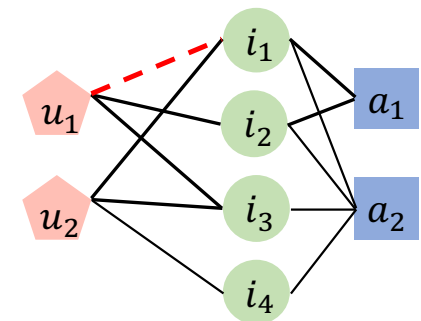
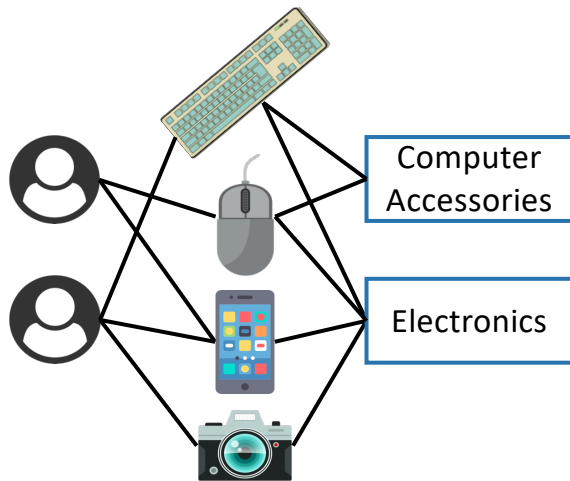
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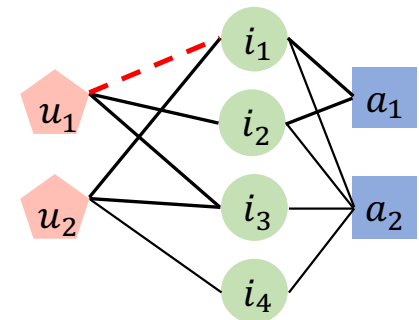
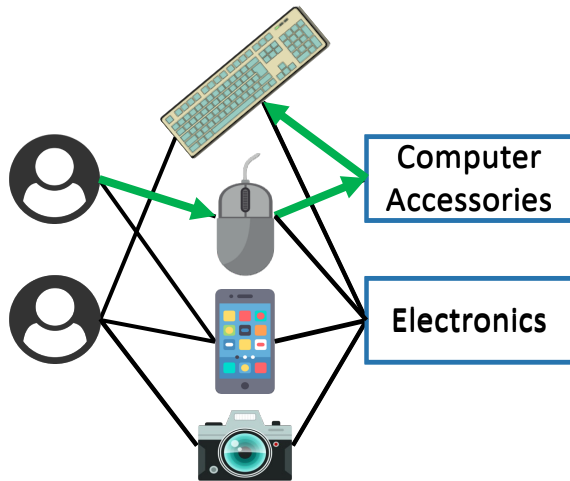
- Natural human-interpretable explanations boil down to paths.





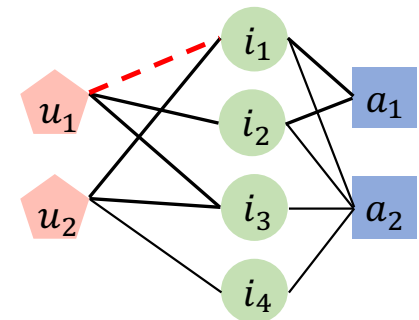
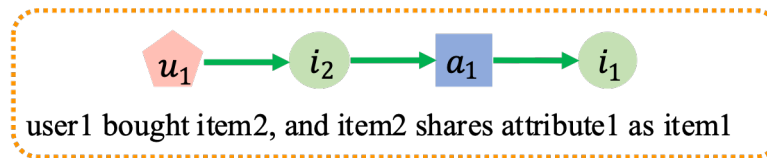
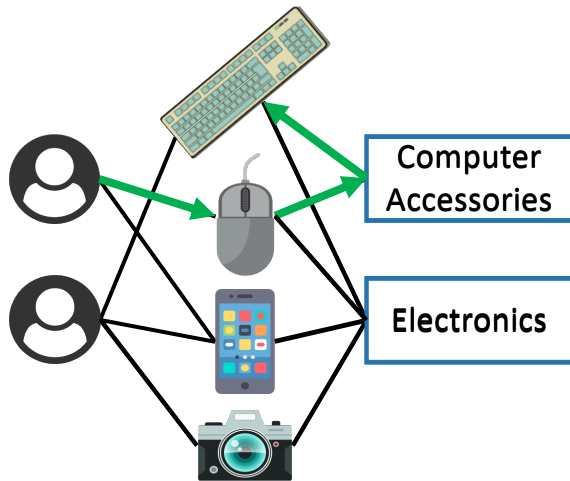
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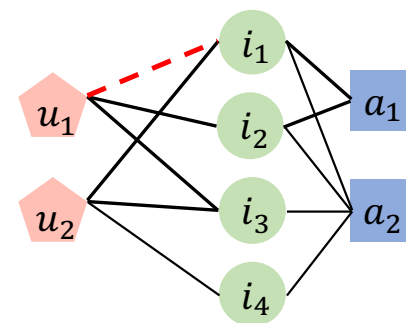
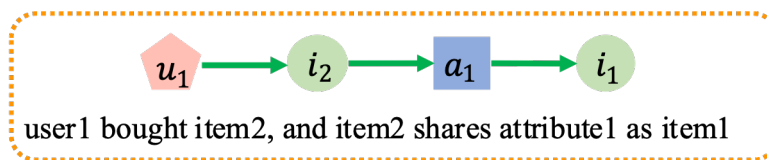
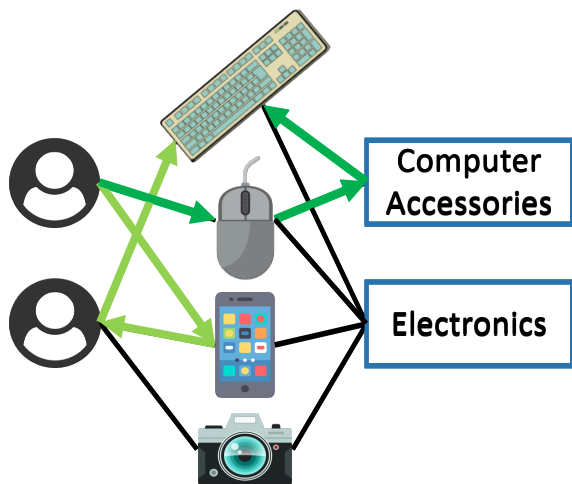
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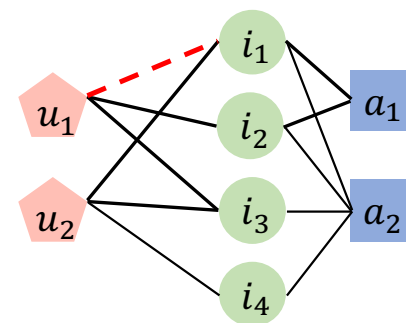
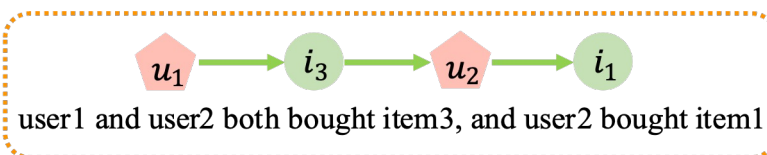
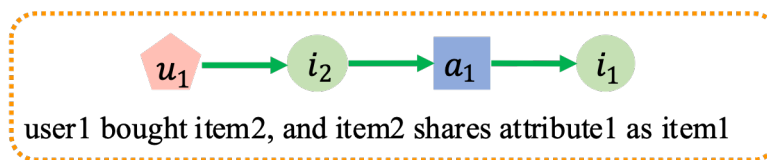
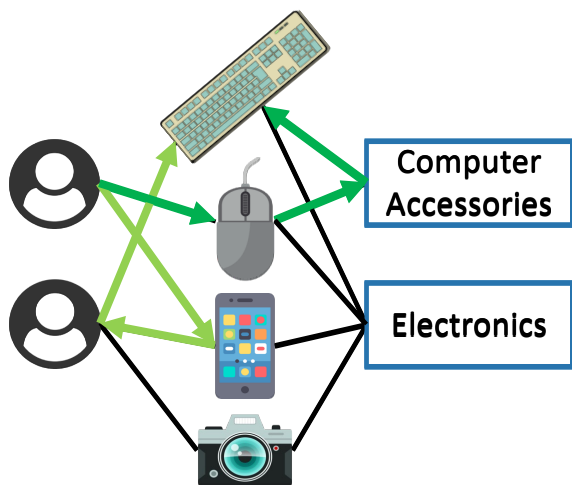
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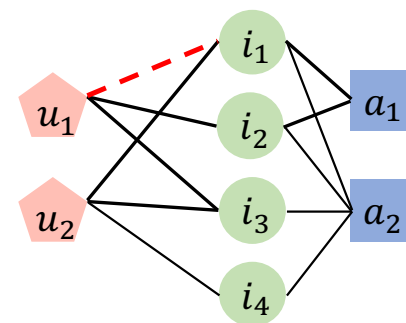
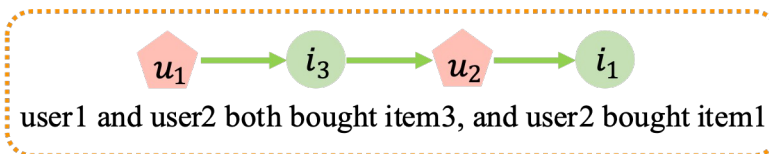
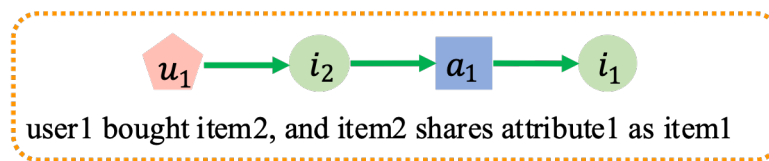
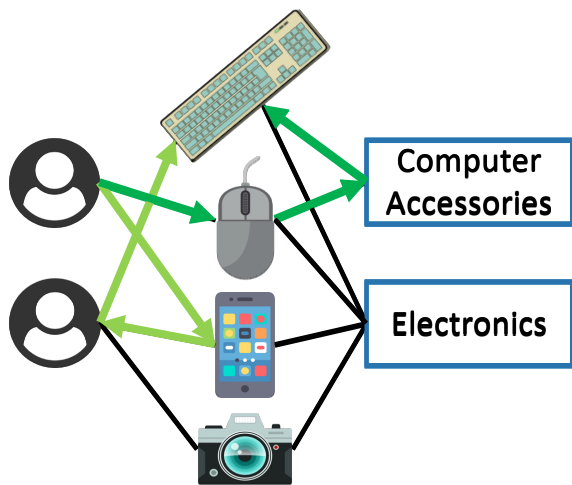
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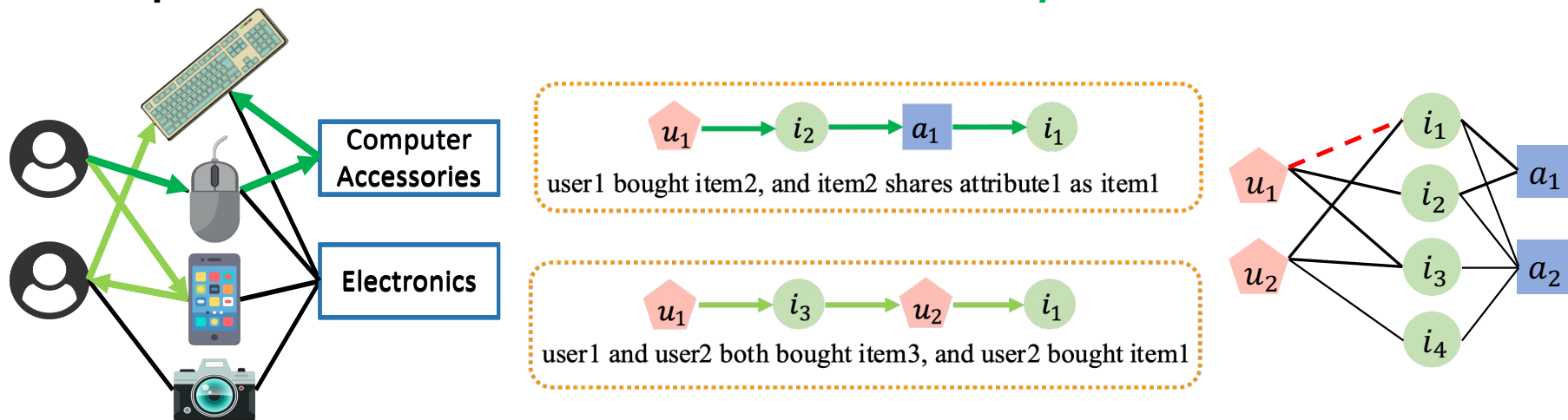
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- Paths form a much smaller search space compared to general subgraphs.
- Define explanations as *concise* and *informative* paths that are *influential to the prediction*.

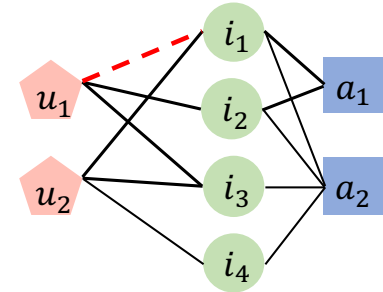


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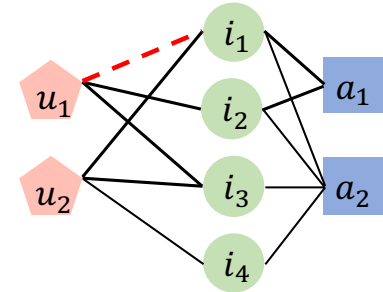
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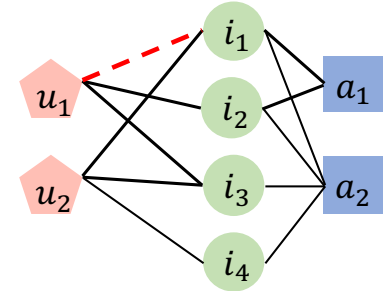
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- Challenges for finding good paths.



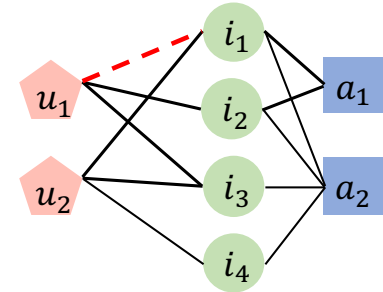
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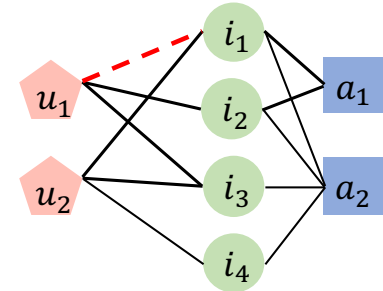
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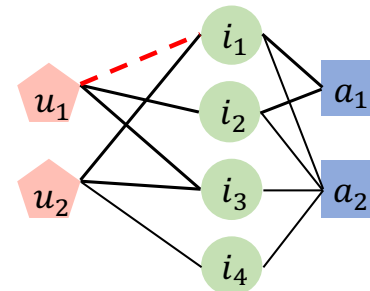
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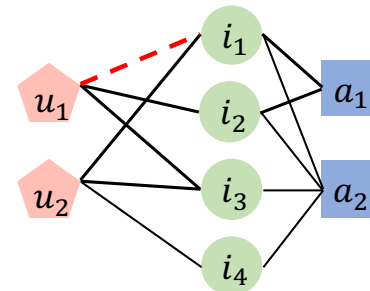
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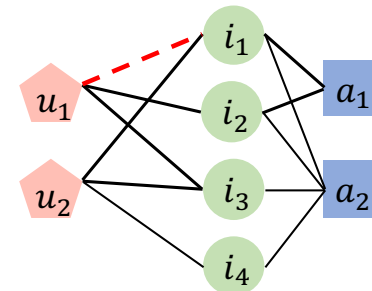
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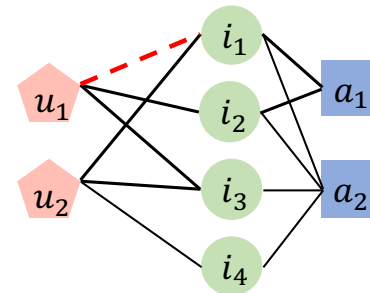


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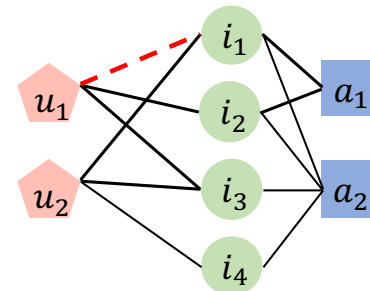
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- Pruning: more informative paths and efficiency.

# Experiments

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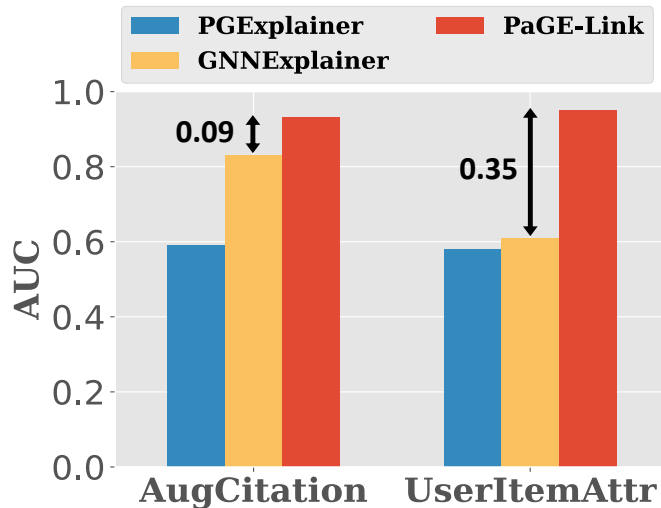
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- ROC-AUC: 9%-35% improvement over baselines.

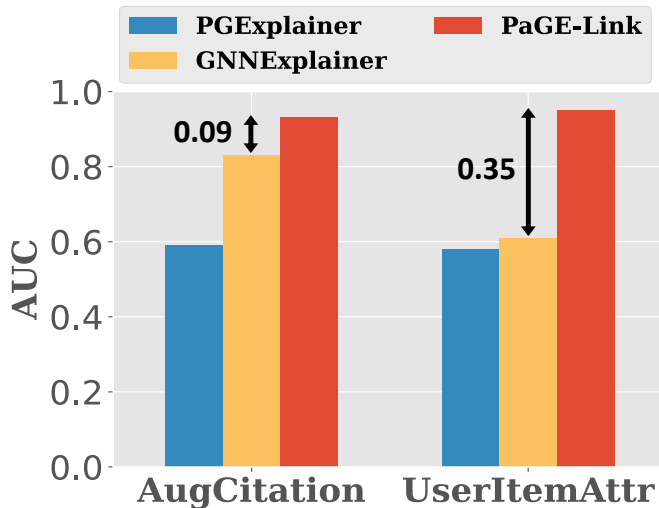
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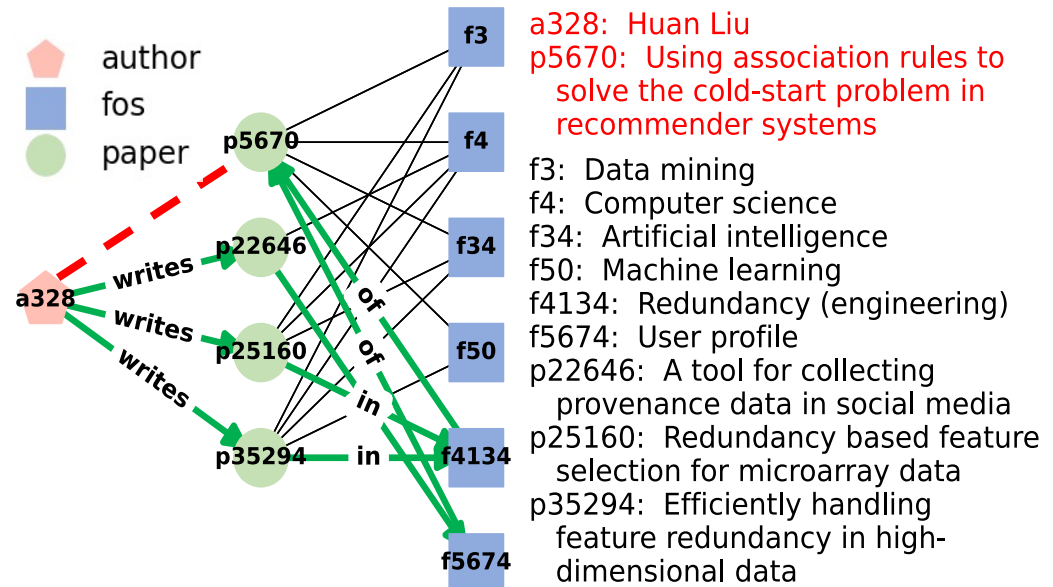
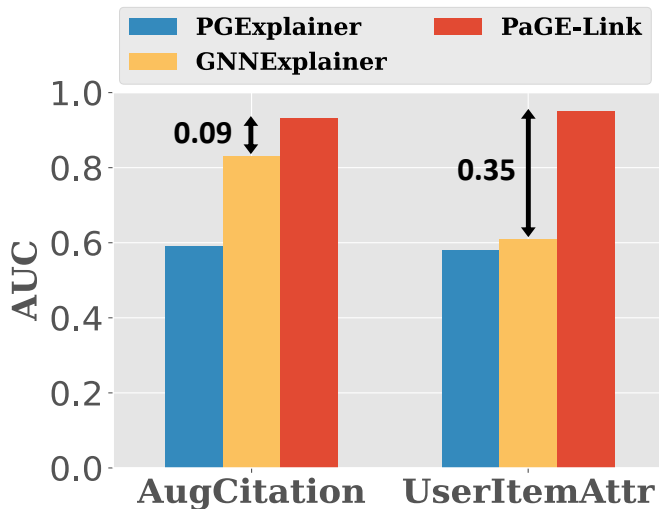
# Experiments

- ROC-AUC: 9%-35% improvement over baselines.
- Concise paths without generic nodes.



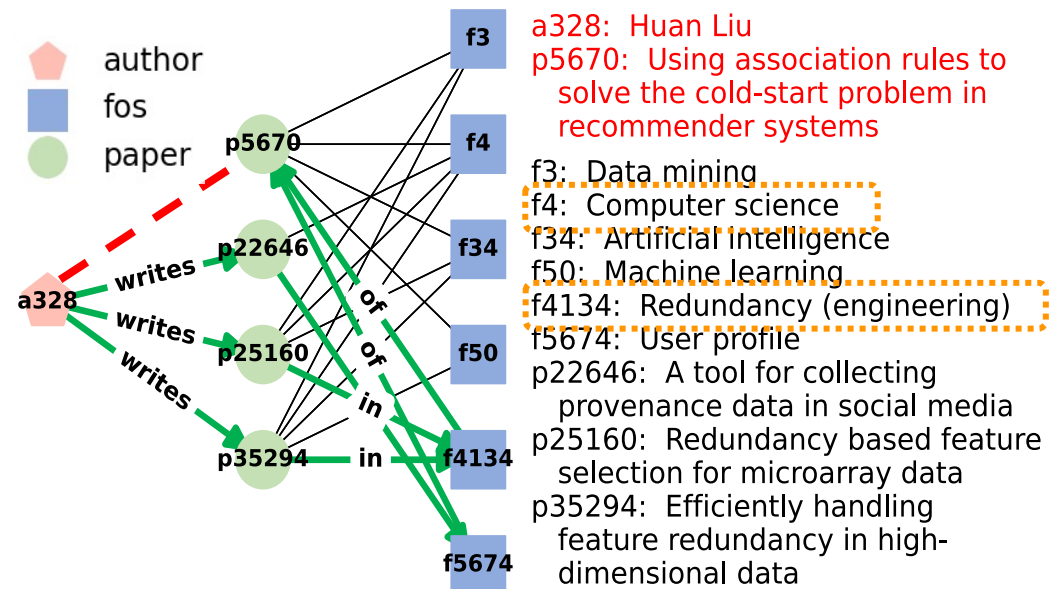
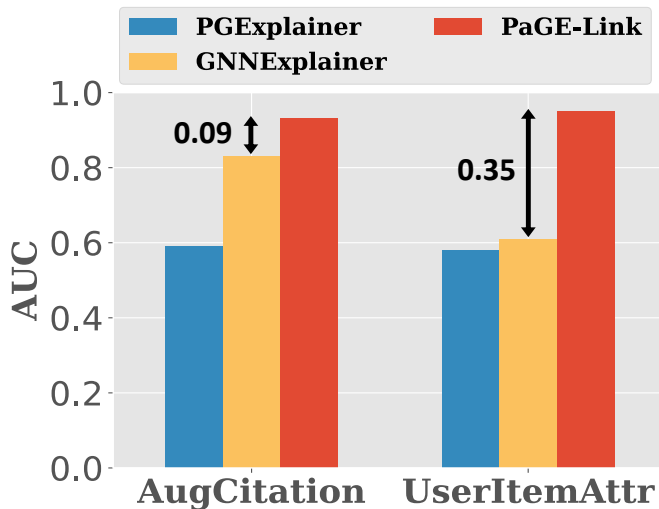
# Experiments

- ROC-AUC: 9%-35% improvement over baselines.
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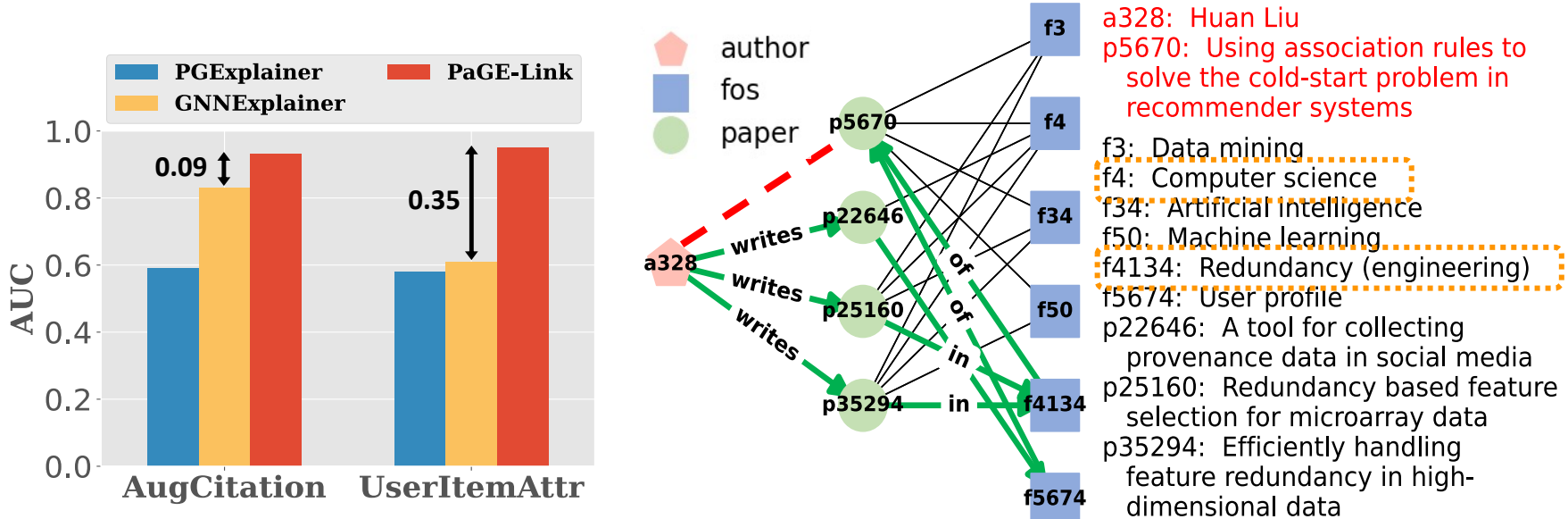
# Experiments

- ROC-AUC: 9%-35% improvement over baselines.
- Concise paths without generic nodes.



# Experiments

- ROC-AUC: 9%-35% improvement over baselines.
- Concise paths without generic nodes.
- Human evaluation: 78.79% responses selected our method as the best compared to baselines.





# Thank you!

## Q & A

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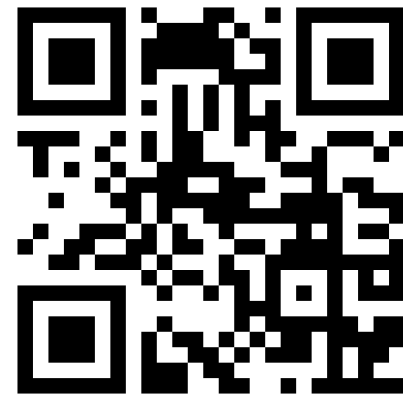
**Paper**



**Code**



**Contact author**



# Appendix

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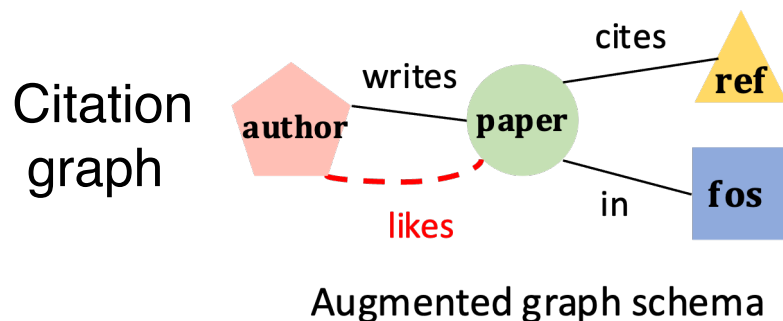
# Experiments: Dataset Generation

Generate datasets new evaluation

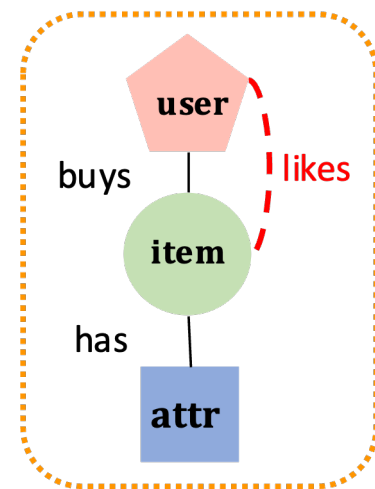
- Create a new edge  $s-t$  if they are connected by a concise and informative path  $p$

$$\mathcal{P} = \{p \mid p \text{ is a } s-t \text{ path with max length } l_{max} \text{ and max node degree } D_{max}\}$$

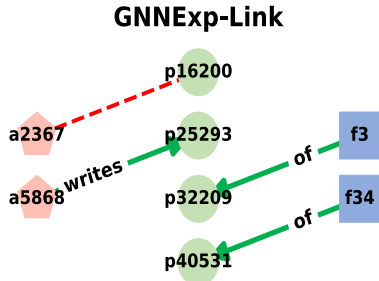
- Use  $p$  as the ground truth for evaluating the prediction of  $(s, t)$



User-item graph

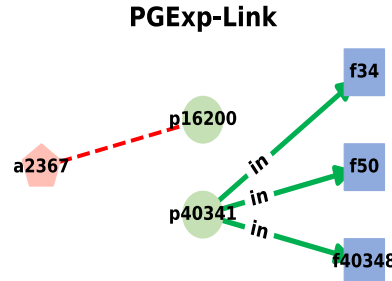


# Experiments: Visualization

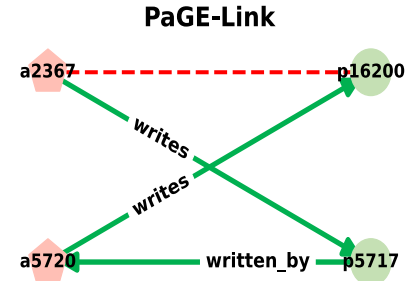


a2367: Vipin Kumar  
 p16200: Fast and exact network trajectory similarity computation: a case-study on bicycle corridor planning

a5868: Pang-Ning Tan  
 f3: Data mining  
 f34: Artificial intelligence  
 p25293: Selecting the right interestingness measure for association patterns  
 p32209: Generalizing the notion of support  
 p40531: Tripoles: A New Class of Relationships in Time Series Data



f34: Artificial intelligence  
 f50: Machine learning  
 f40348: Environmental change  
 p40341: Incremental Dual-memory LSTM in Land Cover Prediction



a5720: Shashi Shekhar  
 p5717: Correlation analysis of spatial time series datasets: a filter-and-refine approach

# Proposition and Theorems

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- Paths form a much smaller search space

**Proposition 4.1.** *Let  $\mathcal{G}(n, d)$  be a random graph with  $n$  nodes and density  $d$ , i.e., there are  $m = d\binom{n}{2}$  edges chosen uniformly randomly from all node pairs. Let  $Z_{n,d}$  be the expected number of paths between any pair of nodes. Let  $S_{n,d}$  be the expected number of edge-induced subgraphs. Then  $Z_{n,d} = o(S_{n,d})$ , i.e.,  $\lim_{n \rightarrow \infty} \frac{Z_{n,d}}{S_{n,d}} = 0$ .*

- Asymptotic normality of the k-core

**Theorem 5.1** (Pittel, Spencer and Wormald [28]). *Let  $\mathcal{G}(n, d)$  be a random graph with  $m$  edges as in Proposition 4.1. Let  $\mathcal{G}^k(n, d) = (\mathcal{V}^k(n, d), \mathcal{E}^k(n, d))$  be the nonempty  $k$ -core of  $\mathcal{G}(n, d)$ . Then  $\mathcal{G}^k(n, d)$  will contain  $\delta_{\mathcal{V}}(n, d, k)n$  nodes and  $\delta_{\mathcal{E}}(n, d, k)m$  edges with high probability (w.h.p.) for large  $n$ , i.e.,  $|\mathcal{V}^k(n, d)|/n \xrightarrow{P} \delta_{\mathcal{V}}(n, d, k)$  and  $|\mathcal{E}^k(n, d)|/m \xrightarrow{P} \delta_{\mathcal{E}}(n, d, k)$  with  $\xrightarrow{P}$  stands for convergence in probability.*