CIKM 2021

Topic-aware Heterogeneous Graph Neural Network for Link Prediction

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Heterogeneous graphs (HGs)

- Multiple types of nodes and edges;
- Rich and diverse semantics;

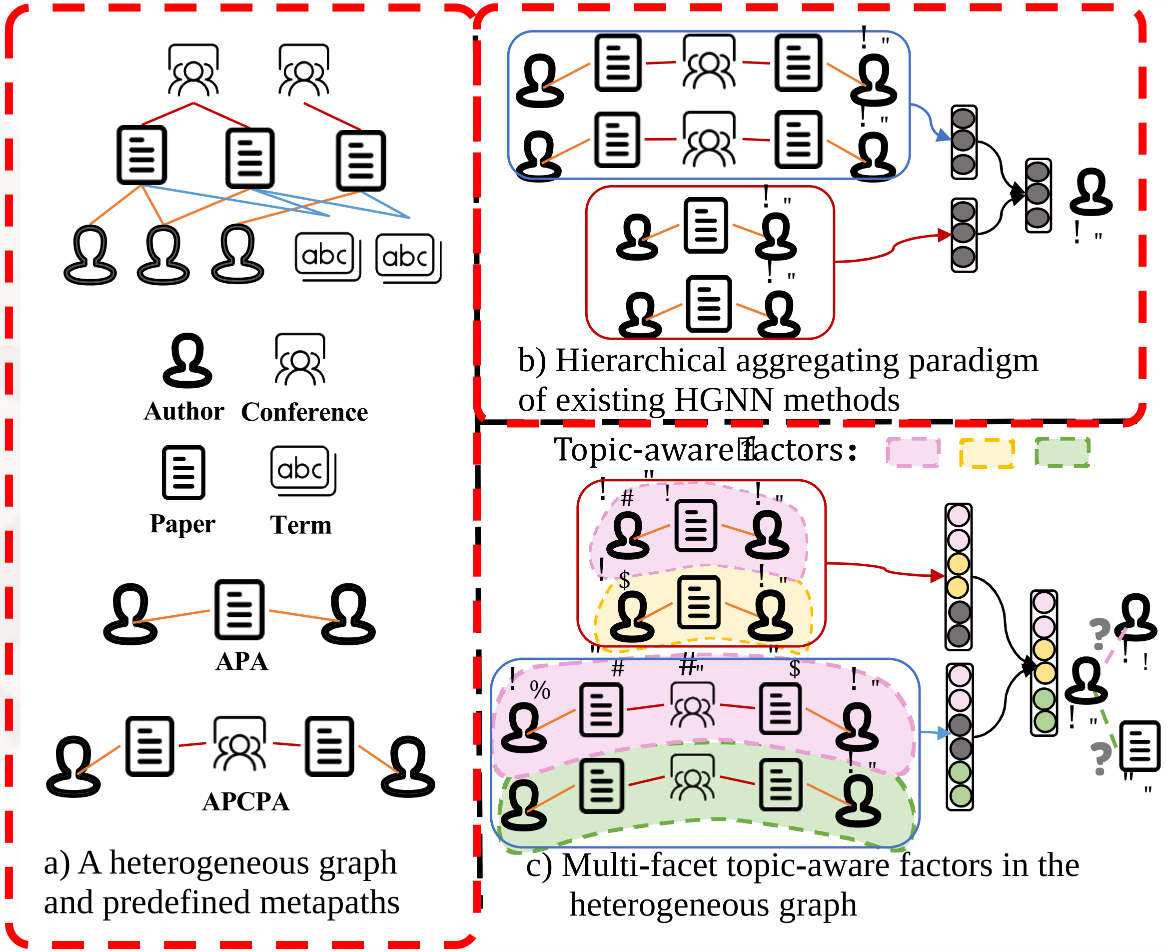
Heterogeneous graph neural networks (HGNNs)

- Defines and leverages metapaths

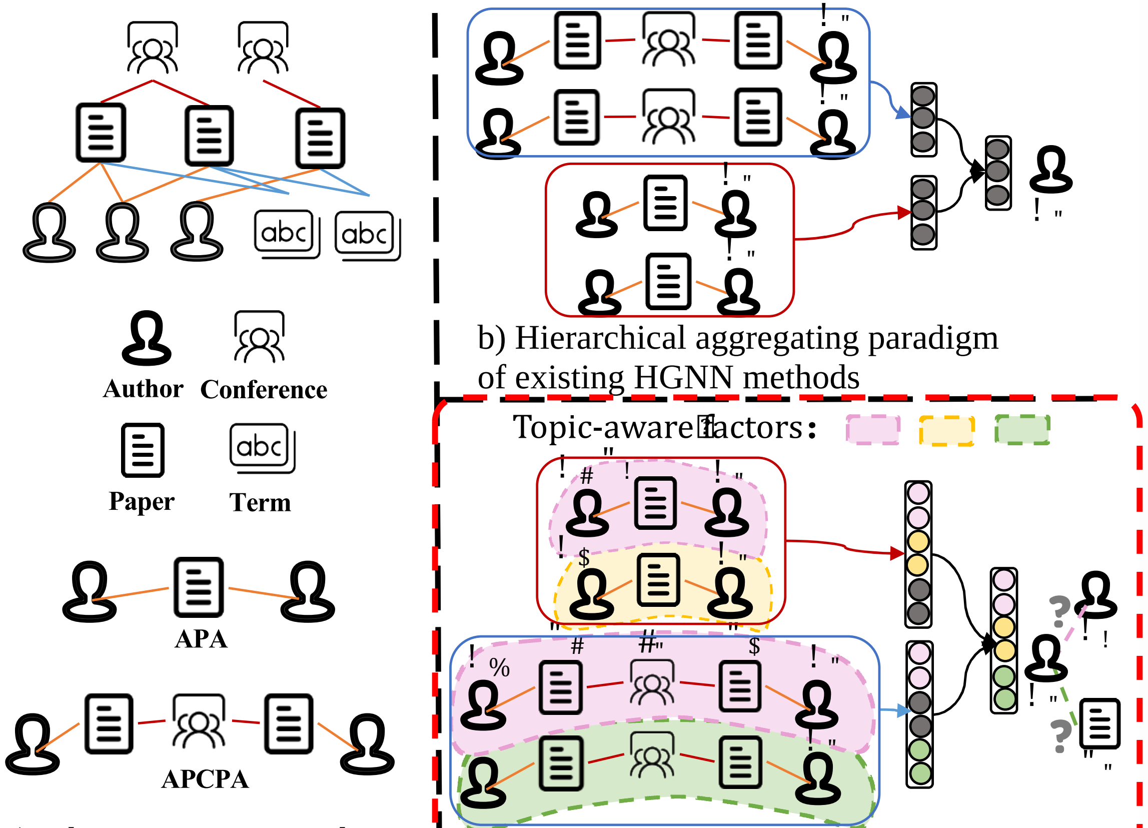
  preserve semantics and model heterogeneous structure

- Classical paradigm

  hierarchical aggregation at node and semantic level



- Rich unstructured text content carried by nodes such as paper abstracts, descriptions or reviews, are also pervasive in HGs.
- Text content is often a mixture of semantics arising from multi-facet topic-aware factors, which fundamentally manifest why nodes of different types would connect and form a specific heterogeneous structure.
- Such topic-aware semantics are more fine-grained than structural semantics for link prediction.



a) A heterogeneous graph and predefined metapaths

b) Hierarchical aggregating paradigm of existing HGNN methods

c) Multi-facet topic-aware factors in the heterogeneous graph

Disentangled learning in HGNNs

Only focuses on a coarse-grained level to automatically factorize structural semantics.

Only focuses on local level avoid metapath selection only from neighbor nodes.

Cannot further recognize and unveil more fined-grained semantics underlying the bare node connections.

Our approach

Exploit both heterogeneous structures and unstructured text content ⇨ Identify the potential but fundamental topic-aware factors ⇨ learn multi-facet topic-aware representations for link prediction

Challenges

1. No explicit labels indicating the topic-aware factors
   - **Method**: Intra-metapath decomposition
2. How to combine both structural and topic-aware semantics
   - **Method**: Inter-metapath mergence
3. How to to preserve the global characteristics of topic-aware semantics
   - **Method**: Topic prior guidance

Topic-aware Heterogeneous Graph Neural Network (THGNN)

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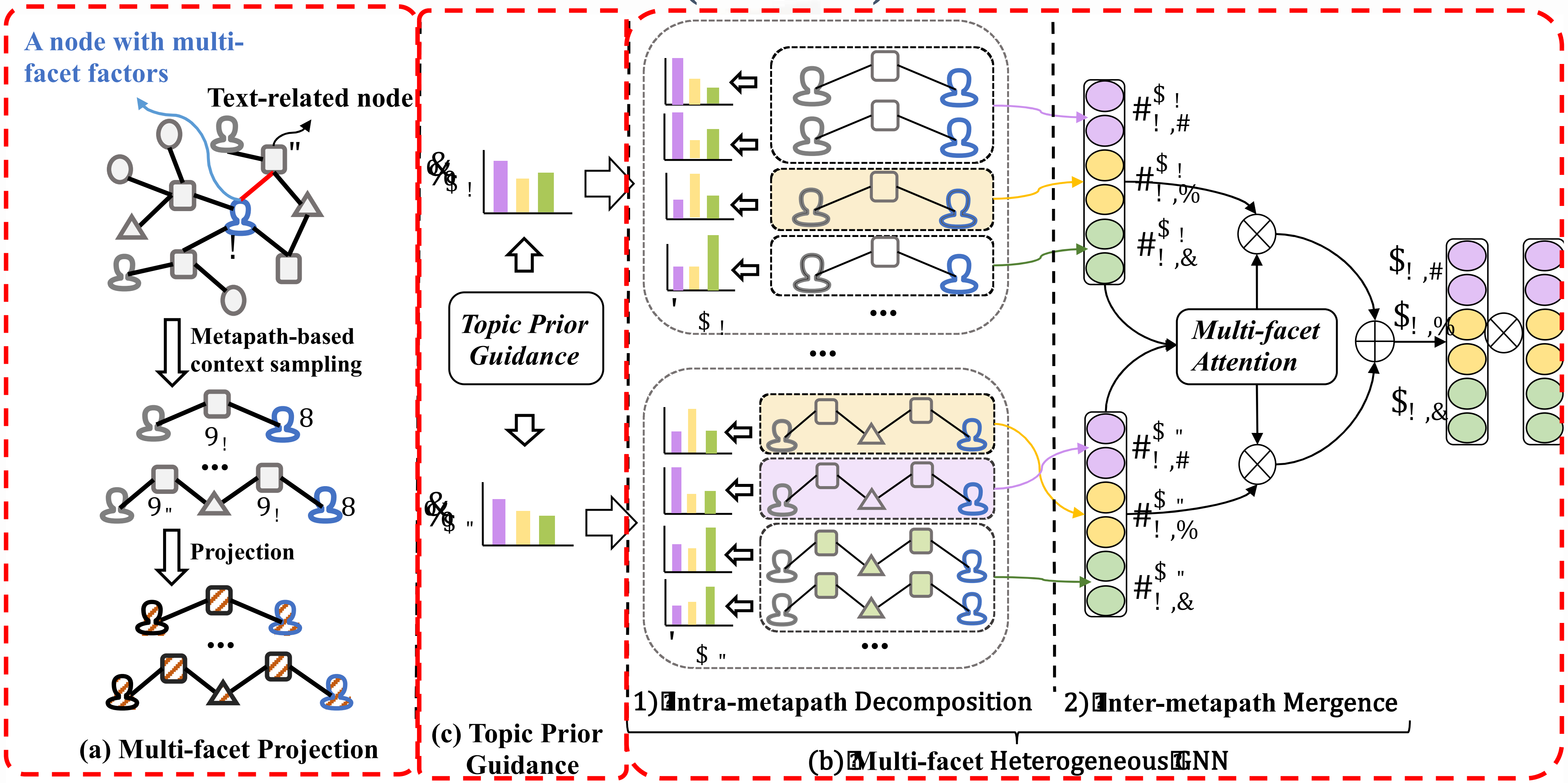
Topic-aware Heterogeneous Graph Neural Network (THGNN)



Multi-facet Projection

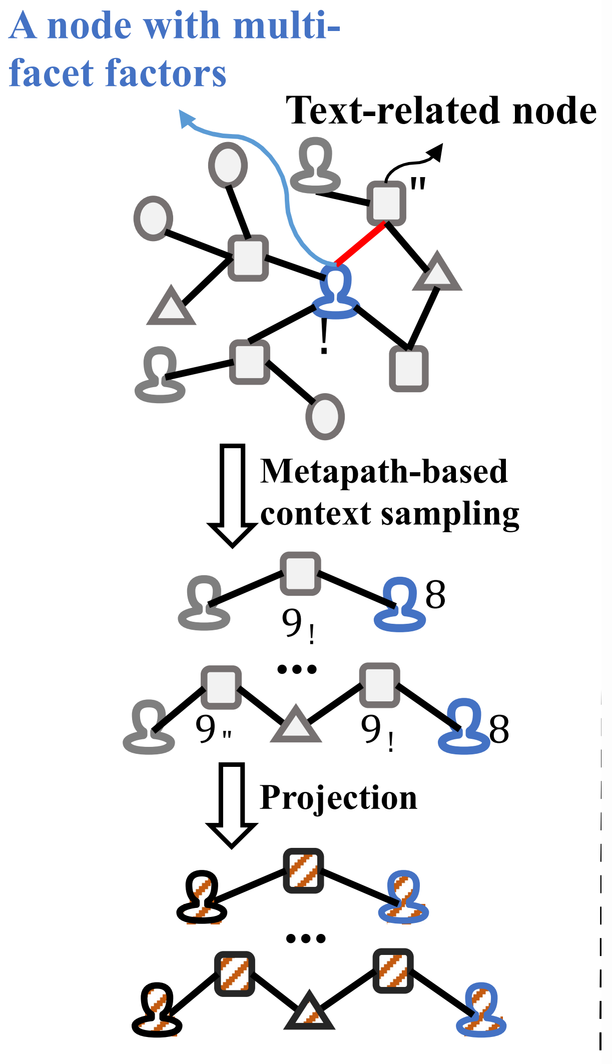
- There exists K potential topic-aware subspaces in the HG:

$$\mathbf{h}_{u,k} = \mathbf{P}_k^{\varphi(u)} \cdot \mathbf{x}_u,$$

- Sampling Strategy :

Given a node u with multi-facet factors in the HG, sample some metapath-based contexts via different metapaths

$$p_{c_u} = \frac{\sum_{v_s, v_{s+1} \in c_u^{text}} \cos(\boldsymbol{\lambda}_{v_s}^{c_u}, \boldsymbol{\lambda}_{v_{s+1}}^{c_u})}{\sum_{c'_u \in C_u^M} \sum_{v_s, v_{s+1} \in c_u'^{text}} \cos(\boldsymbol{\lambda}_{v_s}^{c'_u}, \boldsymbol{\lambda}_{v_{s+1}}^{c'_u})},$$



(a) Multi-facet Projection

Multi-facet Heterogeneous Graph Neural Network

- Intra-metapath Decomposition. (step 1)

$$\mathbf{h}_{u,k}^{c_u} = f(\{\mathbf{h}_{v,k}, \forall v \in c_u\}),$$

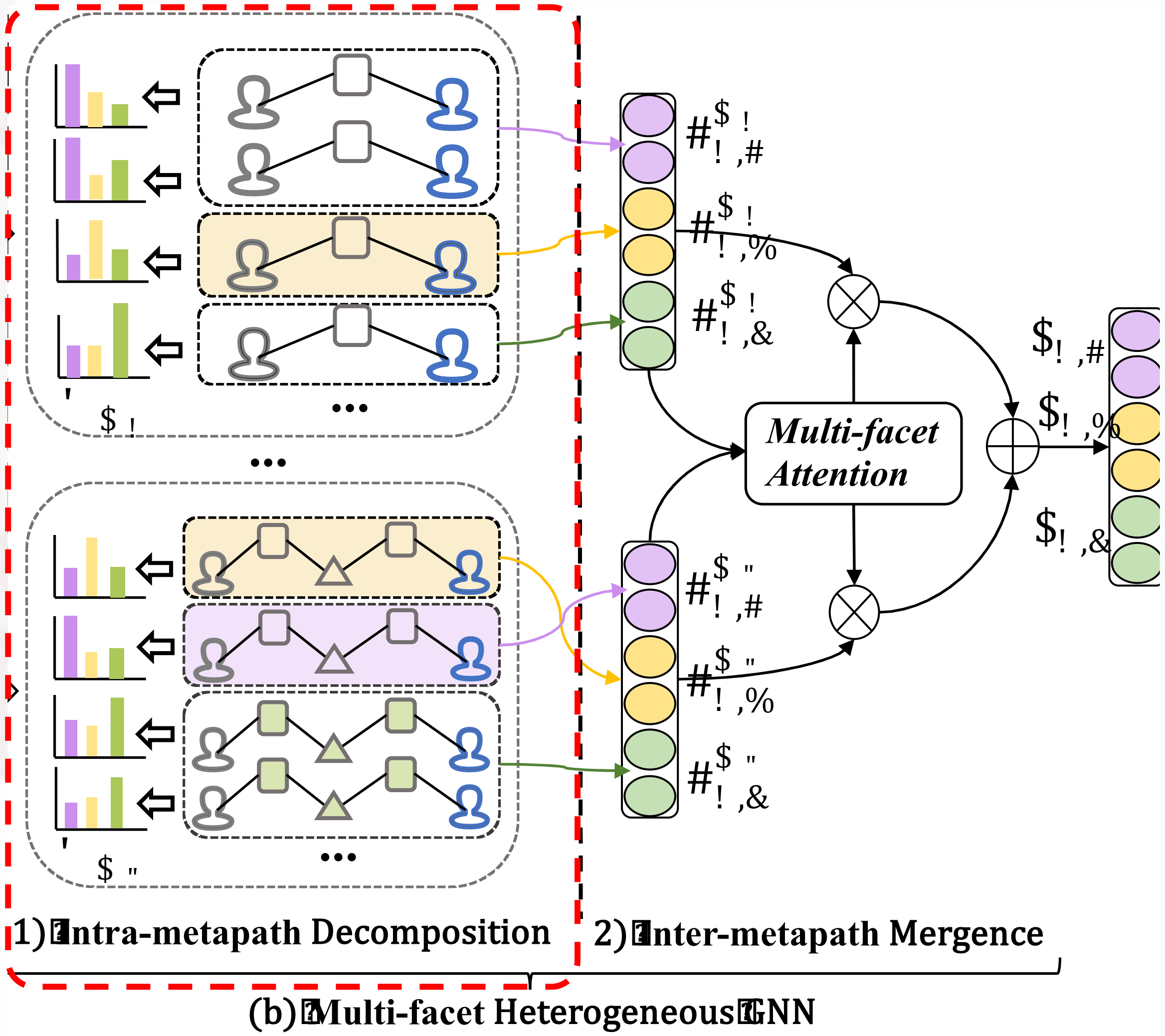
$$p_{k|c_u} = \frac{\exp(\cos(\mathbf{h}_{u,k}, \mathbf{h}_{u,k}^{c_u}))}{\sum_{k'=1}^{K} \exp(\cos(\mathbf{h}_{u,k'}, \mathbf{h}_{u,k'}^{c_u}))},$$

$$\mathbf{h}_{u,k}^{M_i} = L2\_Norm(\sum_{c \in C_u^{M_i}} p_{k|c_u} \cdot \mathbf{h}_{u,k}^{c_u}),$$

the set of selected metapaths: $\mathcal{M} = (M_1, M_2, \cdots, M_P)$ for u,

It generates P groups of metapath-specific multi-facet topic-aware representations for u, denoted as:

$$\{[\mathbf{h}_{u,1}^{M_1}, \mathbf{h}_{u,2}^{M_1}, \cdots, \mathbf{h}_{u,K}^{M_1}], [\mathbf{h}_{u,1}^{M_2}, \mathbf{h}_{u,2}^{M_2}, \cdots, \mathbf{h}_{u,K}^{M_2}], \cdots, [\mathbf{h}_{u,1}^{M_P}, \mathbf{h}_{u,2}^{M_P}, \cdots, \mathbf{h}_{u,K}^{M_P}]\}.$$



Multi-facet Heterogeneous Graph Neural Network

- Inter-metapath Mergence. (step 2)

$$\mathbf{s}_k^{M_i} = \frac{1}{|B|}\sum_{u\in B}\tanh(\mathbf{W}\cdot\sigma(\mathbf{h}_{u,k}^{M_i})),$$

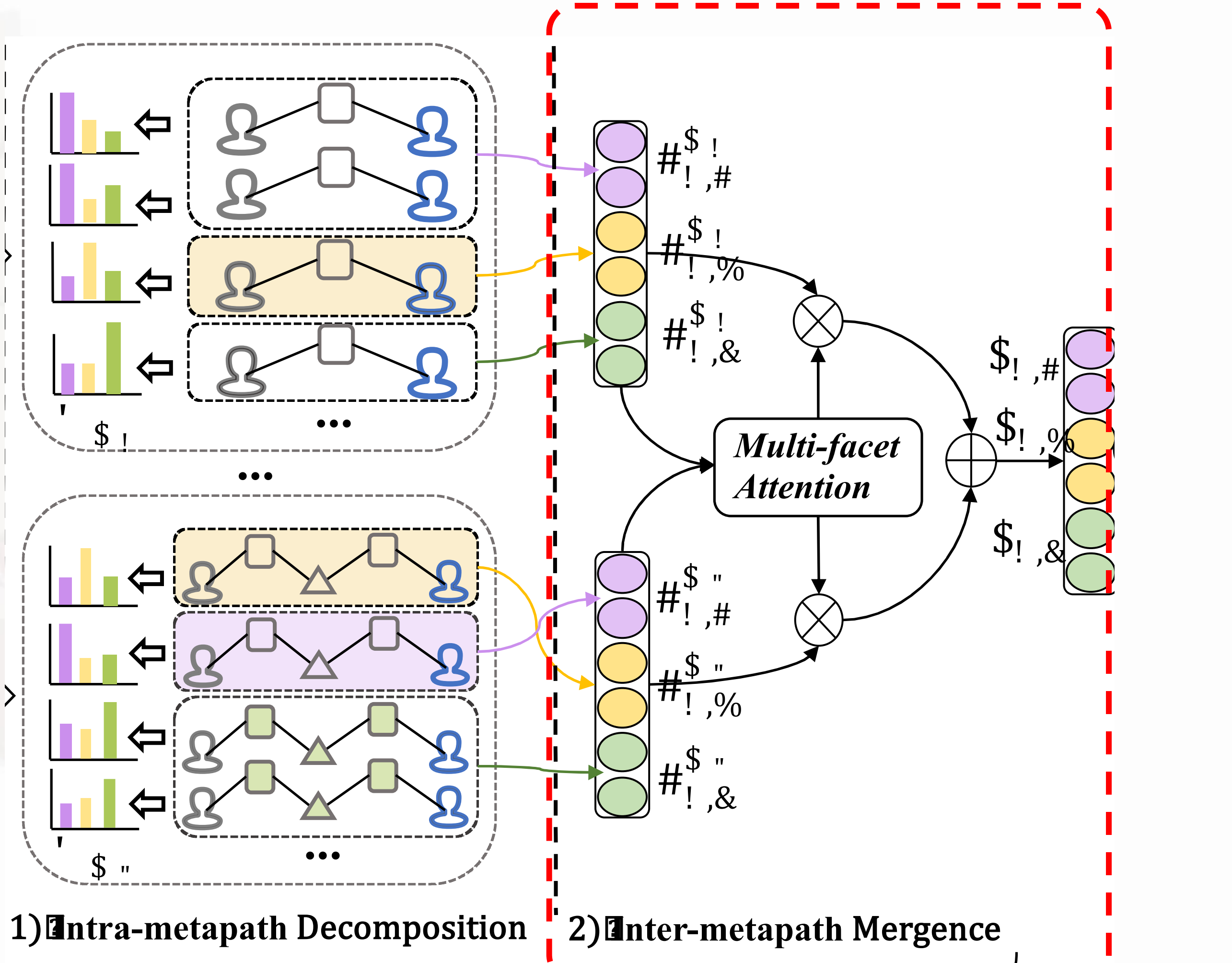
$$e^{M_i} = \sum_{k=1}^{K}\mathbf{q}_k^T\cdot\mathbf{s}_k^{M_i},$$

$$\beta^{M_i} = \frac{\exp(e^{M_i})}{\sum_{M\in\mathcal{M}}\exp(e^{M})},$$

$$\hat{\mathbf{h}}_{u,k} = \sum_{M_i\in\mathcal{M}}\beta^{M_i}\cdot\mathbf{h}_{u,k}^{M_i},$$

$$\mathbf{z}_{u,k} = \sigma(\hat{\mathbf{h}}_{u,k}^{(T)})$$

For a text-related node v, let $\mathbf{z}_{v,k} = \sigma(\mathbf{h}_{v,k})$ without any iteration



(b) Multi-facet Heterogeneous GNN

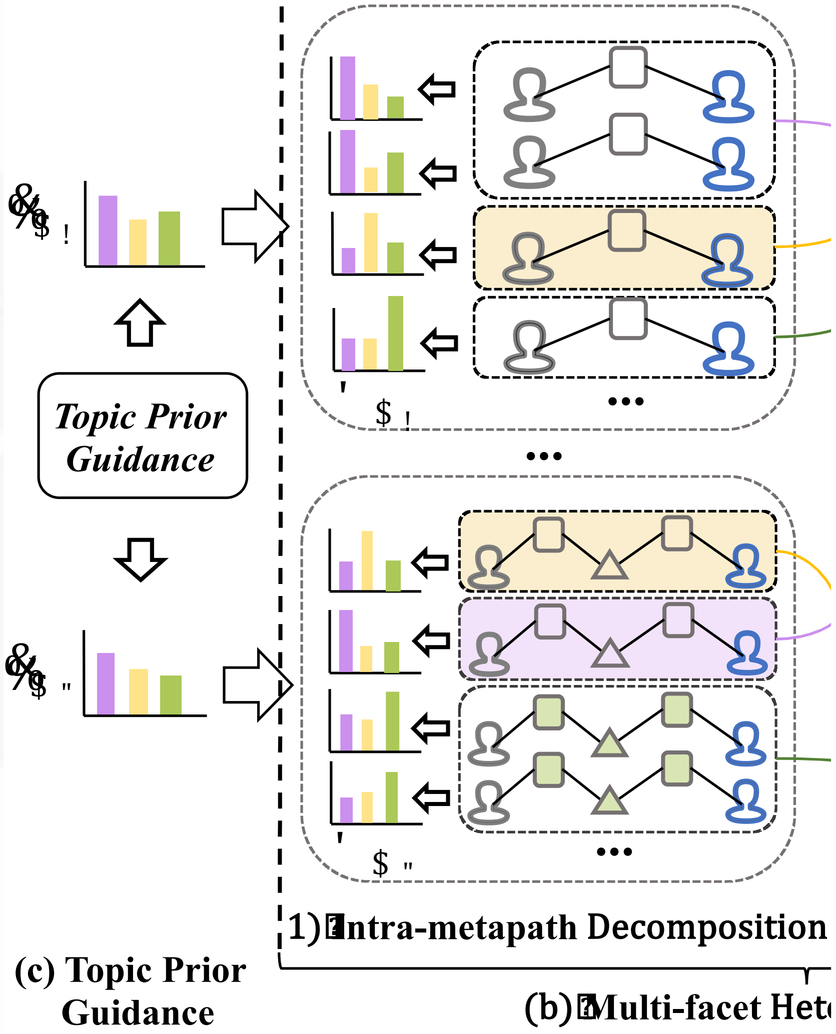
Topic Prior Guidance

- There might be still confounding among different topic-aware subspaces.

- It's difficult to capture global knowledge from K potential topic-aware subspaces we assume.

$$\mathcal{L}_T = \frac{1}{|\mathcal{M}|}\sum_{M_i \in \mathcal{M}} \left\| \frac{\Phi_{M_i}^T \Phi_{M_i}}{\| \Phi_{M_i}^T \Phi_{M_i} \|_F} - \frac{\bar{\lambda}_{M_i}}{\| \bar{\lambda}_{M_i} \|_F} \right\|_F,$$

$$\bar{\lambda}_{M_i} = \frac{1}{|C^{M_i}|}\sum_{c \in C^{M_i}} \lambda_{d_1}^{c},$$



Model Training

- We estimate the similarity for a training pair (u, v) through $s_{uv} = \sum_{k=1}^{K} \mathbf{z}_{u,k}^{T} \cdot \mathbf{z}_{v,k}$,
- The loss of graph reconstruction in two major learning paradigms:
  - Only one node with multi-facet factors in training pair (u,v): assuming that u is the only node with multi-facet factors , then

$$\mathcal{L}_{G,\mathcal{B}} = -\sum_{(u,v)\in\mathcal{B}^+} \log\sigma(s_{uv}) - \sum_{(u,v')\in\mathcal{B}^-} \log\sigma(-s_{uv'}),$$

  - Both are nodes with multi-facet factors in training pair (u,v):

$$\mathcal{L}_{G,\mathcal{B}} = -\sum_{(u,v)\in\mathcal{B}^+} \log\sigma(\frac{1}{K}s_{uv}) - \sum_{(u',v')\in\mathcal{B}^-} \log\sigma(-\frac{1}{K}s_{u'v'}),$$

- The overall training loss:

$$\mathcal{L}_{\mathcal{B}} = \mathcal{L}_{G,\mathcal{B}} + \gamma\mathcal{L}_{T}.$$

CONTENTS

- Q1: How does THGNN perform in link prediction task compared with state-of-the-art methods?
- Q2: How does topic prior guidance affect the result of THGNN?
- Q3: Can THGNN capture multi-facet topic-aware semantics?

Datasets

Dataset	Relation (A-B)	#A	#B	#A-B
DBLP	Paper-Author	11,248	11,569	32,534
	Paper-Conference	11,248	16	11,248
	Paper-Term	11,248	2,463	65,818
YELP	Business-User	2,203	1,430	27,793
	Business-City	2,203	66	2,157
	Business-Category	2,203	347	9,787
Amazon	Movie-User	1,754	2,476	34,042
	Movie-Brand	1,754	293	734
	Movie-Category	1,754	95	4,913

Table 2: The performance comparison of link prediction. The underlined means the best performance in baselines.

Models	DBLP (A-P) AUC	DBLP (A-P) AP	DBLP (A-A) AUC	DBLP (A-A) AP	YELP (U-B) AUC	YELP (U-B) AP	Amazon (U-M) AUC	Amazon (U-M) AP
DeepWalk	0.7754	0.7782	0.7488	0.7568	0.6200	0.6281	0.7684	0.7840
Mp2vec	0.7213	0.7243	0.7600	0.7484	0.6792	0.6872	0.7812	0.7834
HERec	0.8186	0.7927	0.7565	0.7871	0.8383	0.8215	0.8085	0.8083
GraphSage	0.8218	0.8341	0.8524	0.8817	0.8874	0.8810	0.8236	0.8327
GAT	0.8322	0.8367	0.8579	0.8805	0.8915	0.8847	0.8329	0.8343
DisenGCN	0.8301	0.8352	0.8692	0.8936	0.8957	0.8838	<u>0.8435</u>	0.8390
HAN	0.8535	0.8719	0.8744	<u>0.9046</u>	0.9013	0.8722	0.8418	0.8414
DisenHAN	0.8496	0.8654	<u>0.8868</u>	0.8947	0.8976	0.8843	0.8426	<u>0.8419</u>
MAGNN	<u>0.8543</u>	<u>0.8727</u>	0.8671	0.9035	<u>0.9123</u>	<u>0.8926</u>	0.8378	0.8278
$\text{THGNN}_{\backslash MA}$	0.8546	0.8683	0.8712	0.8939	0.9154	0.8945	0.8578	0.8502
THGNN	**0.8807**	**0.9000**	**0.8996**	**0.9174**	**0.9243**	**0.9037**	**0.8634**	**0.8515**

- Our model consistently performs better than all baselines on three datasets.
- It indicates the effectiveness of both structural and topic-aware semantics.

Analysis of Topic Prior Guidance (Q2)

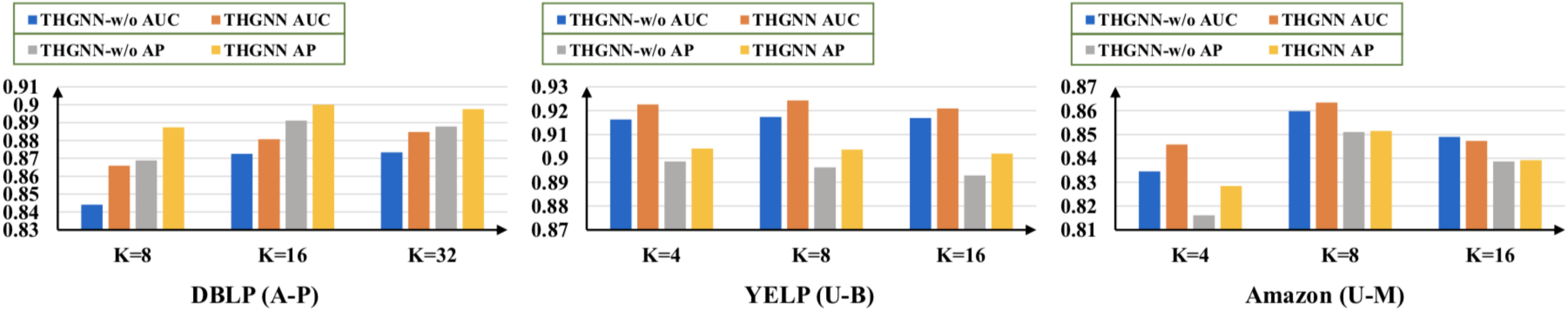
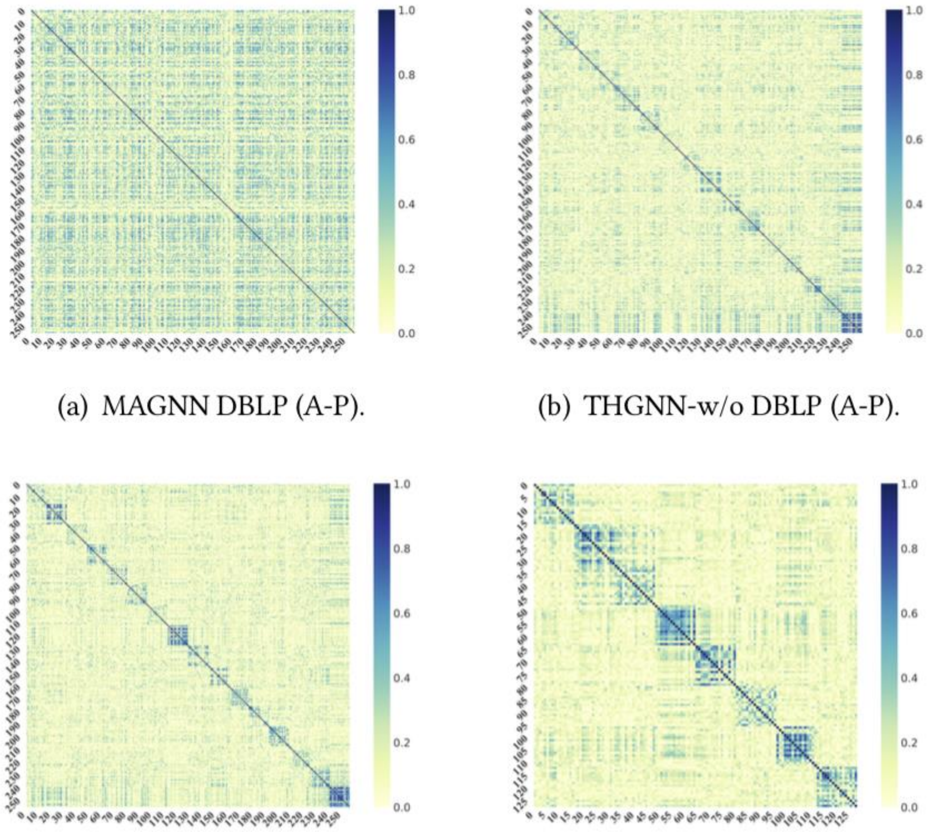


Figure 3: Effect of the topic prior guidance module. THGNN-w/o means THGNN without topic prior guidance.

Multi-facet Embedding Visualization (Q3)



(a) MAGNN DBLP (A-P). (b) THGNN-w/o DBLP (A-P).

(c) THGNN DBLP (A-P). (d) THGNN Amazon (U-M).

Figure 4: The magnitude of the correlations between the elements of the 256-dimensional representations for DBLP (A-P), and 128-dimensional representations for Amazon (U-B).

- The topic prior guidance plays an important role on giving more orthogonality and keeping the quality of multi-facet topic-aware embeddings.

CONTENTS

- We proposed to identify and reason multi-facet topic-aware factors underlying the bare connections between associated nodes, by taking advantage of both heterogeneous structures and unstructured text content in HGs;
- We proposed a novel framework THGNN for link prediction to distinctively aggregate rich heterogeneous information according to the inferential multi-facet topic-aware factors ;
- We incorporated a topic prior guidance module, which aims to leverage global knowledge from unstructured text content, to further improving the quality of multi-facet topic-aware embeddings；
- Experiments show that the learned multi-facet topic-aware node embeddings are more predictive and interpretable.

Thank you !

More materials in http://shichuan.org