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

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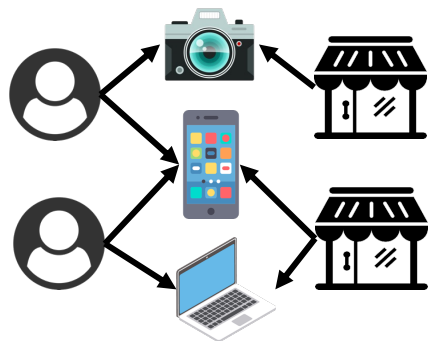
# Outline

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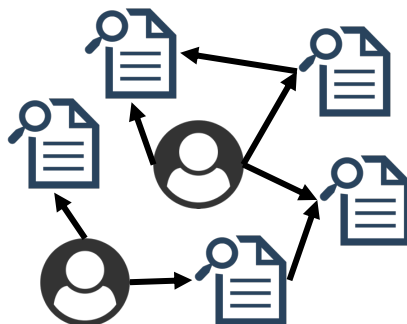
- Machine Learning on Graphs
  - Graph Neural Networks (GNNs)
  - GNNs for Link Prediction
- Model Explainability
- PaGE-Link
  - Main Idea
  - Path-Enforcing Mask
  - Experiments

# Machine Learning on Graphs

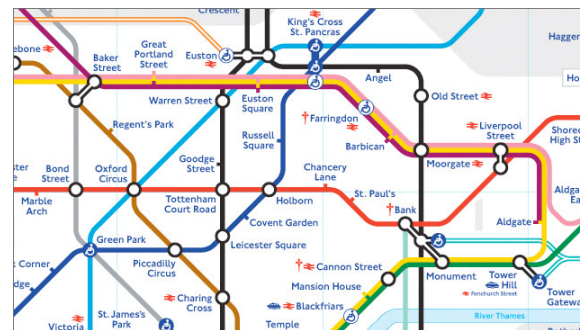
Graphs are a general language for modeling entities with relations



E-commerce graphs



Citation graphs



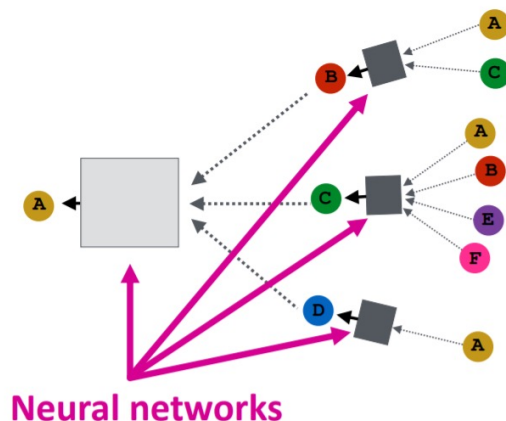
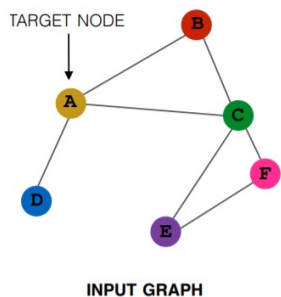
Transportation graphs

(Image Credit: [www.visitlondon.com](http://www.visitlondon.com))

Molecule graphs, code graphs, scene graphs, and many more ...

# Graph Neural Networks

GNNs: a family of neural-network-based models for machine learning on graphs



(Hamilton, W. L., Ying, R., & Leskovec, J. 2017)

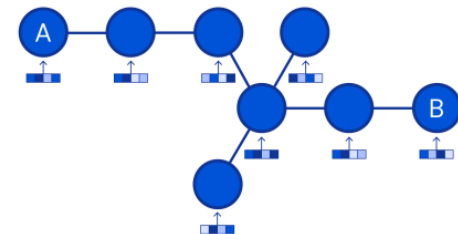
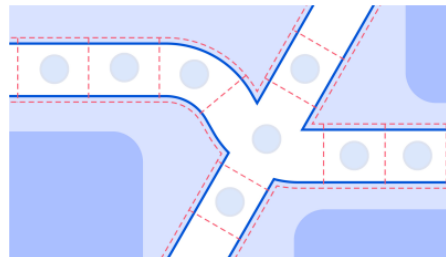
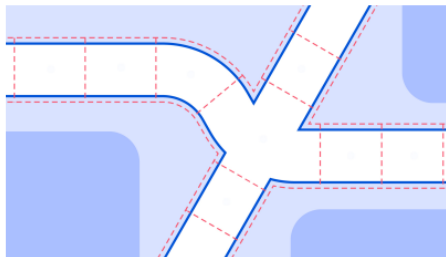
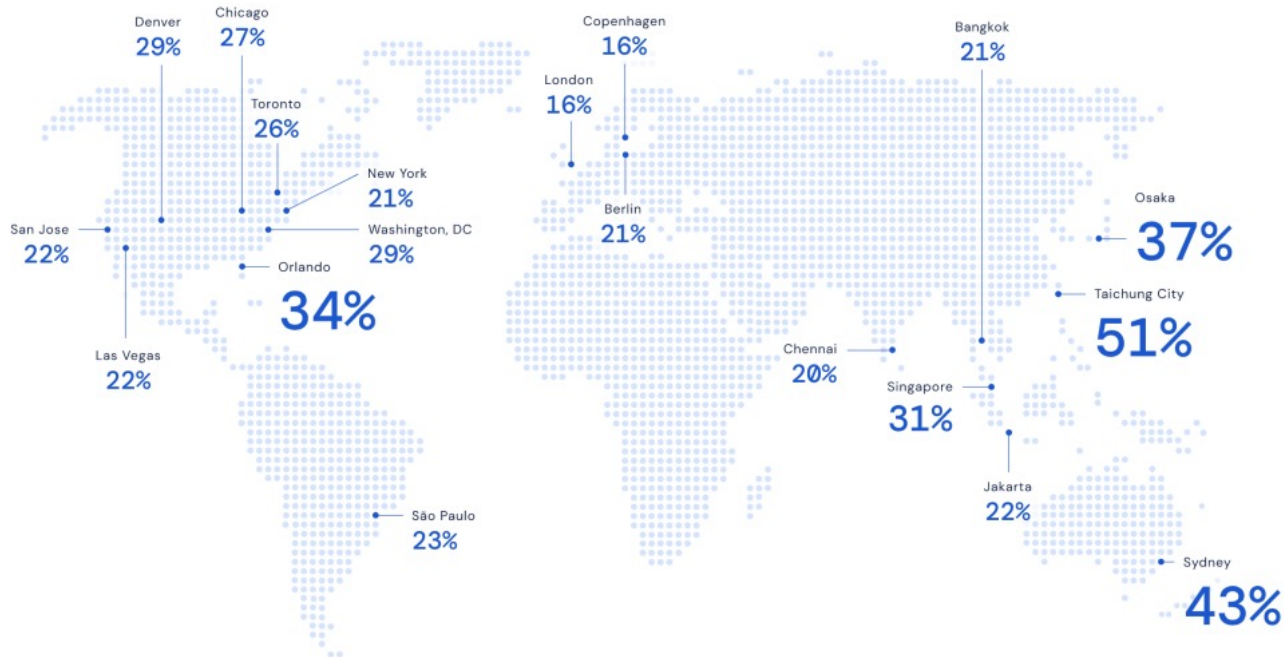
## Message passing

Each node aggregates messages from its neighbors and recursively extends to multi-hop neighbors

Node A with neighbors  $\mathcal{N}(A)$  aggregates messages at step  $l$ :

$$\mathbf{h}_A^{(l)} = \text{AGGR}(\mathbf{h}_A^{(l-1)}, \{\mathbf{h}_i^{(l-1)} | i \in \mathcal{N}(A)\})$$

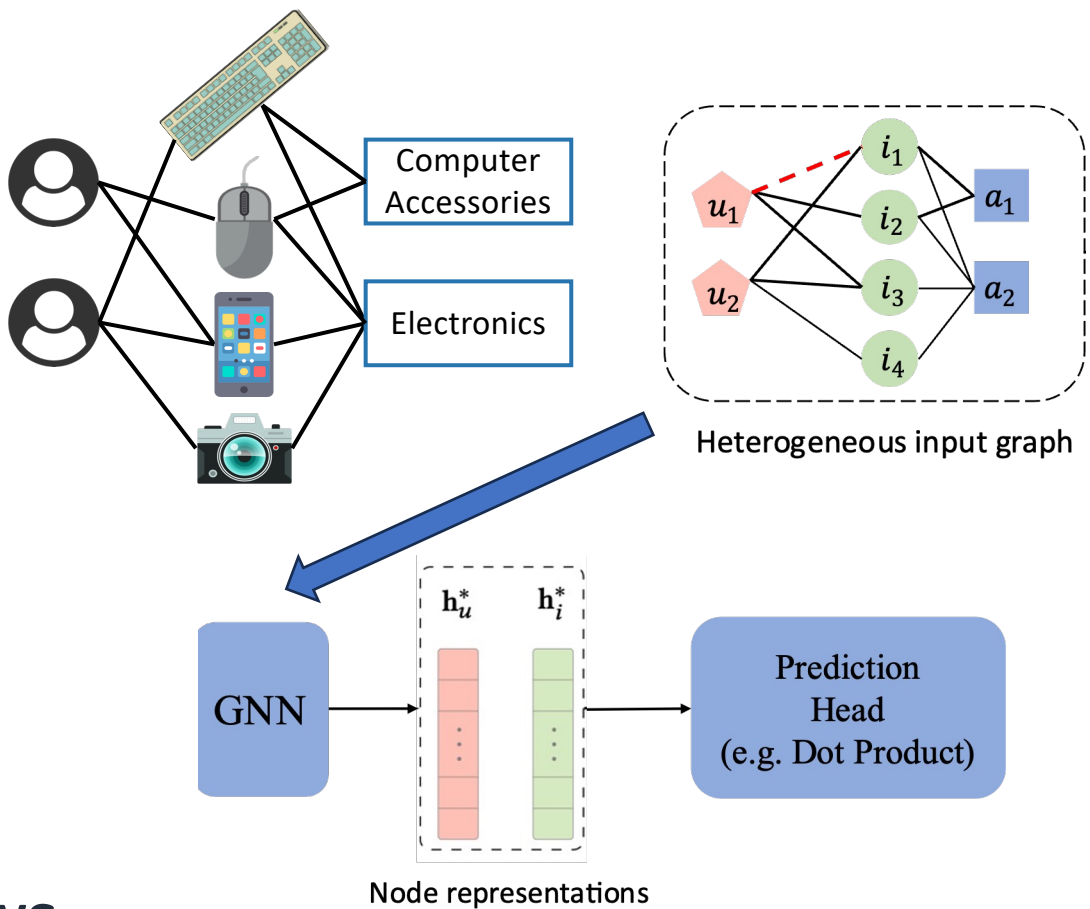
# GNNs for Google Map ETA Prediction



Derrow-Pinion, Austin, et al. "ETA prediction with graph neural networks in google maps." CIKM. 2021.

# GNNs for Link Prediction

- Link Prediction: Recommend items to users



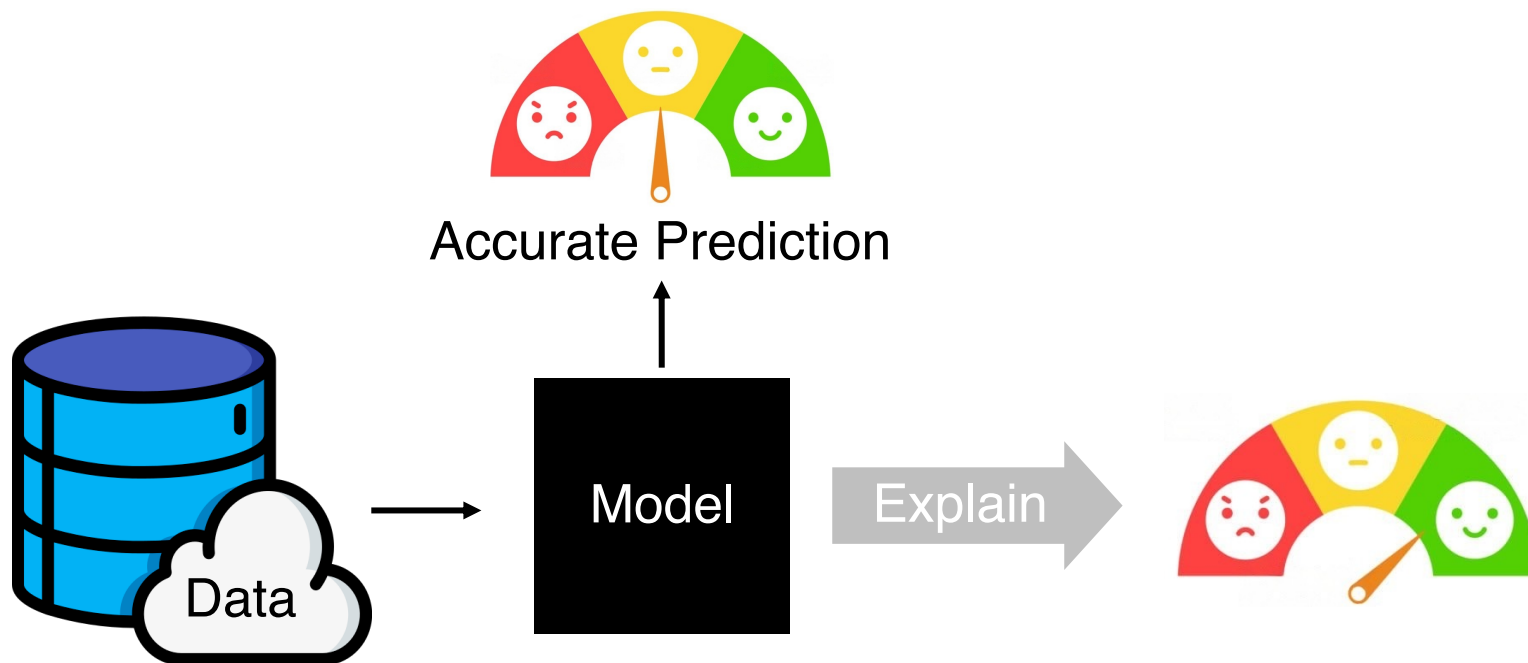
Traditional models (matrix factorization & shallow embedding) **GNNs**

Model	Amazon-Books	
	Recall@20	NDCG@20
MF-BPR	0.0338	0.0261
CML	<u>0.0522</u>	<u>0.0428</u>
ENMF	0.0359	0.0281
DeepWalk	0.0346	0.0264
LINE	0.0410	0.0318
Node2Vec	0.0402	0.0309
NGCF	0.0344	0.0263
NIA-GCN	0.0369	0.0287
LR-GCCF	0.0335	0.0265
LightGCN	0.0411	0.0315
DGCF	<u>0.0422</u>	<u>0.0324</u>
UltraGCN <sub>Base</sub>	0.0504	0.0393
UltraGCN	<b>0.0681</b>	<b>0.0556</b>

GNN achieve SOTA link prediction/recommendation results (Mao et al. CIKM 2021).

# Model Explainability

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



# A Real Amazon Recommendation

Query



Manhattan Wired Computer Keyboard, Black - Basic Keyboard - with 5ft USB-A Cable, 104-keys, Foldable Stands - Compatible for Windows, PC, Laptop - 3 Year Warranty - 179324

Visit the Manhattan Products Store  
 ★★★★★ 4,773 ratings | 30 answered questions

**\$11.99**

Get Fast, Free Shipping with Amazon Prime & FREE Returns

Get \$50 off instantly: Pay \$0.00 \$14.99 upon approval for the Amazon Rewards Visa Card. No annual fee.


Available at a lower price from other sellers that may not offer free Prime shipping.

Keyboard Description Ergonomic

## Recommendation without explanation

## Recommendation with explanation


More items to explore



<p>Mouse Pads 11 x 8.7 inches - Stitched Edges Premium-Textured Large Mouse Pads Mat Natur...</p> <p>★★★★★ 2,729</p> <p><b>\$4.98</b></p> <p>Get it as soon as <b>Thursday, Jun 30</b></p>	<p>Sponsored</p> <p>Rii RK907 Ultra-Slim Compact USB Wired Keyboard for Mac and PC, Windows 10/8 / 7 / ...</p> <p>★★★★★ 5,554</p> <p><b>\$9.99</b></p> <p>List: <del>\$11.99</del> (17% off)</p> <p>Get it as soon as <b>Thursday,</b></p>	<p>Sponsored</p> <p>Computer Keyboard Wired, Plug Play USB Keyboard, Low Profile...</p> <p>★★★★★ 119</p> <p><b>\$14.59</b></p> <p>Get it as soon as <b>Thursday,</b></p>	<p>Sponsored</p> <p>Verbatim Slimline Wired Keyboard and Mouse Combo, Optical Wired...</p> <p>★★★★★ 5,989</p> <p><b>\$13.99</b></p> <p>Get it as soon as <b>Thursday,</b></p>	<p>ALTEC Lansing Computer 6 Button USB Ergonomic Mouse</p> <p>★★★★★ 215</p> <p><b>\$14.99</b></p> <p>Get it as soon as <b>Thursday,</b></p>
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4 stars and above


Sponsored



<p>Rii RK907 Ultra-Slim Compact USB Wired Keyboard for Mac and PC, Windows 10/8 / 7 / ...</p> <p>★★★★★ 3,551</p> <p><b>\$9.99</b> ✓prime</p>	<p>Computer Keyboard Wired, Plug Play USB Keyboard, Low Profile Chiclet Keys, Large Nu...</p> <p>★★★★★ 119</p> <p><b>\$14.59</b> ✓prime</p>	<p>Verbatim Slimline Wired Keyboard and Mouse Combo, Optical Wired Mouse, Full-Size Ke...</p> <p>★★★★★ 5,989</p> <p><b>\$13.99</b> ✓prime</p>	<p>BTO USB Wired Keyboard, 104 Keys with Numeric Pad, Anti Spill and Dust Proof, Slim ...</p> <p>★★★★★ 604</p> <p><b>\$9.99</b> ✓prime</p>	<p>Basic Keyboard and Mouse, Rii RK203 Ultra Full Size Slim USB Basic Wired Mouse and K...</p> <p>★★★★★ 57</p> <p><b>\$14.99</b> ✓prime</p>
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Products related to this item

Sponsored



<p>Rii RK907 Ultra-Slim Compact USB Wired Keyboard for Mac and PC, Windows 10/8 / 7 / ...</p> <p>★★★★★ 3,551</p> <p><b>\$9.99</b> ✓prime</p>	<p>2020 Apple MacBook Air Laptop: Apple M1 Chip, 13" Retina Display, 8GB RAM, 512GB SS...</p> <p>★★★★★ 15,214</p> <p><b>\$1,149.99</b> ✓prime</p>	<p>Cordless Electric Air Duster, 2-Gear 43000RPM Portable Air Blower, Replaces...</p> <p>★★★★★ 16</p> <p><b>\$59.99</b> ✓prime</p>	<p>Manhattan USB Wired Computer Keyboard - with 4.5 ft USB-A Cable, 104-keys, Full-Siz...</p> <p>★★★★★ 869</p> <p><b>\$15.99</b> ✓prime</p>	<p>2021 Apple MacBook Pro (14-inch, Apple M1 Pro chip with 10-core CPU and 16-core GPU...</p> <p>★★★★★ 869</p> <p><b>\$2,349.00</b> ✓prime</p>
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Customers who searched for "keyboard" ultimately bought

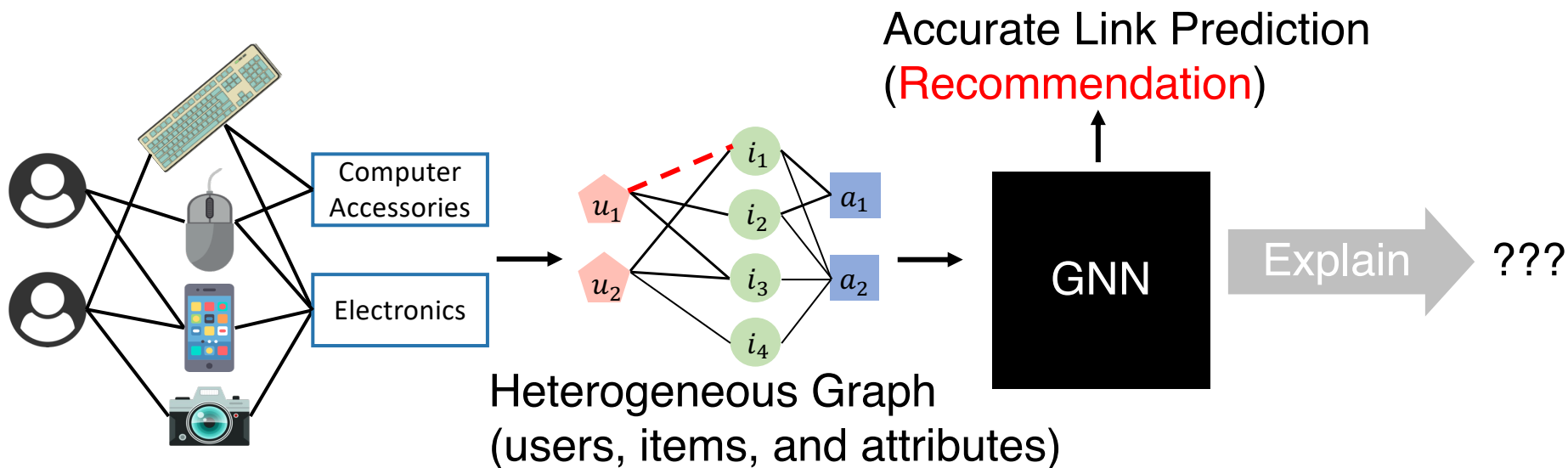


<p>Verbatim Slimline Full Size Wired Keyboard USB Plug-and-Play - Compatible with PC, Laptop - Black</p> <p>★★★★★ 5,989</p> <p><b>\$8.95</b></p> <p>List: <del>\$10.00</del> (11% off)</p> <p>Get it as soon as <b>Thursday,</b></p>	<p>Logitech MK270 Wireless Keyboard And Mouse Combo For Windows, 2.4 GHz Wireless, Compac...</p> <p>★★★★★ 69,150</p> <p><b>#1 Best Seller</b> in Computer Keyboard &amp; Mouse Combos</p> <p><b>\$27.97</b></p>	<p>Manhattan Wired Computer Keyboard, Black - Basic Keyboard - with 5ft USB-A Cable, 104-keys, Foldable...</p> <p>★★★★★ 4,773</p> <p><b>\$11.99</b></p> <p>Get it as soon as <b>Thursday, Jun 30</b></p>	<p>Computer Keyboard Wired, Plug Play USB Keyboard, Low Profile Chiclet Keys, Large Number Pad, Caps...</p> <p>★★★★★ 119</p> <p><b>\$14.59</b></p> <p>Get it as soon as <b>Thursday, Jun 30</b></p>	<p>Redragon S101 Wired Gaming Keyboard and Mouse Combo RGB Backlit Gaming Keybo...</p> <p>★★★★★ 40,127</p> <p><b>#1 Best Seller</b> in PC Gaming Keyboards</p> <p><b>\$35.98</b></p> <p>Get it as soon as <b>Thursday,</b></p>
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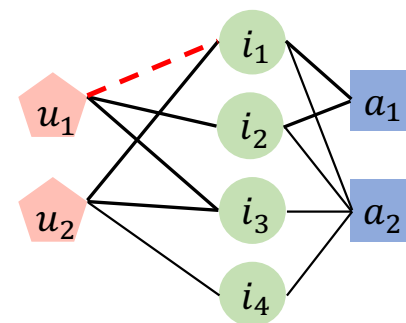
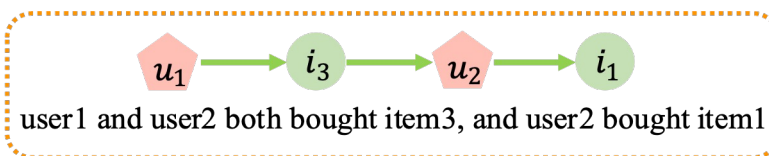
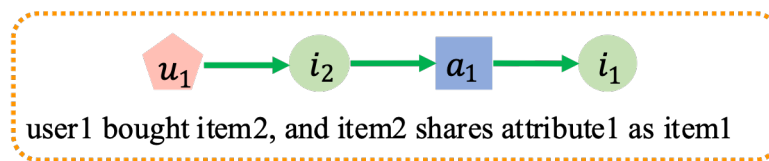
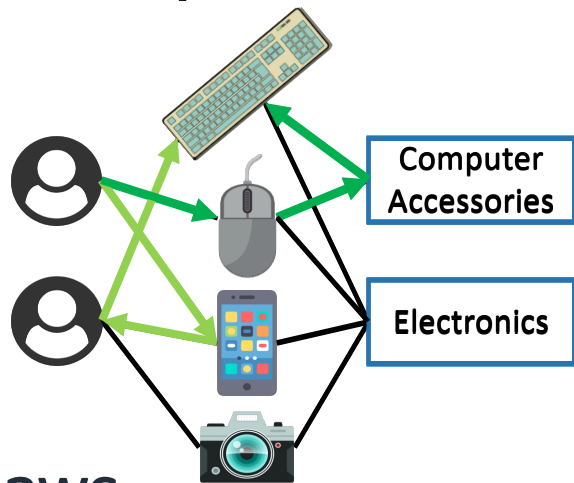
# GNN Explainability

- Data: Heterogeneous graphs.
- Model: GNNs for link prediction.
- Explanation: Why recommend an item to a user? (Why predict a user-item link?)



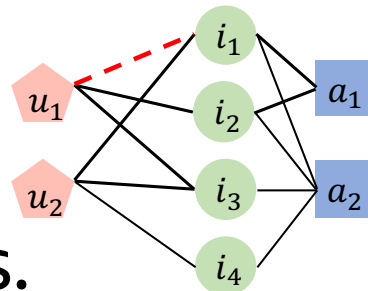
# Main Idea: Paths As Explanations

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



# PaGE-Link: Path-Enforcing Mask

- Challenges for finding good paths.
  - Many path candidates.
  - Criterion for selecting good paths.
- Learn an edge mask to select meaningful edges.
  - Edges form short paths with low-degree nodes.



$$\mathcal{L}_{path}(\mathcal{M}) = - \sum_{r \in \mathcal{R}} (\alpha \sum_{\substack{e \in \mathcal{E}_{path} \\ \tau(e)=r}} \mathcal{M}_e^r - \beta \sum_{\substack{e \in \mathcal{E}, e \notin \mathcal{E}_{path} \\ \tau(e)=r}} \mathcal{M}_e^r)$$

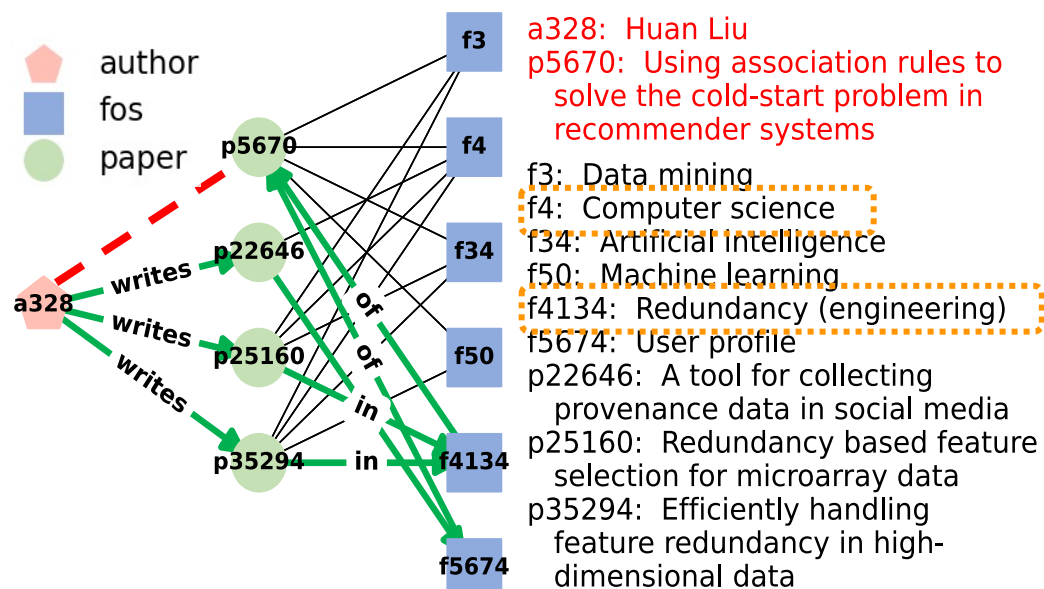
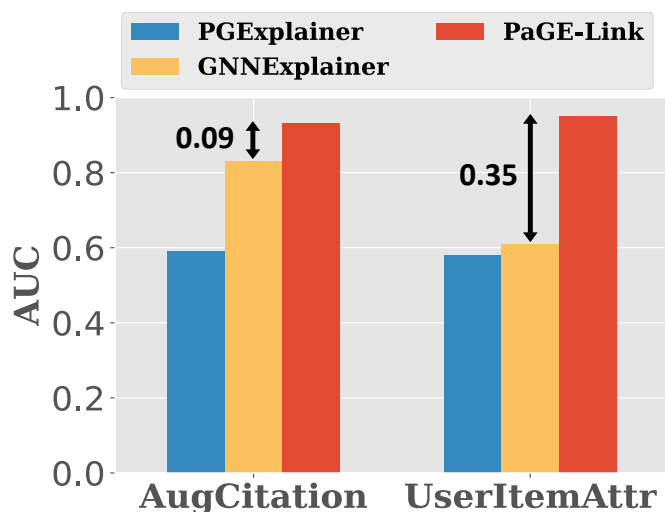
- Edges maximize the mutual information.

$$\mathcal{L}_{pred}(\mathcal{M}) = -\log P_{\Phi}(Y = 1 | \mathcal{G} = (\mathcal{V}, \mathcal{E} \odot \sigma(\mathcal{M})), (s, t))$$

- Pruning: more informative paths and efficiency.

# 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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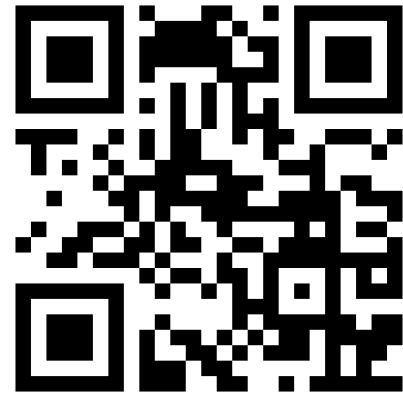
**Paper**



**Code**



**Contact author**



# Appendix

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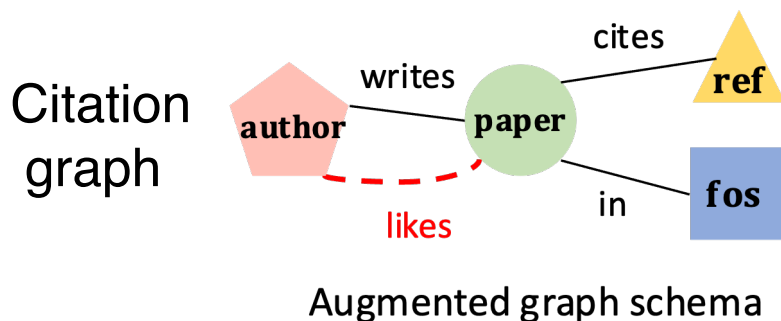
# Experiments: Dataset Generation

Generate datasets new evaluation

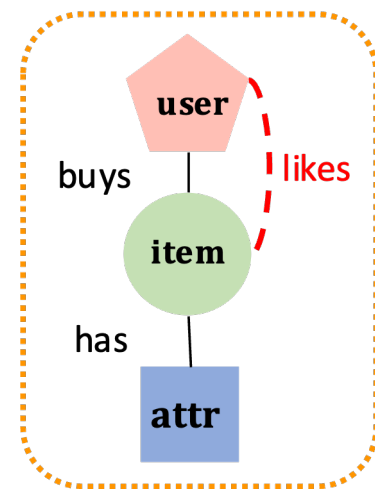
- Create a new edge  $s-t$  if they are connected by a concise and informative path  $p$

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

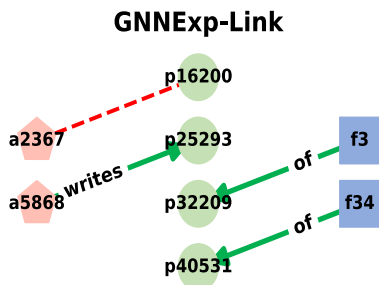
- Use  $p$  as the ground truth for evaluating the prediction of  $(s, t)$



User-item graph

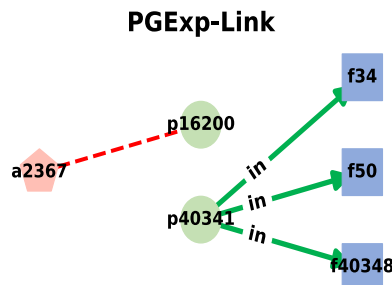


# Experiments: Visualization

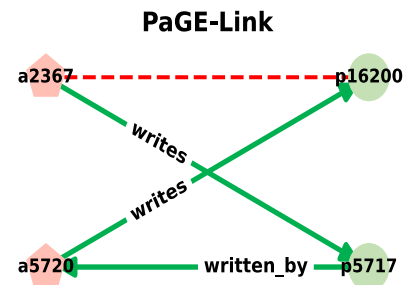


a2367: Vipin Kumar  
 p16200: Fast and exact network trajectory similarity computation: a case-study on bicycle corridor planning

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.*