Heterogeneous Graph Attention Network

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Abstract

Abstract

- Heterogeneous graph
  - Contains different types of nodes and links(=edges)
  - Has not been considered. But so important.
- Challenges
  - Heterogeneity
  - Semantic information
- Recently, the most exciting mechanism: Attention mechanism
- 따라서 hierarchical attention에 기반한 novel heterogeneous GNN 소개
  - Node level과 semantic level attention 모두 포함하는 network
  - Node level = meta-path based neighbors의 중요도를 학습
  - Semantic level = meta-paths의 차이점을 학습
- 우리가 제안한 모델은 heterogeneous graph에서 뛰어난 성능 뿐만 아니라 그래프 분석에 있어 해석 가능성의 잠재력을 보여준다.

Introduction

Introduction

- Attention mechanism
  - Deals with variable sized data(가변량 데이터를 다룸)
  - Focus on the most salient parts of data(데이터의 가장 두드러진 부분에 집중)
  - 따라서 다양한 applications에 적용

- Meta-path?
  - a composite relation connecting two objects
  - to capture the semantics.

- Meta-path 예시
  - Movie, Actor, Director의 관계(=links, edges)를 설명해보자.
  - 두 영화에 동일한 배우가 출연했다면 Movie-Actor-Movie로 관계를 표현할 수 있다.
  - 그렇다면 Movie-Director-Movie 관계는 무엇을 의미할까?
  - 두 영화를 같은 감독이 제작했다는 것을 알 수 있다.
  - 따라서 다른 의미를 가질 수 있는 edges를 meta-path라고 정의한다.

Introduction

- 주요 challenge : heterogeneity
  - Actor node has age, sex, and nationality features.
  - Movie node has story and actors features.

- How to handle such complex structural information ?

Introduction

❑ Node-level attention

- aims to learn the importance of meta-path "based neighbors" and assign different attention values to them.
- Meta-path로 생성된 neighbors 중 유익한 neighbors를 구분할 수 있어야 한다.
- 예시) Movie-Director-Movie, Movie-Director-Movie 라는 두 meta-path 존재 (same director)
  - 따라서 만약 두 영화가 타이타닉과 터미네이터라면, 같은 감독이 제작했기 때문에 edges 형성.
  - 하지만 목적이 터미네이터2 영화 장르 구분이라면, 타이타닉보단 터미네이터가 더 큰 weight(=attention values)를 가져야 한다.

❑ Semantic-level attention

- aims to learn the importance of each "meta-path" and assign proper weights to them
- 예시) 두 영화가 존재(node), 두 영화 모두 주연배우가 동일 & 동일한 년도에 제작됨.
  - 따라서 두 영화의 관계는 (Movie-Actor-Movie) 이나 (Movie-Year-Movie) 의 meta-paths에 의해 설명될 수 있다.
  - 하지만 목적이 영화의 장르 구분이라면 제작년도 보다는 출연한 배우가 조금 더 중요한 가중치를 가진다. 따라서 Movie-Actor-Movie meta path가 더 큰 weights를 가져야한다.

Introduction

❑ 학습방법

- Input : node features
- Type-specific transformation matrix를 사용하여 same space에 project
- Node-level attention 진행(attention values 학습. Neighbors를 기반으로)
- Semantic-level attention 진행(attention values 학습. Different math-path 기반)
- 최적화 진행 및 backpropagation 진행

❑ Brief conclusion:

- heterogeneous graph를 다루고, variable data size를 다룰 때 node feature data가 있다면 해당 모델 사용가능!
- 다만 사전 정의된 node type이 있어야하고, 해당 type에 맞는 type-specific transformation matrix가 필요함.

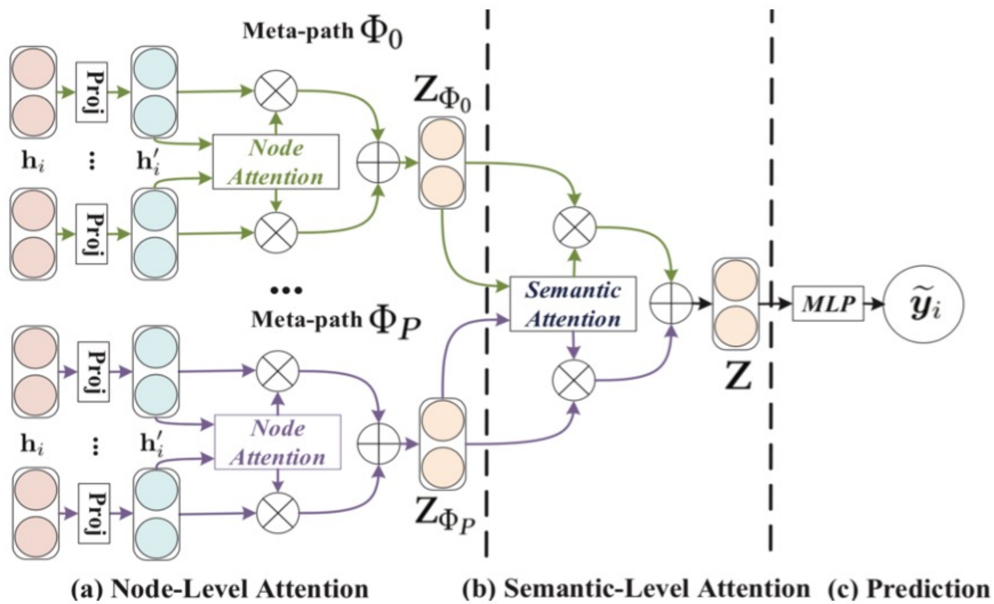
PRELIMINARY

Notations

- Heterogeneous Graph
  - $G = (V, E), V = \ object\ set, E = \ link\ set$
  - $\varphi : mapping\ function, node\ to\ predefined\ node\ type$
    - $\varphi : V \ \rightarrow \ \mathcal{A}\ , \mathcal{A} = predefined\ node\ type$
  - $\psi : mapping\ function, link\ to\ predefined\ link\ type$
    - $\psi : E \ \rightarrow \ \mathcal{R}\ , \mathcal{R} = \text{predefined link type}$
- Meta-path(Φ)
  - $\Phi : A_1 \xrightarrow{R_1} A_2 \xrightarrow{R_2} \dots \xrightarrow{R_n} A_n$ 와 같은 하나의 path를 의미(not edge, link), A는 object
  - Different meta-paths always reveal different semantics
- Meta-path based neighbors(N_i^{Φ})
  - $Given\ node\ i, meta\ path\ \Phi \ \rightarrow \ N_i^{\Phi}$
  - Set of nodes which connect with node i via meta-path Φ (includes itself)

4. PROPOSED MODEL

❑ The overall framework of the proposed model



h_i : $input(= node\ feature)$

h_i' : $projected\ node\ feature$

- Node level attention : Meta-path based neighbors의 weight를 학습
  - Output으로 semantic-specific node embedding을 얻음.
- Semantic-level attention : task에 최적화된 node embedding 조합을 얻을 수 있음.
  - Meta-paths의 차이점을 알아낼 수 있다.(semantic-level)

4.1 Node-level Attention

Node-level Attention

- Goal:
  - Meta-path based neighbors가 특정 task에 따라 다른 중요성을 가짐을 알아내는 것

- Challenge:
  - Different type of nodes have different feature spaces.
  - Solution: use type-specific transformation matrix(M_{ϕ_i})
    - Project the features of different types of nodes into the same feature space.
    - $h_i' = M_{\phi_i} * h_i$

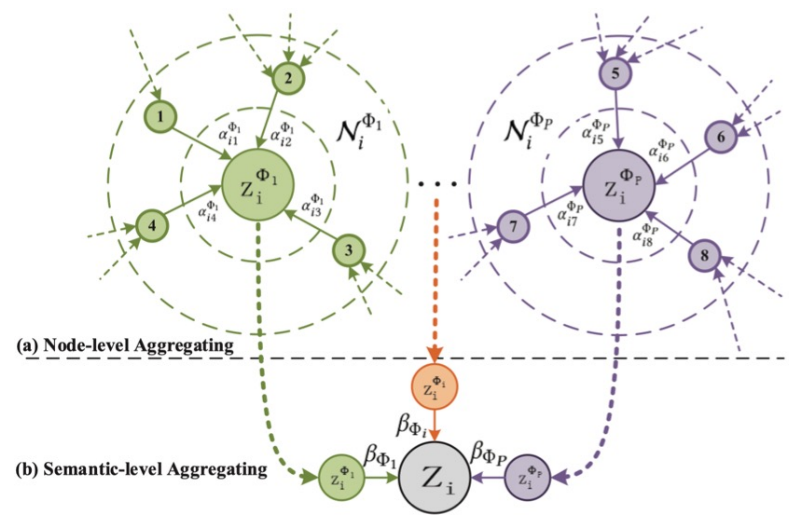
- 모든 feature가 same space에 존재하도록 project 후, importance($e_{i,j}^{\Phi}$) 학습
  - $e_{i,j}^{\Phi}$: meta-path Φ 로 연결된 두 object(=node i,j)의 importance
  - 즉 node i에 대해 node j 가 미치는 영향력.
  - $e_{i,j}^{\Phi}$ = $att_{node}(h_i', h_j'; \Phi)$
  - Asymmetric(node i에 node j가 미치는 영향력은 j 에 i가 미치는 영향력과는 다르다)
    - Critical property of heterogeneous graph

Node-level Attention

- Normalize $e_{i,j}^{\Phi}$ by softmax function
  - $\alpha_{i,j}^{\Phi} = softmax(e_{i,j}^{\Phi})$
  - Asymmetric.

- Generate embedding node i (z_i^{Φ})
  - $z_i^{\Phi} = \sigma(\sum_{j \in N_i^{\Phi}} \alpha_{i,j}^{\Phi} * h_j')$
  - z_i^{Φ} 는 node i의 $n$eighbors(node j)의 noramlize된 importance$(\alpha_{i,j}^{\Phi})$를 aggregate.

Heterogeneous Graph Attention Network



이때 $\alpha_{i,j}^{\Phi}$는 generated by single meta − path. 따라서 semantic information 포함

4.2. Semantic-level Attention

Semantic-level Attention

- Challenge:
  - Heterogeneous graph contains multiple types of semantic information.

- Goal:
  - To learn a more comprehensive node embedding.
  - Solution: use meta-paths & novel semantic-level attention

- $\left(\beta_{\Phi_1}, \ldots, \beta_{\Phi_p}\right) = att_{sem}(Z_{\Phi_1}, \ldots, Z_{\Phi_p})$
  - Z_{Φ_1} : node embedding(Z) p개
  - att_{sem} : semantic-level attention score를 계산하는 deep neural network
  - β_{Φ_1} : learned weights of each meta-path

Semantic-level Attention

- MLP와 같은 transformation을 이용하여 semantic-specific embedding으로 변형
  - semantic-level attention Vector(q)를 사용하여 embedding끼리의 similarity 계산
  - 이는 곧 특정 embedding의 중요도(= 높은 similarity)

- 이후 embedding similarity의 average 계산.
  - Each meta-path importance를 설명하기 위해 비교하는 기준점(=average)으로 활용

- 이후 구한 each meta-path importance를 normalize 진행(via softmax function)
  - 이는 곧, 각 특정 task에 대해 meta-path의 기여도(=importance)이다.
  - Task에 따라 해당 importance는 다르게 계산될 수 있다.

- Final embedding(Z)
  - $Z = \sum_{p=1}^{P} \beta_{\Phi_p} * Z_{\Phi_p}$, node embedding(Z_{Φ_p})에 각 meta-path의 importance(β_{Φ_p}) aggregate

- 결과적으로 node i 에 대한 node j(neighbors)의 importance와, 각 meta-path의 importance의 정보가 포함된 embedding 생성.

Semantic-level Attention

- Loss function은 task마다 다르게 정의
  - 본 예시에서는 node classification에서 minimize the cross-entropy 사용.

- 학습은 semi-supervised learning으로 labeled data를 사용하여 back propagation 진행.

4.3. Analysis of the Proposed Model

Analysis of the Proposed Model

- Benefit:
  - 다양한 유형의 node embedding으로 상호 통합 혹은 상호 향상이 될 수 있다.
  - Highly efficient and can be easily parallelized.
    - Attention 연산은 모든 node 혹은 meta-path에서 개별적으로 수행 가능
  - Type-specific matrix shared parameters for the whole heterogeneous graph
    - Parameter 수가 graph scale에 의존하지 않음.
  - good interpretability
    - Meta-path based neighbors
    - Meta-path importance 표현
    - Large value = more important for our task

5. EXPERIMENTS

EXPERIMENTS

❑ Datasets

- 1. DBLP
  - Node : papers(P), authors(A), conferences(C), terms(T)
    - Authors are divided into fours area : database, data mining, machine learning, information retrieval
    - Hence, meta-path set : APA, APCPA, APTPA
- 2. ACM
  - Node : papers(P), authors(A) and subjects(S)
    - Papers are divided into three class : database, wireless communication, data mining
    - Hence, meta-path set : PAP, PSP
- 3. IMDB

❑ Compare with baselines

- 동일한 datasets에 대해 본 논문에서 소개한 모델과 기존 방법들을 비교

EXPERIMENTS

❑ Compare with baselines (fair comparison : embedding dim(=64))

Table 3: Qantitative results (%) on the node classification task.

Datasets	Metrics	Training	DeepWalk	ESim	metapath2vec	HERec	GCN	GAT	HAN_{nd}	HAN_{sem}	HAN
ACM	Macro-F1	20%	77.25	77.32	65.09	66.17	86.81	86.23	88.15	89.04	**89.40**
		40%	80.47	80.12	69.93	70.89	87.68	87.04	88.41	89.41	**89.79**
		60%	82.55	82.44	71.47	72.38	88.10	87.56	87.91	**90.00**	89.51
		80%	84.17	83.00	73.81	73.92	88.29	87.33	88.48	90.17	**90.63**
	Micro-F1	20%	76.92	76.89	65.00	66.03	86.77	86.01	87.99	88.85	**89.22**
		40%	79.99	79.70	69.75	70.73	87.64	86.79	88.31	89.27	**89.64**
		60%	82.11	82.02	71.29	72.24	88.12	87.40	87.68	**89.85**	89.33
		80%	83.88	82.89	73.69	73.84	88.35	87.11	88.26	89.95	**90.54**
DBLP	Macro-F1	20%	77.43	91.64	90.16	91.68	90.79	90.97	91.17	92.03	**92.24**
		40%	81.02	92.04	90.82	92.16	91.48	91.20	91.46	92.08	**92.40**
		60%	83.67	92.44	91.32	92.80	91.89	90.80	91.78	92.38	**92.80**
		80%	84.81	92.53	91.89	92.34	92.38	91.73	91.80	92.53	**93.08**
	Micro-F1	20%	79.37	92.73	91.53	92.69	91.71	91.96	92.05	92.99	**93.11**
		40%	82.73	93.07	92.03	93.18	92.31	92.16	92.38	93.00	**93.30**
		60%	85.27	93.39	92.48	93.70	92.62	91.84	92.69	93.31	**93.70**
		80%	86.26	93.44	92.80	93.27	93.09	92.55	92.69	93.29	**93.99**
IMDB	Macro-F1	20%	40.72	32.10	41.16	41.65	45.73	49.44	49.78	**50.87**	50.00
		40%	45.19	31.94	44.22	43.86	48.01	50.64	52.11	50.85	**52.71**
		60%	48.13	31.68	45.11	46.27	49.15	51.90	51.73	52.09	**54.24**
		80%	50.35	32.06	45.15	47.64	51.81	52.99	52.66	51.60	**54.38**
	Micro-F1	20%	46.38	35.28	45.65	45.81	49.78	55.28	54.17	55.01	**55.73**
		40%	49.99	35.47	48.24	47.59	51.71	55.91	56.39	55.15	**57.97**
		60%	52.21	35.64	49.09	49.88	52.29	56.44	56.09	56.66	**58.32**
		80%	54.33	35.59	48.81	50.99	54.61	56.97	56.38	56.49	**58.51**

GAT : 기존 homogeneous graph를 위해 제작된 model
HAN : 본 논문에서 소개한 heterogeneous graph를 위한 GAT 모델

EXPERIMENTS

- Details for HAN
  - Initialize parameters and optimize : Adam
  - Learning rate : 0.005
  - The dimension of the semantic-level attention vector : 128
  - Number of attention head : 8
  - Dropout of attention : 0.6
  - Early stopping patience : 100
    - Validation loss doesn't decrease

- GCN, GAT, HAN : same training set, validation set and test set

- DeepWalk, Esim, metapath2vec and HERec (based random walk based methods)
  - Window size : 5
  - Walk length : 100
  - Walks per node : 40
  - Number of negative samples : 5

EXPERIMENTS

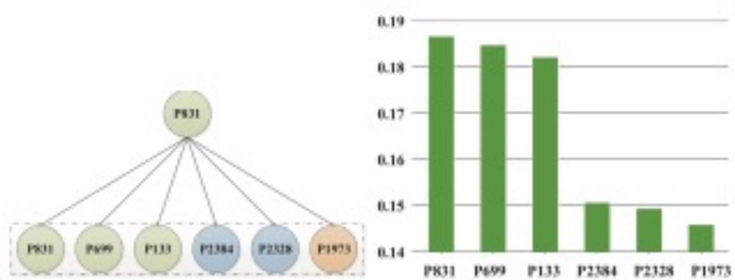
❑ Clustering

Table 4: Qantitative results (%) on the node clustering task.

Datasets	Metrics	DeepWalk	ESim	metapath2vec	HERec	GCN	GAT	HAN_{nd}	HAN_{sem}	HAN
ACM	NMI	41.61	39.14	21.22	40.70	51.40	57.29	60.99	61.05	**61.56**
	ARI	35.10	34.32	21.00	37.13	53.01	60.43	61.48	59.45	**64.39**
DBLP	NMI	76.53	66.32	74.30	76.73	75.01	71.50	75.30	77.31	**79.12**
	ARI	81.35	68.31	78.50	80.98	80.49	77.26	81.46	83.46	**84.76**
IMDB	NMI	1.45	0.55	1.20	1.20	5.45	8.45	9.16	10.31	**10.87**
	ARI	2.15	0.10	1.70	1.65	4.40	7.46	7.98	9.51	**10.01**

- 역시나 기존 다른 방법들보다 성능이 뛰어남을 확인할 수 있다.

❑ Example of ACM



(a) Meta-path based neighbors of P831 (b) Attention values of P831's neighbors

Figure 4: Meta-path based neighbors of node P831 and corresponding attention values (Different colors mean different classes, e.g., *green* means Data Mining, *blue* means Database, *orange* means Wireless Communication).

-> Good interpretability

EXPERIMENTS

❑ Analysis of Hierarchical Attention Mechanism

- 1. Analysis of node-level attention
  - Large attention values = important neighbors for the specific task

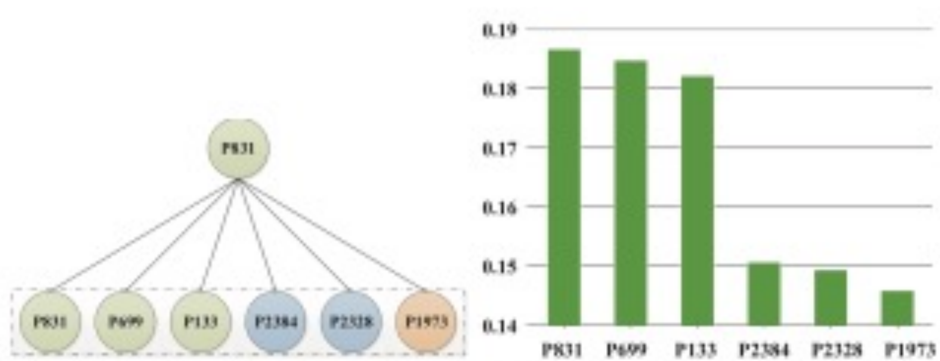


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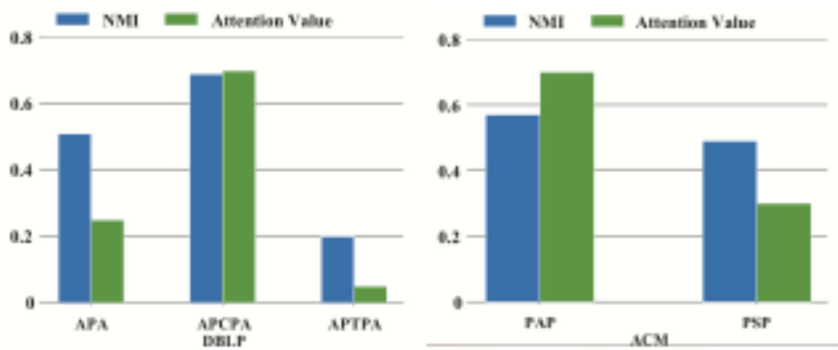
Figure 4: Meta-path based neighbors of node P831 and corresponding attention values (Different colors mean different classes, e.g., *green* means Data Mining, *blue* means Database, *orange* means Wireless Communication).

- PAP meta-path가 주어졌을 때
- Measure attention values(P831 이웃 nodes)
- Itself attention value를 제외하면 P699, P133
  - Green color(=Data mining)
- 두 paper를 모두 제작한 author 라는 meta-path에 based neighbors의 중요도는 당연히 비슷한 장르(Data mining)의 이웃 노드 P699, P133이 높은 importance를 가진다.

EXPERIMENTS

❑ Analysis of Hierarchical Attention Mechanism

- 2. Analysis of semantic-level attention.



(a) NMI values on DBLP (b) NMI values on ACM

Figure 5: Performance of single meta-path and corresponding attention value.

- NMI 는 clustering 결과
- Attention value는 meta-path의 importance
- Task in DBLP : author's research area
  - APCPA meta-path is most important
  - C(conference)

EXPERIMENTS

- Visualization

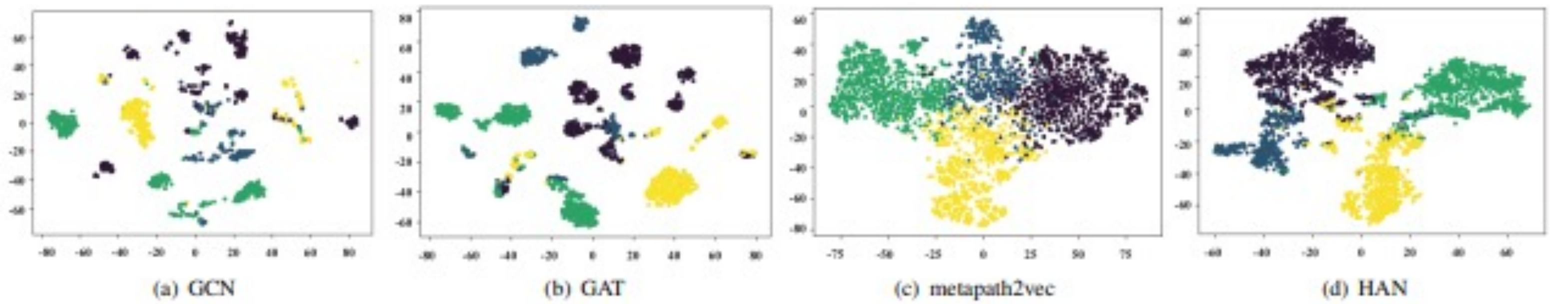
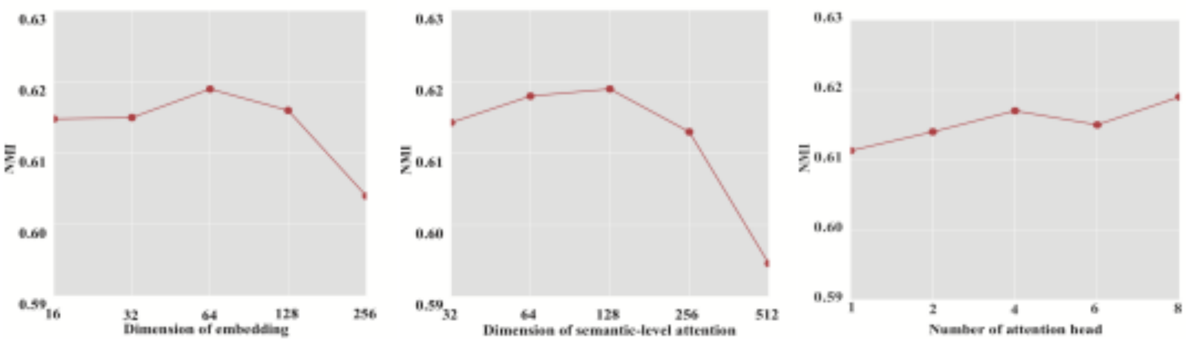


Figure 6: Visualization embedding on DBLP. Each point indicates one author and its color indicates the research area.

EXPERIMENTS

Y축 : NMI
= results of clustering



(a) Dimension of the final embedding **Z** (b) Dimension of the semantic-level attention vector **q** (c) Number of attention head K.

Figure 7: Parameter sensitivity of HAN w.r.t. Dimension of the final embedding Z, Dimension of the semantic-level attention vector q and Number of attention head K.

❑ Parameters Experiments

- Dimension of the final embedding Z(=64)
  - HAN needs a suitable dimension to encode the semantics information
  - Larger dimension may introduce additional redundancies
- Dimension of semantic-level attention vector(=128)
  - Test various dimension. The result is 128.
- Number of attention head(K)
  - Change of performance is slightly

6. CONCLUSION

CONCLUSION

- In this paper, propose heterogeneous GNN based on attention network(HAN)
- HAN can capture complex structures and rich semantics
- 계층구조. Node-level attention -> semantic-level attention
- Experimental results :
  - Classification good
  - Clustering good
- HAN has good interpretability
- **Heterogeneous graph & variable data size -> HAN**
  - **Then, we need type-specific transformation matrix**

Thank you