# SynHIN: Generating Synthetic Heterogeneous Information Network for Explainable AI

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#### **Abstract**

Graph Neural Networks (GNNs) excel in various domains, from detecting e-commerce spam to social network classification problems. However, the lack of public graph datasets hampers research progress, particularly in heterogeneous information networks (HIN). The demand for datasets for fair HIN comparisons is growing due to advancements in GNN interpretation models. In response, we propose SynHIN, a unique method for generating synthetic heterogeneous information networks. SynHIN identifies motifs in real-world datasets, summarizes graph statistics, and constructs a synthetic network. Our approach utilizes In-Cluster and Out-Cluster Merge modules to build the synthetic HIN from primary motif clusters. After In/Our-Cluster mergers and a postpruning process fitting the real dataset constraints, we ensure the synthetic graph statistics align closely with the reference one. SynHIN generates a synthetic heterogeneous graph dataset for node classification tasks, using the primary motif as the explanation ground truth. It can adapt and address the lack of heterogeneous graph datasets and motif ground truths, proving beneficial for assessing heterogeneous graph neural network explainers. We further present a benchmark dataset for future heterogeneous graph explainer model research. Our work marks a significant step towards explainable AI in HGNNs.

#### 1 Introduction

Graph neural networks (GNNs) have demonstrated impressive performance in various domains, such as community analysis (Shchur and Günnemann 2019), chemical bond analysis (Stokes et al. 2020), and recommendation systems (Cui et al. 2020). They effectively address node classification and link prediction challenges within graphs (Chami et al. 2022). However, compared to other machine learning domains like natural language processing (NLP) and computer vision (CV), the available public datasets for GNNs are limited. The scarcity of public datasets is especially noticeable in heterogeneous information network graph datasets, making it more challenging for GNN models to generalize and prone to overfitting due to the small number of available datasets (Palowitch et al. 2022). Many researches have been focused on enhancing the interpretability of GNNs.

They aim to develop methods that provide insights into the decision-making processes of GNNs. These efforts encompass various aspects, such as self-explainable classification models (Dai and Wang 2021) and post-hoc interpretation techniques (Ying et al. 2019; Luo et al. 2020; Lin et al. 2022). However, one of the significant obstacles in investigating interpretable GNNs is the need for datasets with explanatory ground truths. Furthermore, a limited amount of real datasets with similar structures and attributes lack diverse features, potentially causing overfitting and biased results in research and hindering progress in this field, as mentioned by Lin et al. (Lin et al. 2022). Simulating real datasets proves beneficial to surmount these challenges and enhance interpretable GNNs. An effective synthetic dataset should mirror vital attributes of the actual data, including graph size, edge distribution, node features, and label dispersion. Essential ground truth explanations, like primary motifs, should also be included. The current synthetic dataset generation method (Ling, Yang, and Zhao 2021) demands substantial human involvement. Therefore, an automated process is highly desirable for scalability, offering an efficient approach to generating datasets. In light of the above issues, we develop a novel approach to generate synthetic graphs. We extract primary motifs from real-world datasets and apply a *Merge* strategy, creating clusters with explanatory ground truths and combining meaningful clusters into a full synthetic heterogeneous graph dataset as benchmark datasets for future explanatory models. Our main contributions are summarized as follows:

- We proposed SynHIN with a novel approach of *In-Cluster Merge* and *Out-Cluster Merge* for generating synthetic heterogeneous graph datasets. It closely emulates heterogeneous real-world graph structures and characteristics, enabling realistic synthetic generation.
- We are the first to generate heterogeneous graphs with explanatory ground truths and devise benchmark datasets for heterogeneous GNN explainers to the best of our knowledge.
- We provide a modularized synthetic graph dataset generation framework, including motif extraction, subgraph building, In-Cluster Merge, Out-Cluster Merge, and pruning. Each module can be substituted or expanded according to the requirements.

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## 2 Related Work

# **Synthetic Graph Generation**

There are some existing tools to generate graph datasets artificially. Snijders et al. (Snijders and Nowicki 1997) proposed to generate a graph edge between two nodes based on the clusters they belong. Other approaches involve extracting subgraphs from real-world graphs and using them as predefined graphs to evaluate the capability of graph neural networks in identifying specific substructures within random Stochastic Block Model (SBM) graphs (Dwivedi et al. 2020). SBM is one of the most popular methods used to generate clustering (Snijders and Nowicki 1997). The concept of SBM is to maintain a high correlation between nodes with the same pre-marked label in the graph structure. By considering the characteristics of the graph structure, it generates a graph dataset that aligns with these specifications.

SBM has many variants, including unsupervised (Tsitsulin et al. 2020) and semi-supervised ones (Rozemberczki et al. 2021). GraphWorld (Palowitch et al. 2022) designs these graph dataset benchmark based on the Degree-Corrected Stochastic Block Model (DC-SBM) model (Abbe 2017) and uses different parameter adjustments to design diverse graph datasets. Therefore, different graph neural network classification models can be evaluated clearly and fairly without overfitting a small number of datasets.

Currently, these works all focus on homogeneous graphs, and most synthetic graph methods do not provide the ability for interpretation, lack the ground truths of interpretation, and cannot be easily extended to heterogeneous graphs.

## **Explainer for Graph Neural Networks**

The field of GNN explainable models has seen a burgeoning growth, focusing primarily on node classification and graph classification (Ying et al. 2019; Luo et al. 2020; Yuan et al. 2021; Lin et al. 2022). These models can be divided into inherent self-explanation and post-hoc interpretation. Self-explanatory models, such as ProtGNN (Dai and Wang 2021), use top-K similarity to identify analogous subgraphs contributing to predictions, with these similar subgraphs serving as the explanation itself. On the other hand, post-hoc interpretation models aim to capture significant subgraphs (Luo et al. 2020; Yuan et al. 2021) and key features (Ying et al. 2019), necessitating a further layer of interpretation after the model has been applied. These models utilize a variety of techniques and definitions to isolate subgraphs. For instance, GNNExplainer (Ying et al. 2019) is trained on each instance, generating an output that masks the graph structure as its explanation. It strives to identify the most consequential portions of the node feature simultaneously. Similarly, PGExplainer (Luo et al. 2020) uses mutual information to maximize the similarity between the masked graphs in the prediction results. SubgraphX (Yuan et al. 2021) employs Monte Carlo Tree Search (MCTS) to locate vital subgraphs.

#### **Graph Explanatory Evaluation Issues**

Conventional evaluation of graph explanatory models heavily depended on molecular datasets or artificial community datasets, which were often scarce. Consequently, overfitting

was a common occurrence in these datasets. Datasets like BA-Shape and MUTAG achieved remarkable accuracies exceeding 98% (Luo et al. 2020; Lin et al. 2022), reached a plateau where further improvements are difficult to attain, leading to a loss of generalizability. These synthetic explanatory datasets are composed of artificially defined motifs and random graphs in advance. In BA-Shape, the motif component comprises elements like houses, grids, cycles, and more (Ying et al. 2019). The generation process involves defining the desired motif structure and quantity and generating the random graph portion. Moreover, the motif is randomly connected to the random graph part, with edge addition or removal occurring randomly. Since the graphs generated through this method can be considered random noise, it becomes challenging to distinguish the significant elements from them. As a result, it becomes difficult to define the explanatory ground truths in the graph. Furthermore, only evaluating the motif parts could lead to overestimating the performance of explanatory models.

# 3 Methodology

In this research, we proposed SynHIN, a novel synthetic heterogeneous graph generation approach. We utilize realworld datasets as the reference to extract the primary motif. Then use the proposed Merge technologies to create synthetic heterogeneous graph datasets that mimic real-world ones with primary motifs that serve as the explanatory ground truths, specifically designed for evaluating heterogeneous GNN explainers of node classification. The synthetic heterogeneous datasets generated by SynHIN can relieve the lacking of datasets for explainable AI studies of HINs. This study includes several critical modules, including Motif Extraction, Subgraph Building, In/Out Cluster Merge, and Pruning. The module detail is introduced in the following chapters. For clarity, we use the IMDB <sup>1</sup> heterogeneous graph dataset as a reference dataset to explain our proposed algorithm and implementation details and illustrate the effectiveness of SynHIN. IMDB is a movie dataset with information such as movies, keywords, actors, and directors. The goal is to predict the movie genre tags. The graph schema is shown on the left of Figure 2.

#### **Motif Extraction**

To extract the primary motif as explanatory ground truths, we use the graphlet searching method (Milo et al. 2002) to capture common subgraphs on the real graph. The graphlet model captures the number of occurrences on the IMDB dataset. We organize the most frequently occurring graphlets as follows, G9, G10, G11, and G20. The graphlet notations follow the paper (Milo et al. 2002). Figure 3 shows the shape of the graphlets. The first three shapes, G9: simple straight lines, G10: Y-shape, and G11: crossed shape, are prevalent across the datasets. Therefore we did not use them as primary motifs. However, G20 is a unique graphlet in the dataset, a three 2-hop path with the same node type for start and end (Figure 2). For IMDB, the start and end

<sup>&</sup>lt;sup>1</sup>https://www.kaggle.com/datasets/karrrimba/moviemetadatacsv

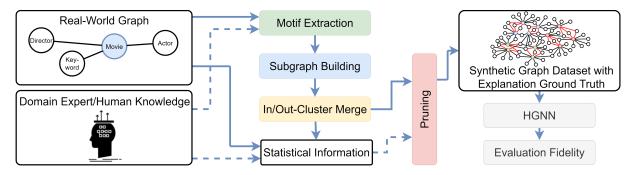


Figure 1: Overall SynHIN Structure

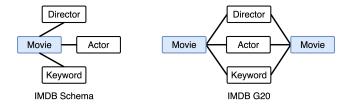


Figure 2: IMDB Schema and a Primary Motif

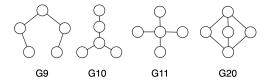


Figure 3: Graphlet G9, G10, G11, and G20

nodes are movies, and the nodes between two movies could be directors, actors, or keywords. G20 would be a stronger connection between two target nodes and more interpretable to humans. Coincidentally, this connection method is consistent with studies based on meta-paths and meta-graphs (Zhang et al. 2020), used to capture the critical paths in the connection between two target nodes. Hence, G20 is especially suitable as an explanatory motif. In practice, to imitate the situation in the real world and increase flexibility for explanatory ground truths. The number of non-target nodes within G20, connections between two target nodes, could be sampled through a Poisson distribution to generate primary motifs.

#### **Subgraph Building**

After designing the primary motifs, we randomly add non-target nodes to the motifs as secondary nodes. Adding these secondary nodes can make the motifs more in line with the real-world target graph because a target node would not only be connected to nodes that are connected to other target nodes. Many non-target nodes might only be connected to one target node in the real-world dataset. Additionally, we leverage the actual degree distribution of target nodes from the real-world reference graph, considering different edge types, as a basis for sampling the number of secondary nodes. These secondary nodes are subsequently introduced

and attached to target nodes. For example, most movies are connected with one director, three actors, and five keywords in the graph. This process results in a subgraph that attaches to the degree distribution of the real-world dataset, ensuring that each target node is connected to a non-target node following the real-world dataset degree distribution.

After adding the secondary node to the primary motif, all the target nodes in subgraphs will be marked with labels. Furthermore, the two target nodes in the same primary motif will be assigned the same label. The subgraphs would be organized into multiple clusters. Motifs in different clusters can be of different labels. In addition to agreeing with the graph datasets, most of the nodes with the same label are strongly connected, and it is also more in line with human interpretation.

#### **Connect or Merge the Subgraphs**

We can observe from the graph schema that HIN has a specific connection structure; not every edge type between two nodes is legal. Suppose we directly applied traditional graph generation methods (BA and SBM) to generate HIN. Illegal connections may appear in the generated graph because the connection method does not provide such a guarantee. Additionally, different edge types on the graph will also have different distributions. It is challenging to determine how to connect the nodes via edges. Moreover, conventional methods for generating homogeneous graphs restrict the ability to apply distinctive processing for different edge types.

To resolve these issues, we approach the problem with a brand-new perspective: we consider the operation of Merge between subgraphs and nodes instead. Specifically, we propose a novel approach wherein two nodes of the same type are merged into a single node. It offers two distinct advantages: Firstly, it ensures all edges generated during the process adhere to the established constraints, thereby maintaining legality. Secondly, it upholds a heterogeneous merge probability/threshold/ratio, effectively emulating the inherent variability in the distribution of different node types in the real-world reference graph. Concurrently, it preserves the intrinsic structure and characteristics of the motif, thereby ensuring a faithful representation of the target dataset. Two types of Merge are described below: In-Cluster Merge and Out-Cluster Merge, where each type has a different use and purpose.

# **In-Cluster Merge**

We perform the In-Cluster Merge (IC Merge) for the subgraphs in the same label. In an IC Merge, we randomly arrange the subgraphs with the same label and merge the subgraphs into the cluster one by one in a greedy manner. When merging, the non-target nodes in the merged subgraphs will be sampled via a uniform distribution probability U(0,1). Only the nodes that are sampled in the process will be merged. Within the sampled nodes, we randomly merge these nodes into the same type of nodes in the cluster. The target node type will not participate in the IC Merge to avoid destroying the structure of the primary motifs. In addition, we avoid merging two motifs with the same label to avoid multiple explanatory ground truths for the same target node. Also, the greedy method allows subgraphs to have different opportunities to be merged. When every time a subgraph merges into a cluster, the subgraphs added earlier in the cluster will have more opportunity to be sampled to become the merged object; This mimics the 'Superstar' phenomenon, which is common in actual community graphs (Abbe 2017; Albert and Barabási 2002).

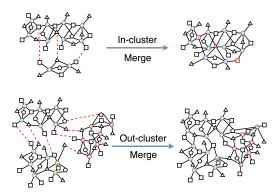


Figure 4: In and Out-Cluster Merges

## **Out-Cluster Merge**

In contrast to the IC Merge method, we employ a distinct approach for Out-Cluster Merge (OC Merge) in different labels, considering the different characteristics of merging between clusters. If we still use the greedy method of IC Merge for OC Merge, some clusters that join the graph first will have more chances to merge, making the clusters easier to connect with others. The clusters that join later are less likely to be closely connected with others. The 'Superstar' phenomenon should not be observed in out-cluster behaviors. In the actual graph, connections between clusters of different labels generally have a more uniform distribution. Therefore, we adopt a one-time method approach to OC Merge. Our approach carefully segregates all nodes based on their type, creating distinct clusters. Subsequently, a probability of merging is computed for each pair of nodes from different clusters,

$$M \sim \mathcal{U}(0,1),\tag{1}$$

where M represents a symmetric  $N \times N$  matrix, and N corresponds to the total number of nodes in a node type. The

element in the i-th row and j-th column of matrix M signifies the probability of a OC Merge operation between node i and node j. In our OC Merge step, we ensure that node pairs originating from the same cluster have a zero merge probability, thereby avoiding any potential re-merging within the same cluster. Our approach views the OC Merge threshold as the proportion of nodes involved in the merging process. We can determine the number of node pairs to be merged based on the OC Merge threshold and subsequently perform Merge operations on the node pairs with the highest probabilities according to the Merge probability matrix M,

$$k = (1 - OC\_Merge\_Threshold) * N,$$
 (2)

where k represents the count of node pairs undergoing Merge, and N corresponds to the total number of nodes. By adopting this strategy, we strike a balance between the OC Merge threshold's influence and the IC Merge threshold's interpretation. This method enables us to merge the graph dataset comprehensively, accurately capturing the intricate connections between various node types.

In the *OC Merge* phase, we set whether the target node type participates in the merge according to different task objectives. In a multi-label classification task, the target node is allowed to be merged now. After the *OC Merge*, this node can be marked with the labels from the original two nodes. Different motifs can be used as explanatory ground truths according to different labels in the multi-label. As such, a multi-label dataset can be created.

#### **Pruning**

Pruning is to regularize the synthetic graph to fit the restrictions or constraints of the reference real-world graph. Most real-world graph databases are derived from non-graphical raw databases. There are some restrictions from the nature of the raw dataset that limit the graph schema and edge-type degree distributions. The pruning step can help synthetic graphs satisfy such raw data constraints. For instance, due to raw data constraints, the public IMDB dataset only connects one movie to at most three actors. In ACM (Wang et al. 2019) and DBLP 2, one paper should be published in one conference, and thus there will be only one connection to the conference. In the pruning step, we remove edges according to the node degree upper limit from raw data constraints with a well-designed approach. If pruning is done randomly, it will easily destroy the primary motif structure, affecting the explanatory ground truths. Therefore, we identify the nodes with degrees exceeding the upper limit and randomly drop the non-primary motif edges until the degree fits the upper limit degree. If the node degree is still too high, we allow some flexibility in the node degree to ensure the primary motif can maintain a complete structure. Keeping the complete structures of primary motifs is more crucial since they serve as the essential explanation of ground truths.

#### **Node Feature Generation**

Following the node features generation approach (Tsitsulin et al. 2022; Palowitch et al. 2022), we generate the node fea-

<sup>&</sup>lt;sup>2</sup>http://web.cs.ucla.edu/ yzsun/data/

tures from a within-cluster multivariate normal distribution. The features in the same cluster will be sampled from the same prior multivariate normal distribution with unit covariance. The feature center of each group will first be sampled from a multivariate normal distribution with the feature center distance defined by the user. The ratio of feature center distance to cluster covariance can be regarded as a signal-to-noise ratio. In the multi-label node classification task, we first overlay the probability distribution functions of the labels of the node. Afterward, we draw samples from this combined distribution to determine the features of the nodes. The effect of the feature center distance parameter will be discussed in the experiment.

# Fidelity for Heterogeneous Graph

Fidelity is a metric commonly used to evaluate the performance of the explanation model (Yuan et al. 2021; Li et al. 2022). It measures how closely related the explanations are to the model's predictions. The idea behind fidelity is that the performance of GNN models should be reduced if important characteristics or subgraphs are removed. If the critical information is included in the subgraph, the classification model prediction probability should be close to the original prediction. We use fidelity as the evaluation metric to support that the primary motifs can be excellent explanations of ground truths. Nevertheless, we extend fidelity scoring to multi-label tasks, which to our knowledge has not been done before. The following are the details of the fidelity score:

$$Fidelity = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{L} \sum_{l=1}^{L} \left\| f(G_i)_{y_i} - f(\hat{G}_i)_{y_i} \right\|, \quad (3)$$

where  $f(G_i)_{y_i}$  and  $f(\hat{G}_i)_{y_i}$  denote the predition probability of  $y_i$  of the original graph  $G_i$  and motifs  $\hat{G}_i$ , respectively. We denote N as the total number of target node samples and L as the number of node labels i.

# 4 Experiment Settings

As the SynHIN framework is flexible and can be highly customized according to the characteristic of the reference datasets, we conduct a series of experiments to examine the influence of different tunable parameters on the synthetic IMDB dataset generated by SynHIN. Following the prior graph generation research (Palowitch et al. 2022), we delve into the interplay between tunable parameters, classification model efficacy, and fidelity. We employ micro-F1 and macro-F1 for the HGNN model accuracy and fidelity for interpretations.

# **SynHIN Parameter Settings**

The tunable parameters of the SynHIN framework for generating the synthetic graphs include the following:

- Number of primary motifs: It affects the number of target nodes and the size of the final generated graph. In the experiments, we set it similar to the reference dataset.
- Number of clusters: We determine the cluster number depending on the reference dataset. Also, we generate

- data in a balanced manner removing class imbalance issues. In the experiment, we set it as the reference dataset.
- In-Cluster Merge threshold: The threshold is the probability of sampling from a uniform distribution. It can be seen as the proportion of nodes that are not merged. The lower the *IC Merge* threshold, the more nodes are merged, and links within the cluster will be stronger. We grid search *IC Merge* threshold from 0.1 to 0.8 with an interval of 0.1.
- Out-Cluster Merge threshold: The *OC Merge* affects the closeness between clusters. If the threshold is lower, the links between different clusters will be denser. We grid search from 0.2 to 0.9 with an interval of 0.1.
- Feature dimension: The dimension size of the feature is set as the same as the reference real-world dataset feature dimension.
- Feature center distance: Feature center distance determines the information richness of the features, which can be regarded as the signal-to-noise ratio of the feature due to the use of the unit covariance. We perform a grid search from 0.1 to 1.0 with an interval of 0.1.

# **Heterogeneous Graph Neural Network Models**

We used three different concept HGNN models to validate the synthetic graphs. Model parameters follow paper recommendations. The following briefly introduces the models: (1) HGT (Hu et al. 2020) adopted a transformer-based design for handling different node and edge types without manually defining the meta-path for the HGNN model. (2) Simple-HGN (Lv et al. 2021) introduce the attention mechanism, project different node-type features to the share feature space, and then use GAT as the HGNN backbone. (3) TreeXGNN (Hong et al. 2023) leverage the decision tree-based model XGBoost to enhance the node feature extraction, assisting the HGNN model in getting more prosperous and meaningful information.

#### 5 Experiment Results

We first experimented with the effect of the combination of IC Merge and OC Merge thresholds on the performance of the node classification model. We set the OC Merge threshold larger than the IC Merge threshold. This assumption is from the observations of real-world graph datasets that the proportion connected to the same group must be more than different groups (Palowitch et al. 2022). The results are shown in Table 1. We also visualize the results in Figure 5. When the IC Merge threshold decreases or the OC Merge threshold increases, the performance of the prediction model would be better. The less the noise of the corresponding connection, the better the performance. Moreover, when the feature center distance is larger, the higher the information contained in the node feature, the better the prediction performance. We adjust the number of different motifs, thereby affecting the number of target nodes and the size of the synthetic graph dataset. Since we follow the original parameter setting of the HGNNs, rather than fine-tune for each synthetic graph dataset, when we halve the reference dataset size, the model tends to be over-fitted and declines in performance.

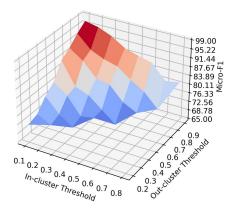


Figure 5: HGT Macro-F1 in different IC/OC Merge thresholds

#### **Fidelity**

Figures 6a and 6b illustrate the fidelity comparison between HGT, Simple-HGN, and TreeXGNN under the same settings. Simple-HGN and TreeXGNN exhibit lower fidelity, indicating higher model stability than HGT. Figure 6b is evident that the fidelity decreases as the OC Merge threshold increases while maintaining a fixed IC Merge threshold. This decrease can be attributed to noise reduction, resulting in higher predicted performance. Consequently, the models become more stable, leading to a corresponding decrease in fidelity. Figure 6a presents the fidelity results for a fixed OC Merge threshold. Notably, the fidelity remains stable regardless of changes in the IC Merge threshold. The observation indicates that the model predominantly relies on the primary motif designed as the prediction foundation. While the amount of noise in the dataset remains constant, different in-cluster connections are formed based on varying IC Merge thresholds. It implies the presence of additional effective information beyond the designed primary motif. However, despite the presence of this additional information, the fidelity of the model does not significantly change. This finding confirms that the primary motif designed indeed serves as the primary cause for the model's predictions.

When the number of nodes surpasses the reference dataset's count (2000 motifs), the model's prediction perfor-

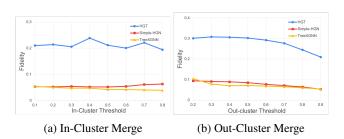


Figure 6: Threshold to Fidelity results

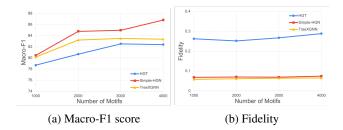


Figure 7: Different graph size results

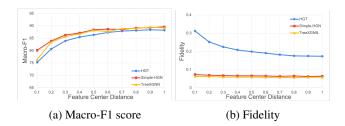


Figure 8: Different center distance results

mance remains steady, shown in Figure 7a, though the classification model's hyperparameters were not fine-tuned for this condition. Similarly, changing the number of motifs, reflective of the graph's size, maintains a relatively consistent signal-to-noise ratio across the graph. Consequently, Figure 7b shows fidelity performance remains stable.

Figure 8a presents the relationship between fidelity and feature center distance. It can be observed that as the feature center distance increases, the amount of information associated with all node features also increases. Consequently, when the graph structure and primary motif design remain unchanged, the primary motif incorporates more node feature information. While the model's performance improves due to the increased information, Figure 8b shows that the fidelity decreases as well. It can be attributed to more information present in the node features. The increased feature center distance introduces more informative node features into the dataset and primary motif, decreasing fidelity.

#### Visualization

We visualize the examples of synthetic graphs with varied parameters. Dark blue represents non-target nodes shown in Figures 9a, 9b, and 9c, while other colors indicate different label target nodes. Figures 9a and 9b show that when the *IC Merge* threshold is constant, an increase in the *OC Merge* threshold reduces noise, enhancing groupings and relaxing divisions in the graph. When the *OC Merge* threshold is constant, shown in Figures 9b and 9c, raising the *IC Merge* threshold leads to reduced information, resulting in looser connections within the group and less conspicuous grouping in the graph.

#### **Applying SynHIN to Other Datasets**

We demonstrate the adaptability of SynHIN to different reference datasets, ACM and DBLP. The prediction object of DBLP is different from ACM; the graph schema of ACM

HGT Macro-F1 (%)		Out-Cluster Threshold							
		0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
	0.1	72.05	73.37	78.14	81.43	88.02	90.63	94.23	97.05
	0.2	-	70.51	72.13	77.16	78.28	86.61	88.71	95.83
	0.3	-	-	68.11	69.84	76.10	80.67	86.18	93.45
In-Cluster	0.4	-	-	-	70.97	71.42	79.42	84.65	89.80
Threshold	0.5	-	-	-	-	66.72	73.50	80.41	88.07
	0.6	-	-	-	-	-	70.55	76.80	86.64
	0.7	-	-	-	-	-	-	70.95	80.38
	0.8	-	-	-	-	-	-	-	81.40

Table 1: HGT Macro-F1 in different IC/OC Merge thresholds

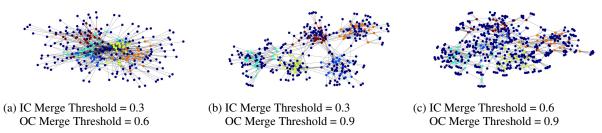


Figure 9: SynHIN synthetic graph example

	ACM					
	Micro-F1 (%)	Macro-F1 (%)	Fidelity			
HGT	92.90	92.85	0.3525			
Simple-HGN	96.39	96.37	0.1452			
TreeXGNN	98.24	98.23	0.1606			
		DBLP				
HGT	84.89	84.95	0.1246			
Simple-HGN	92.29	92.33	0.0920			
TreeXGNN	90.50	90.53	0.1347			

Table 2: Micro/Macro-F1 and Fidelity in ACM/DBLP

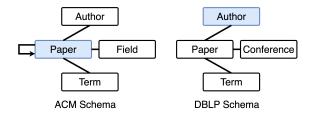


Figure 10: ACM and DBLP graph schema

and DBLP are shown in Figure 10. We perform a similar process to IMDB. Notably, we avoid merging the target node during the *OC Merge* for the single-label datasets.

The performance is shown in Table 2. Under the same parameter settings, compared to the multi-label dataset IMDB, single-label ACM and DBLP perform better in micro/macro-F1 because a single-label task is relatively simple. Moreover, the number of labels in ACM and DBLP is less than in IMDB, making the task easier. In addition, the degree distribution in ACM and DBLP also has a higher average, making the graph structure more closely connected. Based on the above reasons, the classification models perform better in ACM and DBLP than IMDB.

#### 6 Conclusion

We present SynHIN, a novel method for generating synthetic graph datasets that address the limitations of existing approaches. We leverage real-world datasets and employ the graphlet model to identify primary motifs that serve as ground truth explanations. These primary motifs are then connected with additional nodes to form subgraphs, ensuring the degree distribution aligns with the reference dataset. Subgraphs with the same pre-defined label are clustered through the IC Merge step. Later, the OC Merge step combines different clusters to form a complete synthetic graph. Finally, pruning is applied to align the output graph with the limitations of the reference real-world dataset, resulting in a HIN dataset with explicit ground truth explanations. In this work, we address the scarcity of heterogeneous graph datasets and overcome the need for such datasets in the domain of GNN explanations. Furthermore, our approach resolves the challenges faced by GNN explanations in homogeneous graphs, such as the absence of explanatory ground truths for many nodes in most explanation datasets and the repetitive and limited nature of primary motif design. To the best of our knowledge, our work introduces the first synthetic heterogeneous graph dataset with ground truth explanations, offering a multi-label functionality previously unavailable in generated graph datasets. Additionally, we design a comprehensive and diverse benchmark that provides a solid foundation for future research on heterogeneous GNN explanations.

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