Hypergraph Pre-training with Graph Neural Networks

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ABSTRACT
Despite the prevalence of hypergraphs in a variety of high-impact applications, there are relatively few works on hypergraph representation learning, most of which primarily focus on hyperlink prediction, and often restricted to the transductive learning setting. Among others, a major hurdle for effective hypergraph representation learning lies in the label scarcity of nodes and/or hyperedges. To address this issue, this paper presents an end-to-end, bi-level pre-training strategy with Graph Neural Networks for hypergraphs. The proposed framework named HyperGene bears three distinctive advantages. First, it is capable of ingesting the labeling information when available, but more importantly, it is mainly designed in the self-supervised fashion which significantly broadens its applicability. Second, at the heart of the proposed HyperGene are two carefully designed pretext tasks, one on the node level and the other on the hyperedge level, which enable us to encode both the local and the global context in a mutually complementary way. Third, the proposed framework can work in both transductive and inductive settings. When applying the two proposed pretext tasks in tandem, it can accelerate the adaptation of the knowledge from the pre-trained model to downstream applications. The extensive experimental results demonstrate that: (1) HyperGene achieves up to 5.69% improvements in hyperedge classification, and (2) improves pre-training efficiency by up to 42.80% on average.

1 INTRODUCTION

Hypergraph, as a generalization of the regular graph data, is ubiquitous in various domains, and has drawn increasing attention recently [26, 36, 37]. Different from traditional regular graphs, which consist of nodes and edges to represent pairwise relations between nodes, the hyperedges in the hypergraphs contain a collection of nodes, which represent high-order relations. For example, in the clinical studies of the pharmacological mechanism [24, 26], the effects of medical treatment is often the result of the combined interactions of a set of drugs. Here the combination of drugs for one disease could consist of one hyperedge. In the bioinformatics research, protein/multi-protein complexes, which consist of different collections of protein molecules, display different functions [22]. Here a collection of protein molecules could be one hyperedge. In the social network domain, a group of users who participate in the same event could be an one hyperedge of that event [31, 32]. In the academic domain, authors of the same academic paper could be an hyperedge of the paper they jointly publish [16].

Representation learning on hypergraph offers a potentially promising way to streamline various hypergraph applications. However, the traditional representation learning methods on regular graphs are not directly applicable in capturing the high-order relations of the hypergraphs. To date, relatively few works on hypergraph representation learning exist, most of which primarily focus on hyperlink prediction (e.g. [25], [37], [26], [31]). The major difficulties of representation learning on hypergraph are two-fold. First, the labels of diverse downstream tasks are usually very scarce, which makes it difficult for training the downstream neural models. Second, most of the recent hypergraph representation learning methods only work in the transductive learning setting (e.g. [26], [31], [14], [19], [36], [30]). Specifically, these methods require all data to be seen during the training for feature generation or representation learning in the model, which renders the inability of these methods to handle unseen data. For example, in the hyperlink prediction problem, many methods require that all candidate hyperlinks to be seen during training for hyperlink prediction on unlabeled hyperlinks.

In this paper, inspired by the recent advances of pre-training strategies developed in Natural Language Processing (NLP) community [3] and Graph Neural Networks (GNN) research (e.g. [7], [11], [8]), we propose HyperGene (i.e. a Hypergraph pre-training framework with Graph Neural Networks), and target on both inductive and transductive hyperedge classification. Compared with existing methods, our proposed method is characterized by the following three distinctive advantages. First, the proposed pre-training framework is capable of leveraging labeled data (with supervised pre-training) as well as unlabeled data (with self-supervised pre-training), to learn transferrable knowledge for diverse downstream tasks without the help of extra domain-specific hypergraph datasets [7, 15]. Second, our method explores bi-level (i.e. node-level and hyperedge-level) self-supervised pretext tasks, which aims at capturing the intrinsic high-order relationships of nodes and hyperedges respectively. Third, the proposed HyperGene can work in both inductive and transductive settings. The pre-training strategy proposed for transductive setting is adaptation-aware, in a sense that the pre-trained model could be more adaptive to the downstream tasks compared to traditional pre-training methods, and meanwhile more efficient.

The main contributions of the paper are summarized as follows.

- **Novel Framework.** We propose a bi-level pre-training framework for hypergraph representation learning named HyperGene, equipped with two mutually complementary self-supervised pretext tasks. The proposed framework can be applied to both transductive and inductive settings. For the transductive setting, the proposed HyperGene further embraces an adaptation-aware pre-training strategy to accelerate the knowledge transfer from the pre-trained model to the downstream applications.

- **Empirical Evaluations.** We perform extensive experiments to demonstrate the efficacy of HyperGene. In particular, the proposed HyperGene (1) outperforms all baselines across
all datasets for inductive hyperedge classification, with an up to 5.69% improvements over the best competitor, and (2) improves pre-training efficiency by up to 42.8% on average. In addition, the proposed HyperGene has been successfully applied to a real-world large online e-commerce application, namely inconsistent variation family (IVF) classification, outperforming the current baseline models therein.

The rest of the paper is organized as follows. Section 2 formally describes the problem studied by the paper. Section 3 presents the proposed model and Section 4 shows the experiments on public datasets and the real-world case study is shown in Section 5. Related work is introduced in Section 6. The paper is finally concluded in Section 7.

2 PROBLEM DEFINITION

The main notations used in this paper are summarized in Table 1. We first define the hypergraphs as follows.

Definition 1. Hypergraph: A hypergraph is represented by \( G = (\mathcal{V}, \mathcal{E}, F(\mathcal{V})) \), in which \( \mathcal{V} = \{v_1, v_2, ..., v_n\} \) is the set of \( n \) nodes and \( \mathcal{E} = \{e_1, e_2, ..., e_m\} \) is a set of \( m \) hyperedges. \( e_i = \{v_{i1}, v_{i2}, ..., v_{ik}\}, 1 \leq j \leq n \) represents the \( i \)-th hyperedge in which the nodes \( v_{ij}(i) \in \mathcal{V} \). We say that node \( v_j \) is inside hyperedge \( e_i \). \( F(\mathcal{V}) \) is the feature matrix\(^1\) for nodes.

A hypergraph incidence matrix \( M \in \mathbb{R}^{n \times m} \) is defined such that \( M(i,j) = 1 \) if node \( i \) appears in hyperedge \( j \) and otherwise 0. From \( M \), we can build an adjacency matrix \( A = M^T \cdot M \), in which \( A(i,j) \) indicates the number of nodes that appear in both hyperedge \( i \) and hyperedge \( j \). \( A = 0 \) when hyperedges do not share nodes.

Before giving the definition of inductive hyperedge classification, we provide brief preliminaries on Graph Neural Networks.

Preliminaries on Graph Neural Networks. GNNs are powerful deep learning models on graphs. Representative models include Graph Convolutional Networks (GCN) [13], Graph Isomorphism Networks (GIN) [29], Graph Attention Networks (GAT) [27], etc. The intuition behind the GNN model is to learn the node representation by convolutionally aggregating both the node/edge features and the features of the node’s local neighbors through neural networks. Message passing is often adopted as a convenient perspective to describe GNN models [5]. There are two steps in the message passing process: message passing and message updating. In message passing step, the node features are passed to its neighbors. In the message updating step, the received features are passed through an aggregation function (e.g., a neural network) for node representations. Typical message passing can be summarized as:

\[
\begin{align*}
    h_{m\rightarrow w}^{t+1} &= P_t(h_w^{t}, h_w^{t}, c_{vw}), \forall w \in N(v) \quad (1) \\
    h_w^{t+1} &= U_t(h_w^{t}, h_{m\rightarrow w}^{t+1}) \quad (2)
\end{align*}
\]

\( P_t \) and \( U_t \) are the message passing function and node representation updating function of the \( t \)-th iteration respectively. \( h_w \), \( h_{m\rightarrow w} \) are node representations (node \( w \) is the neighbor of node \( v \)), which are initialized as node features. \( c_{vw} \) is the edge feature of edge between nodes \( v, w \). Different GNN models differ in the functions \( P_t() \) and \( U_t() \). For example, GCN model [13], as one of the most representative GNN models, takes the summation of the neighboring nodes in the message passing step and attach a neural network module on the passed message and the node feature itself for feature aggregation. Recently there are also research on sampling strategies during message passing for removing redundant computations [2], so that the \( w \) in Eq. (1) does not always contain the entire neighborhood.

By using GNN as a neural function \( f_{\Theta}() \) for node representations, the inductive hyperedge classification is defined as follows.

Definition 2. Inductive Hyperedge classification: Given a set of hyperedges \( \mathcal{E} = \{e_1, e_2, ..., e_m\} \) which is not seen in the training stage, the goal of GNN model \( f_{\Theta}() \) is to learn embeddings for the downstream classifier\(^2\), \( g_{\Omega_t}() \) to classify them into \( t \) categories. \( g_{\Omega_t}(f_{\Theta}(e_i)) = p_i, i \in \{1, 2, ..., m\} \), and \( p_i \) is the prediction vector for \( e_i \) with a non-zero entry indicating \( e_i \)'s category.

By adopting pre-training strategy, model \( f_{\Theta}() \) is first trained on pretext task(s). Note that there could be more than one pretext task. The fine-tuning module can be represented as \( f_{\Theta_{st}, \Phi}() \) given the pre-trained GNN module \( f_{\Theta}() \). Generally speaking, pre-training \( f_{\Phi}() \) could be either supervised if the labels for the pretext task are available, or unsupervised, such as the self-supervised methods.

### Table 1: Symbols and Definition

| Symbols | Definition |
|---------|------------|
| \( G = (\mathcal{V}, \mathcal{E}, F(\mathcal{V})) \) | a hypergraph of node set \( \mathcal{V} \), edge set \( \mathcal{E} \), and feature \( F(\mathcal{V}) \) |
| \( M \) | the hypergraph incidence matrix |
| \( A \) | the adjacency matrix of hyperedges inferred from \( M \) |
| \( \Theta, \Omega_t \) | GNN module with parameter \( \Theta \) and neural adjustment module with parameter \( \Omega_t \) |
| \( g_{\Omega_t}() \) | a pre-trained GNN module with initialization \( \Theta^t \) |
| \( h_{\epsilon}^{(t)} \) | the hidden representation of hyperedge \( \epsilon \) |
| \( h_{s}^{(t)} \) | the hidden representation of seed node \( s \) |
| \( h_{c}^{(t)} \) | the hidden representation of context \( c \) |
| \( h_{n}^{(t)} \) | the hidden representation of negative example \( n \) |

3 PROPOSED PRE-TRAINING FRAMEWORK

In this section we present the proposed HyperGene framework. We first present the challenges and key ideas in Section 3.1, and then the bi-level self-supervised pretext tasks in Section 3.2 and Section 3.3. Section 3.4 introduces an adaptation-aware pre-training strategy, followed by the overall HyperGene framework architecture in Section 3.5 with analysis.

3.1 Challenges and Key Ideas

The first challenge for pre-training hypergraphs is how to design the self-supervised pretext tasks, since the high-order node relations of hypergraphs are significantly different from regular graphs structurally. Our idea is to incorporate both node-level and hyperedge-level pretext tasks, which aim at capturing local as well as global contextual pattern of hypergraphs. Locally, the node inside one specific hyperedge should be distinguished from nodes outside this hyperedge given the context of node. For one specific

\(^1\)Optionally, there also might be feature matrix for hyperedges \( F(\mathcal{E}) \).

\(^2\)We will also use \( g_{\Omega_t} \) to denote neural adjustment modules (e.g. using MLP) specified for pretext tasks with parameter \( \Omega_t \) after GNN module.
hyperedge and a given inside node, we define the context of the
tnode as all other nodes inside the hyperedge (Figure 1). Globally, the
similarities between hyperedges ought to be preserved. However,
calculating pairwise hyperedge similarities itself is challenging and
costly (with at least $O(m^2)$ time complexity for calculating every
pair of hyperedges if the number of hyperedges is $m$). As an approxi-
mation for learning pair-wise hyperedge similarities, our idea is to
first cluster the hyperedges, based on the features of nodes inside
hyperedges or the hyperedge adjacency matrix when available, and
then to preserve the membership characteristic of the hyperedge
clusters.

The second challenge is how to mitigate the divergence between
the self-supervised pretext tasks and the downstream tasks. Even
with two mutually complementary pretext tasks, such divergence
might still exist, in a sense that the well-trained pre-trained model
might be overly fit on the pretext tasks, and could not optimally
generalize on the downstream tasks. In the transductive setting, our
idea is to design an adaption-aware pre-training strategy, which
targets at learning a well-adaptive pre-trained model for down-
stream tasks. In this strategy, only one self-supervised pretext task
(node-level) is fully trained on the training data, and the other self-
supervised pretext task (hyperedge-level) is applied on the unseen
data for fast adaptation.

![Figure 1: An illustrative example of the hyperedge-level
pretext task (left), and the node-level pretext task (right).
$P_{T1}$ and $P_{T2}$ are probabilities for assigning $e_2$ to cluster 1
and cluster 2. The red area on the right subfigure shows the context
of node $v$, and the gray nodes are the sampled negative examples
of node $v$ and its context. Best viewed in color.]

### 3.2 Node-level Self-supervised Pretext Task

**A - Task Description.** In this pretext task, we aim at predicting
the relationship between a given node and its hyperedge context
(other nodes inside the hyperedge). Intuitively, we expect the node
and the context share similar representation if they belong to the
same hyperedge.

To be specific, in the node-level self-supervised training, we
first uniformly sample a seed node (e.g. $e_i^{(s)}$) inside each hyper-
edge, and obtain its corresponding context (e.g. $C_i$). The combined
node-context pair $(e_i^{(s)}, C_i)$ is a positive example. Next, for each
pair $(e_i^{(s)}, C_i)$, we adopt a negative sampling method for negative
examples ($e_i^{(n)}$) with $P_{Tij}$, the negative sampling probability) of the selected context. We utilize a GNN module inside the *clique-expansion*
of hyperedges for the hidden representation of nodes. The represen-
tation of nodes corresponding to contexts are aggregated by a
pooling layer for the context representations. The node-context
relationship is learned via a binary cross-entropy objective. For
notation simplicity, let $h$ be the representation learned by GNN
module, and $\hat{h} = g_{\Theta_n}(h)$ be the node representation after applying
the neural adjustment function $g_{\Theta_n}(\cdot)$ for node-level pretext task.

$$L^{(n)} = \sum_i \sum_j \log \sigma(h_i^{(s)}) + \log \sigma(h_i^{(n)})$$

where $h_i^{(s)}$ and $h_i^{(n)}$ are the hidden representation of seed node $i$,
context of node $i$, and the negative sample $j$ of node $i$ after using
the adjustment function, respectively. $\sigma(\cdot)$ is a sigmoid function.
$h_i^{(s)}$ is expected to be larger than $h_i^{(n)}$ since the positive seed node-context pair share similar feature distributions.

**B - Negative Sampling Method.** For a given pair of node and
its corresponding context of one hyperedge, one naive negative
sampling method is referred to as the exponential sampling
method (shorted as Exp.) in the rest of the paper.

For a given node $i$ the probability of sampling node $j \neq i$ is given as follows.

$$Pr_{ij} = \frac{\exp(-\gamma \cdot \hat{A}_{ij}^k)}{\sum_{j} \exp(-\gamma \cdot \hat{A}_{ij}^k)}$$

in which $k, \gamma > 0$ and $\gamma$ is a scaling scalar. $\hat{A}$ is the normalized
adjacency matrix, and matrix $\hat{A}^k$ gives the number of $k$-length
paths. We consider the nodes which are not reachable by $k$-length
paths having high and equal probability of being sampled. This
negative sampling method is referred to as the exponential sampling
method (shorted as Exp.) in the rest of the paper.

### 3.3 Hyperedge-level Self-supervised Pretext Task

In this pretext task, different from the local node-level pretext task,
we strive to capture the more global patterns of the relationship
of hypergraphs. As discussed in Section 3.1, we aim at predicting
hyperedges’ cluster membership information. When the adjacency
matrix of hyperedges $A$ exists, the clustering could be conducted
on the regular graph of hyperedges. First the regular graph of
hyperedges is constructed with adjacency matrix $A = M^\top M$, such
that $A(i,j)$ is the number of nodes that exist in both hyperedge
$i$ and $j$. Next, the METIS algorithm [12] is applied to partition
the graph of hyperedges into $q$ clusters. $q$ is empirically selected,
and is usually set larger or equal to the number of categories
of hyperedges in the empirical experiments (see details in Section
4). Similar to the node-level self-supervised pretext task, the GNN
module is applied inside the *clique-expansion* of the hyperedges,
and the representations for hyperedges are obtained by a graph

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3 An objective variant is detailed in the appendix.
where the first stage trains the pretext task until convergence with which the key idea is only performing node-level pre-training on the hyperedge-level self-supervised pretext task.

### 3.4 Adaptation-aware Pre-training Strategy

Traditional pre-training methods use a two-stage procedure, in which the first stage trains the pretext task until convergence with the self-labels, and the second stage trains the downstream task with the task labels. Specifically in our scenario with two self-supervised pretext tasks, the two-stage training can be realized in a serial procedure as follows.

\[
\Theta' = \arg \min_{\Theta} \mathcal{L}^{(n)}(g_{\Theta_n}(f_{\Theta_n}(\mathcal{E}_{\text{train}}, \mathcal{F}(n))); y^{(n)})
\]  

\[
\Theta^{(pre)} = \arg \min_{\Theta} \mathcal{L}^{(h)}(g_{\Theta_h}(f_{\Theta_h}(\mathcal{E}_{\text{train}}, \mathcal{F}(n))); y^{(h)})
\]  

\[
\hat{\Theta} = \arg \min_{\Theta} \mathcal{L}^{(t)}(g_{\Theta_t}(f_{\Theta_t}(\mathcal{E}_{\text{train}}, \mathcal{F}(n))); y^{(t)})
\]

where \(\mathcal{L}^{(t)}\) and \(y_{\cdot i}\) are the loss function and labels for the downstream task respectively. The parameters of GNN module is first obtained by training the node-level pretext task and then by training the hyperedge-level pretext task.

As discussed in Section 3.1, the above strategy in the transductive setting might bring non-negligible divergence between pre-training and downstream task training, which would lead to a sub-optimal model. Moreover, since the hyperedge-level pretext task approximately preserves the pair-wise hyperedge distances, pre-training this task till convergence might result in a large divergence. To address this issue, we propose an adaptation-aware pre-training strategy. The key idea is only performing node-level pre-training on the training set, and utilizing the hyperedge-level pretext task as adaptation steps on the testing set (unseen when training the downstream task) in the transductive setup.

Specifically, we maintain Eq. (6a). But instead of training the hyperedge-level pretext task until convergence (Eq. (6b)), we use it as an adaptation task, which can be represented as \(s\) steps of gradient descent on testing hyperedges \(E_{\text{test}}\), so that Eq. (6b) can be replaced as \(s\) steps of:

\[
\Theta := \Theta - \epsilon \frac{\partial \mathcal{L}^{(h)}(g_{\Theta_h}(f_{\Theta_h}(\mathcal{E}_{\text{test}}, \mathcal{F}(n))); y^{(h)})}{\partial \Theta}
\]

where \(\epsilon\) is the learning rate. Compared with the traditional pre-training method, the advantages of the adaption-aware training strategy is two-fold. First, the pre-trained model for transferring general data knowledge is more adaptive to the downstream tasks. Second, it is a more efficient pre-training strategy, because only one pretext task needs to be fully trained, and the adaption (only a few steps) can be conducted whenever the testing data is available.

### 3.5 Proposed HyperGene Framework

The end-to-end model architecture is illustrated in Figure 2, and the full algorithm is summarized in Algorithm 1 (in Appendix). The negative sampling strategy is first conducted for the input hyperedge set, followed by the node-level pretext task. Two variants of GNN modules are explored. First, the positive and negative hyperedges use different GNN modules for node/context representation (with parameters \(\Theta_1\) and \(\Theta_2\) in Fig. 2). Second, contrarily the positive and negative hyperedges share the parameters of the same GNN module. The proposed pre-training framework could support various types of GNN layers as the GNN module, such as GCN [13], GraphSAGE [6], GIN [29], etc. We use GIN [29] module for clique expansion due to its superior empirical performance in our downstream task (see details in Section 4). After adopting the GNN module, a pooling layer is used for obtaining the context/hyperedge representation, such as mean pooling and set2set [28]. In order to achieve permutation equivariance, set module could be adopted, such as DeepGCN [29].
We use four public datasets to evaluate the proposed model. The statistics of the datasets are summarized in Table 2.

### 4 EXPERIMENTS

In this section we present evaluation results of the effectiveness and efficiency of the proposed framework on public datasets.

#### 4.1 Experimental Setup

**A - Datasets.** We use four public datasets to evaluate the proposed model. The statistics of the datasets are summarized in Table 2.

| Name | # of nodes | # of hyper-edges | Min # of nodes in hyperedge | Max # of nodes in hyperedge |
|------|------------|-------------------|-----------------------------|-----------------------------|
| Cora | 2,708      | 2,427             | 2                           | 169                         |
| Pubmed | 19,717    | 3,887             | 3                           | 20                          |
| Corum | 6,132      | 4,736             | 2                           | 131                         |
| Disgenet | 8,352    | 8,386             | 3                           | 487                         |

- **Cora:** The Cora dataset consists of 2,708 scientific publications (nodes) classified into one of seven classes. The citation network consists of 5,429 edges between publications. The dataset contains text features for each publication, and it is described by a zero/one-valued word vector indicating the absence/presence of the corresponding word from the dictionary. The dictionary consists of 1,433 unique words [16]. Note that the Cora dataset is a regular graph dataset.

- **Pubmed:** The Pubmed Diabetes dataset consists of 19,717 scientific publications (nodes) from PubMed database pertaining to diabetes classified into one of three classes. The citation network consists of 44,338 links. This dataset contains text features for each publication which is described by a TF-IDF weighted word vector from a dictionary which consists of 500 unique words [17]. The Pubmed dataset is also a regular graph dataset.

- **Corum:** The Corum is the dataset of mammalian protein complexes. The dataset contains 6,132 types of proteins (nodes), and each protein complex consists of a collection of proteins. No direct connections between proteins in the complexes exist. The Corum dataset is a hypergraph dataset.

- **Disgenet:** The Disgenet dataset contains 8,352 genes (nodes) and each disease (hyperedge) consist of a collection of genes. Each disease is classified into one of 23 MeSH codes. 21 of these codes are used as the hyperedge categories. Note that this dataset is highly unbalanced.

**B - Experimental Setups.** We pre-process two versions of Cora and Pubmed datasets as Cora/Pubmed-clean/noisy. The training details, hyper-parameter setting, dataset pre-processing and baseline adjustments are in Appendix for space.

#### 4.2 Effectiveness Results on Public Datasets

The results for hyperedge classification are presented in Table 3. The metric is the multi-class classification accuracy. The results are mean and standard deviation values over ten runs. All supervised methods share the same training, validation, and testing ratio of 6:2:2. The best results are shown in bold fonts, and the second best results are shown with underlines. We adopt the two-GNN module for the inductive setting (no Ada. in Table 3), and one-GNN module for the transductive setting (Ada. in Table 3) because of overall better performance. Both exponential and uniform sampling are evaluated (shorted as Exp. and Uni. in Table 3). Other results of model variants are detailed in the Appendix. For baselines, Hyper-SAGNN, SAGE, DHNE and Joint Training use inductive setting, and DW and Deep-Hyperedge use transductive setting.

From the table, we can make the following observations. First, for inductive setting, HyperGene outperforms all current baselines on all datasets (by up to 5.69%), and for transductive setting, HyperGene outperforms all current baselines on five out of six datasets (by up to 4.75%). The framework with adaptation-aware pre-training outperforms the traditional pre-training method in five out of six datasets. The exponential sampling method is competitive with the uniform negative sampling method when no adaptation stage is used, but it achieves significant improvements when adaptation-aware pre-training is applied. The performance of the joint training model is competitive compared with the current baselines. In the current baselines, Deep Hyperedge, Hyper-SAGNN and DeepWalk have relatively better performance over the rest of the baseline methods because DHNE is originally for hyperlink prediction. Note that compared with Deep Hyperedge, which requires hyperedge association, HyperGene does not use such information in downstream tasks, but still outperforms Deep Hyperedge in five datasets, and is also competitive on Disgenet. For Disgenet dataset, the relatively low accuracy is due to the highly imbalanced data with 21 hyperedge categories.

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### Appendix

#### Table 2: The summary of datasets

| Name   | # of nodes | # of hyper-edges | Min # of nodes in hyperedge | Max # of nodes in hyperedge |
|--------|------------|-------------------|-----------------------------|-----------------------------|
| Cora   | 2,708      | 2,427             | 2                           | 169                         |
| Pubmed | 19,717     | 3,887             | 3                           | 20                          |
| Corum  | 6,132      | 4,736             | 2                           | 131                         |
| Disgenet | 8,352    | 8,386             | 3                           | 487                         |

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3https://www.disgenet.org/downloads

4https://mips.helmholtz-muenchen.de/corum/
In this section we conduct ablation study on the following setups. First, we compare the hyperedge classification performance by using different GNN modules in our framework. For all the different versions of GNN modules, we apply the adaptation-aware pre-training strategy, and the exact same hyper-parameters for the rest of the framework. The results are shown in Table 4. The results are the mean and standard deviation values of ten runs. We can see that the GIN module overall shows the best performance over the rest of the GNN modules in our framework for the hyperedge classification task. Also, for the same GNN module, we can see that generally the exponential negative sampling method outperforms the uniform negative sampling method.

Second, we conduct the ablation study on the transductive hyperedge classification performance for bi-level self-supervised pretext tasks (Table 5). We apply HyperGene totally without pre-training stage (the first row), with only node-level self-supervised pretext task (the second row), and with only hyperedge-level self-supervised pretext task (the third row). We can observe that the HyperGene framework with both two-level self-supervised pretext tasks shows the best performance, which demonstrates the effectiveness of both levels of self-supervised pretext tasks.

### 4.4 Parameter Sensitivity Results

Here we study the hyper-parameter sensitivity of our proposed framework. First, we show the results of the sensitivity of the number of clusters in the hyperedge-level pretext task in Fig. 3 and Fig. 4. Note that we use the same model architecture with one-GNN module for all experiments in this subsection, whose setting is different from effectiveness experiments. The experiments are conducted in both inductive and transductive settings and with both uniform and exponential negative sampling methods. We observe that: (1) the framework shows relatively stable performance on a large range of the number of clusters; and (2) the framework that uses the exponential negative sampling method with adaptation-aware pre-training strategy overall shows stabler performance compared with the framework that uses uniform negative sampling, and does not use the adaptation-aware pre-training, which indicates better adaptation for the downstream task of the two-level adaption-aware pre-training framework. Second, the results of hyperedge classification accuracy vs. the number of adaptation steps are shown in Fig. 5. The results demonstrate slight performance drop but relatively stable over the tested adaptation steps in the range of $[1, 20]$ for both exponential and uniform negative sampling method.

### 5 A CASE STUDY

In this section, we introduce a real-world application of the proposed model on the inconsistent variation family detection problem in a large online store, and show that how the proposed pre-training
strategy can help to improve base model (without pre-training) as well as baselines, even when direct hyperedge associations are not available (the adjacency matrix \( A \) of hyperedges is a zero matrix).

### 5.1 Preliminaries and Experimental Setup

**A - Preliminaries**

Large E-commerce services such as Amazon, Etsy, and eBay often utilize merchandise relationships such as variations and substitutes to improve their catalog quality. These relationships between merchandise items are the cornerstone of research in the field of relationship science.

Variation family refers to a family of product items which are functionally the same but differ in specific attributes. Such variation families are present in the same detail page. For example, in Fig. 7 the correctly grouped 'Nike Air Max 270 React' shoe family is shown in one detail page. All items inside this family are this particular model but have different sizes and colors. The grouping attributes of a variation family are shared by all items inside the variation family (e.g., brand 'Nike'). The variation theme attributes are attributes which differ from item to item inside the variation family (e.g., size and color). When variation families contain inconsistent items (e.g., an Adidas shoe is grouped into the variation family in Fig. 7), they are called inconsistent variation family (IVF). One of the most important task in the catalog system is the IVF detection.

In order to solve this problem, each variation family can be seen as a hyperedge, in which every item should belong to the same merchandise if it is a consistent family. Then this specific problem is transformed into hyperedge classification problem. As for the pretext tasks, we adopt a task called variation theme learning, which is defined as:

**Definition 3. Variation Theme Learning:** Given a set of variation families (hypergraph \( G = (V, E, F(\pi)) \) with \( E = \{e_1, ..., e_m\} \), the Variation Theme Learning aims at learning the variation theme attributes and grouping attributes of the families (i.e. which rows of \( F(\pi) \) are grouping/variation theme attributes).

Note that variation families are independent, which makes the direct hyperedge associations unavailable. Most baselines from Section 4 become inapplicable, such as SAGE, DW, Deep-Hyperedge, and DHNE. Our idea is to transform this problem as a hyperedge multi-label classification problem since variation families (hyperedges) might have multiple grouping/variation theme attributes. Due to the fact that the labels of grouping/variation theme attributes are available in our catalog system for variation family datasets, this pretext task in the pre-training stage could be supervised. During training, the hyperedge representation produced by HyperGene is first used for the multi-label supervised pretext task (variation

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### Table 4: Accuracy of hyperedge classification for different GNN module (mean ± std in %)

| Models        | Cora-noisy | Cora-clean | Pubmed-noisy | Pubmed-clean | Corum | Disgenet |
|---------------|------------|------------|--------------|--------------|-------|----------|
| GCN (Uni.)    | 75.58±0.98 | 82.09±1.26 | 83.59±0.63   | 85.96±2.27   | 65.23±0.48 | 32.36±0.44 |
| GCN (Exp.)    | 76.88±2.08 | 84.65±3.32 | 84.14±1.62   | 86.06±1.94   | 83.34±0.25 | 32.84±0.18 |
| SAGE (Uni.)   | 75.28±0.69 | 80.68±0.94 | 83.89±1.27   | 86.15±2.71   | 64.98±0.45 | 33.33±0.79 |
| SAGE (Exp.)   | 75.52±1.01 | 81.04±2.09 | 85.18±0.86   | 86.94±3.02   | 66.03±0.28 | 31.69±0.21 |
| GAT (Uni.)    | 73.12±2.56 | 81.31±0.24 | 84.15±1.49   | 86.74±2.67   | 82.70±2.47 | 31.89±2.38 |
| GAT (Exp.)    | 71.21±0.72 | 80.15±1.68 | 84.79±0.72   | 88.49±0.72   | 85.75±1.29 | 29.89±1.48 |
| GIN (Uni.)    | 74.53±1.81 | 83.86±3.55 | 85.52±0.95   | 87.23±0.96   | 84.31±0.99 | 35.05±0.49 |
| GIN (Exp.)    | 78.78±1.28 | 83.77±1.62 | 86.94±0.73   | 90.84±0.29   | 85.33±1.09 | 33.90±2.26 |

### Table 5: Ablation study on two-level self-supervised pretext tasks (mean ± std in %)

| Models            | Cora-noisy | Cora-clean | Pubmed-noisy | Pubmed-clean | Corum | Disgenet |
|-------------------|------------|------------|--------------|--------------|-------|----------|
| No Pre-train      | 69.12±0.48 | 81.48±1.24 | 84.40±1.53   | 84.60±2.49   | 78.25±0.13 | 32.76±1.54 |
| Only Node         | 74.23±0.84 | 82.27±1.25 | 85.04±0.37   | 86.84±1.94   | 82.52±2.14 | 33.75±1.70 |
| Only Hyperedge    | 73.24±1.53 | 82.78±1.30 | 86.29±1.36   | 85.67±0.38   | 84.17±1.56 | 33.40±0.65 |
| HyperGene (Exp.)  | 78.78±1.28 | 83.77±1.62 | 86.94±0.73   | 90.84±0.29   | 85.33±1.09 | 33.90±2.26 |

Figure 5: Accuracy (±std) vs. # of adaptation steps on Cora-clean (left) and Pubmed-clean (right) dataset

Figure 6: Running time comparison of the pre-training stage for traditional and adaptation-aware pre-training strategy.
Table 6: Results of IVF classification for case study (mean ± std in %)

| Dataset          | Category 1 | Category 2 | Category 3 |
|------------------|------------|------------|------------|
|                  | AUC-I      | AUC-C      | AUC-I      | AUC-C      |
| Hyper-SAGNN      | 56.12 ± 1.19 | 88.87 ± 0.93 | 58.72 ± 1.94 | 89.81 ± 1.64 |
| Hyper-SAGNN, pre-train | 60.26 ± 1.42 | 90.12 ± 0.38 | 59.82 ± 0.55 | 89.57 ± 0.21 |
| HyperGene, no pre-train | 60.51 ± 0.89 | 90.32 ± 0.88 | 58.09 ± 0.57 | 89.64 ± 0.79 |
| Joint Training   | 62.80 ± 1.33 | 90.99 ± 0.78 | 56.73 ± 1.41 | 89.55 ± 0.82 |
| HyperGene, Sup. pre-train | 64.06 ± 1.27 | 90.74 ± 1.40 | 59.42 ± 1.78 | 89.84 ± 0.70 |
| HyperGene, Sup. pre-train + Ada. | 61.86 ± 1.32 | 90.31 ± 1.80 | 61.73 ± 1.24 | 90.42 ± 1.74 |

5.2 Results on Datasets of Product Lines
As shown in Table 6, first we can see that by using the supervised pretext task, the model performances are consistently better than those without pre-trained pretext task in all product lines. Second, for both methods using pretext task, the pre-training strategy outperforms the joint training strategy by AUC-I metric and they are very close by AUC-C metric. The Hyper-SAGNN with the adapted pre-training stage also has relatively competitive performance compared with the proposed model. This indicates that in this real-world application of hyperedge classification, pre-training can improve the base model as well as baseline method, and pre-training is generally a better training strategy than joint training. Third, by utilizing the adaptation stage with the node-level self-supervised pretext task (the last row), the model is able to further improve the AUC-I performance on Categoty-2 and Category-3 product lines, which demonstrates the effectiveness of the adaptation-aware pre-training of HyperGene in this application scenario.

6 RELATED WORK
The related work of the proposed model can be roughly divided into three categories, the GNN-related research, the recent pre-training methods, and the hypergraph mining.

A - GNN-related Research. GNN-related works are partially covered in Section 2. It becomes popular since Bronstein et al. introduce geometric deep learning [1] to bring the convolutional network to the graph mining field, and Kipf et al. significantly simplify the graph convolutional process and develop GCN [13]. To name a few representative works, Velivckovic et al. [27] improve GCN by introducing attentions of neighborhoods, which is calculated dynamically at message passing step. Xu et al. study the expressiveness of GNN model compared with the closely related Weisfeiler-Lehman graph isomorphism testing algorithm, and develop Graph Isomorphism Networks [29]. This direction still has numerous challenges.

B - Pre-training Strategy. After the pre-training strategy is first used in NLP communities [3], researches also begin to appear in the graph mining field. Hu et al. develop a new strategy and self-supervised methods for pretraining Graph Neural Networks [7]. The key to the success of this method is to pretrain an expressive GNN at the level of individual nodes as well as entire graphs so that the GNN can learn useful local and global representations simultaneously. Most recently, Hu et al. [8] propose a generative pre-training strategy for GNN models in which a self-supervised attributed graph generation task is introduced. Qiu et al. [23] propose a graph contrastive coding method for the pre-training stage in the

As suggested by [7], through preliminary studies, these two tasks are highly likely to be positively correlated. Briefly, inconsistent variation families contain inconsistent items with different distributions of grouping attributes compared with other items, and vice versa.
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GNN model. Jin et al. [11] summarize and compare commonly used self-supervised training strategies on graphs and point out future directions. However, the pre-training strategy on graph/hypergraph data is still an open question with lots of potential for breakthrough in the immediate future.

C - Hypergraph Mining. The hypergraph mining studies the combined relation pattern of inner-related items. Among some earliest work, Li et al. [14] transform the hyperlink prediction method [9] for ranking the hyperedges. Zhang et al. [36] use a coordinated matrix minimization method for nonnegative matrix factorization in the adjacency space of the hypergraphs for hyperedge prediction. More recently, representation learning and CNN based methods are developed for this direction. Tu et al. propose DHNE [25] which applies auto-encoder and deep neural networks for the representation learning of hyperedges. Hyper-SAGNN by Zhang et al. [37] combines the attention-based dynamic representations and the MLP-based static representations for hyperedge prediction. HGNN by Feng et al. [4] generalizes the convolution operation to the hypergraph by hypergraph Laplacian. Deep Hyperedges [19] by Payne jointly uses contextual and permutation-invariant node memberships of hyperedges for hyperedge classification, which is relevant to the focus of this paper. DHGN by Ji et al. [10] adopts vertex convolution and hyperedge convolution in the dynamic hypergraph representation learning. Yu et al. [34] propose a multi-channel hypergraph convolutional network for social recommendation. Other recent neural hyperlink prediction methods include [30–33].

7 CONCLUSION

In this paper, we study the problem of hypergraph representation learning, and propose an end-to-end hypergraph pre-training framework HyperGene with GNNs. HyperGene incorporates bi-level self-supervised pretext tasks (node-level and hyperedge-level respectively), and enables both transductive and inductive learning settings. The proposed pre-training strategy does not require extra domain-specific datasets, and is adaptation-aware, which helps the pre-trained model more adaptive to downstream tasks compared to traditional pre-training methods. Extensive experiments on public datasets as well as a real-world case study mainly demonstrate that:
1) HyperGene shows significant improvements of downstream task performance and stability over baselines in most public datasets;
2) the proposed pre-training strategy is efficient compared with traditional pre-training method;
3) the proposed framework shows applicability in real-world applications of online stores.

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APPENDIX
We summarize the appendix as follows:

- **Reproducibility**: The detailed experimental setups for training the proposed model, hyper-parameter setting, and dataset pre-processing for reproducibility.
- **Discussions of model variants**: The study of variants of the proposed HyperGene.
- **Additional experimental results**: Additional results on model variants.

A - Reproducibility

**Model Training Details.** First, for HyperGene with uniform negative sampling, we adopt a local sampling method for the negative hyperedges in order to sample negative nodes. Specifically, the uniform sampling is conducted inside each batch of hyperedges of the stochastic gradient descent algorithm (e.g. Adam optimizer). To this end, the node-level self-supervised pretext task captures the local node-context relationship within a batch at each parameter updating. Since the batch is uniformly sampled, this local sampling method eventually equals to the global uniform sampling on all hyperedges for pre-training. Compared with exponential sampling, which calculates $\hat{A}^k$ (Eq. (4)) for globally sampling negative nodes, this uniform negative sampling is more efficient (see Fig. 6).

Second, in order to obtain the hyperedge embeddings from the node embeddings as the outputs of GNN module, mean pooling is adopted on public datasets and Set2set [28] pooling with 1 recurrent layer is adopted on case study because of optimal practical performance. Other sophisticated pooling methods for hypergraphs could be one future direction.

Third, all the adaptation functions which take the node/hyperedge embeddings as inputs for adapting with the self-supervised pretext/downstream tasks are set as MLPs with 0.5 dropout rate. All non-linear activation functions are set as ReLU function.

**Hyper-parameter Setting.** For the model optimization, we adopt Adaptive Moment Estimation (Adam). The hyper-parameters are set such that the downstream task performs well on validation set. Specifically, for the optimizer, we select the batch size as 64, and learning rate as 0.001 with learning rate scheduler that reduces learning rate on plateau. The number of epochs for node-level pretext task and hyperedge-level pretext task (for traditional pre-training) are set to 50. For the effectiveness evaluations on public datasets, the number of clusters for hyperedge-level pretext task is set as 10, 10, 3, 3, 21, 20 for Cora-noisy, Cora-clean, Pubmed-noisy, Pubmed-clean, Corum, Disgenet datasets, respectively. The number of GNN layers is set as 1. The number of adaptation steps are set to 5 for all datasets. The dimension of node/hyperedge embeddings are set as 64.

For baseline methods, the hyper-parameters are empirically optimized based on the literature. For joint training, we set the weighting parameters $\alpha, \beta$ to be equal to 1 in Eq. (8). For Hyper-SAGNN, DHNE, SAGE, and Joint Training methods, we train them using Adam optimization method as well. The learning rate are set as 0.001 with learning rate scheduler. The dimension of node/hyperedge embeddings is set as 64. Other baseline hyper-parameters are set either based on the validation set or original literature guidance.

**Dataset Pre-processing.** Since not all of the datasets are originally hypergraph datasets, i.e. Cora and Pubmed, we need to first process them for generating the hypergraphs. For Cora and Pubmed, we generate two versions of hypergraph datasets as follows. For the first version, we take the ego-network (subgraph of the center node with 1-hop neighbors) of each node as hyperedges, and assign the hyperedge label as the label of the majority in the ego-network. We name this version as the noisy version since the hyperedge might contain nodes with different categories. For the second version, we also take the ego-network of each node as hyperedges, but only keep those whose nodes share the same category. We name this version as the clean version. For Corum and Disgenet, they are originally hypergraph datasets, and do not need processing.

As for the node features, for Cora and Pubmed, we use the text feature vectors as described in the dataset details. For Disgenet, we use the numerical features of genes from the original data (e.g. DSI, DPI, etc.) For Corum, we first construct a regular graph of nodes, in which each edge represents that the end nodes exist in the same hyperedge. Then we adopt the Subsample and Traverse (SaT) Walks [19] strategy for sampling a collection of random walks and use the embedding vectors from DeepWalk [21] method as node features.

**Baselines and Adjustments.** In total we adopt six baselines in our experiments. Five of them are from existing work (Deep Hyperedge [19], DHNE [25], Hyper-SAGNN [37], Graph-SAGE [6], DeepWalk [21]), and one of them is the joint training strategy with the proposed self-supervised pretext tasks (Eq. (8)). Among the baselines from existing work, only Deep Hyperedge is directly designed for hyperedge classification. DHNE and Hyper-SAGNN are originally designed for hyperlink prediction. We keep the major model architecture, and adapt these two methods as follows.

For DHNE, firstly the second-order component is designed for heterogeneous hyperedges. Since our datasets are not homogeneous, we only need to use one auto-encoder in this component. Second, the supervised binary component for hyperlink prediction is modified to multi-class hyperedge classification. For Hyper-SAGNN, we keep the idea of using both static and dynamic embeddings of nodes, and take the summation of the static and dynamic embeddings as the final embeddings of hyperedges for hyperedge classification.

Graph-SAGE and DeepWalk are originally designed for regular graphs. We adapt these two models to make them work on the regular graph of hyperedges. In this regular graph, each vertex represents one hyperedge and there is an edge between two vertexes if two hyperedges share nodes.

**Hardware and Software Details.** All experiments are performed on a machine with an Intel(R) Core(TM) i7-9800X CPU (64.0 GB RAM) and GeForce GTX 1080 GPU. The model is implemented with Python 3.6 and Pytorch 1.5.0 [18].

B - Discussions of Model Variants

**HyperGene Algorithm.** We first present the proposed framework in Algorithm 1.

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Note that if the hypergraph is constructed from regular graph, in which the pairwise node links are known, the links among nodes inside and outside one hyperedge should neither be used for model input, nor be used for feature generation.

For all baselines (except for DeepWalk which does not utilize node features), we use the same node features as model inputs for fair comparison.
Joint Training. Next we briefly describe a natural variant in which the pretext tasks are jointly trained with the downstream task. We also use this training method as a baseline in our experiments (see details in Section 4). The joint training loss can be written as:

$$\mathcal{L}^{(j)\text{Joint}}_{\Theta_{D1, D2, D3}} = \alpha \mathcal{L}^{(n)} + \beta \mathcal{L}^{(h)} + \mathcal{L}^{(t)}$$

where $\mathcal{L}^{(t)}$ represents the loss function for downstream task, hyperedge classification. $\alpha, \beta$ are used for re-weighting the bi-level pretext tasks.

Algorithm 1: The HyperGene framework

Input: \{$E_{\text{train}} = \{e_1, ..., e_m\}$, $E_{\text{test}} = \{e_1, ..., e_q\}$\}: training and testing set for hyperedge classification; pretext tasks’ hyper-parameters.

Output: The pre-trained GNN module $f_\Theta(\cdot)$.

1. for $e \in E_{\text{train}} \cup E_{\text{test}}$ do

2. \hspace{1em} Perform clique expansion for $e$ to obtain new hyperedge $e' \in E'_{\text{train}} \cup E'_{\text{test}}$.

3. end for

4. for each epoch do

5. \hspace{1em} Sample batches $B^{(m)} = \{B_1, B_2, ..., B_s\}$ from $E'_{\text{train}}$.

6. \hspace{1em} for each batch $B_i \in B^{(m)}$ do

7. \hspace{2em} Update GNN module parameters $\Theta$ by $\mathcal{L}^{(n)}$ (Eq. (3)).

8. \hspace{1em} end for

9. end for

10. /* Line 11 - 16: for inductive setting only */

11. for each epoch do

12. \hspace{1em} Sample batch set $B^{(m)} = \{B_1, B_2, ..., B_s\}$ from $E'_{\text{train}}$.

13. \hspace{1em} for each batch $B_i \in B^{(m)}$ do

14. \hspace{2em} Update GNN module parameters $\Theta$ by $\mathcal{L}^{(h)}$ (Eq. (5)).

15. \hspace{1em} end for

16. end for

17. /* Line 18 - 20: for transductive setting only */

18. for each adaptation step do

19. \hspace{1em} Update GNN module parameters $\Theta$ by Eq. (7) on $E'_{\text{test}}$.

20. end for

21. Return Pre-trained GNN module parameter $\Theta$.

Variant I. As discussed in Section 3.5, instead of using one GNN module for both positive and negative nodes in the node-level pretext task, one natural variant is to utilize two GNN modules, which do not share parameters, for positive and negative nodes respectively.

Variant II. For the node-level self-pretext task, we could also learn the hyperedge representation by a ranking-based objective function, which aims at forcing the similar nodes in the feature space to be also close in the representation space, and the dissimilar nodes to having a margin in the representation space. Here we adopt the cosine embedding loss function to replace Eq. (3). For node $i$ and context $j$:

$$\mathcal{L}^{(n)} = \sum_{i,j} (y(1 - \cos(\hat{h}_i, \hat{h}_j^{(C)})) + (1-y)(\max(0, \cos(\hat{h}_i, \hat{h}_j^{(C)}) - \epsilon)))$$

where $\epsilon > 0$ is a margin, $y \in \{-1, 1\}$ is the label, and $\cos(\cdot)$ is the cosine similarity function.

Variant III. For the hyperedge-level self-pretext task, in order to approximate the task of preserving the exact pair-wise hyperedge similarities, we can also try to preserve the approximated pair-wise hyperedge distances in a regression objective as follows to replace Eq. (5):

$$\mathcal{L}^{(h)} = \|g^{(h)}_{\Theta_2}(H) - A^k||_F^2$$

where $g^{(h)}_{\Theta_2}(\cdot)$ is a neural adjustment function for the embeddings of hyperedges, $H$ is the embedding matrix of all hyperedges (with row-wise hyperedge embeddings), $k' > 0$ is a small scalar and $A^k$ is an approximation for pair-wise hyperedge similarities when the incidence matrix can be used for calculating the adjacency matrix $A$. In this Variant, we use the above pretext task as adaptation steps.

Variant IV. In order to adopt GNN technique and learn the representations for hyperedges. Besides expanding each hyperedge as a fully-connected graph (clique expansion), we can also expand a hyperedge as a tree (tree expansion). Intuitively, each hyperedge can be seen as a new root node connecting to all the nodes inside the hyperedge. In the message passing of GNN module, the difference between clique expansion and tree expansion is that the nodes in clique expansion first pass their features to the neighbors in the same hyperedge, but the nodes in tree expansion only pass their features to the root nodes. Clique expansion and tree expansion are two typical methods of adding hypothetical connections to the nodes inside hyperedges for expansion.

C - Additional Experimental Results

We present the experimental results on the four variants which we discuss in the Appendix-B in Table. 8. Compared with HyperGene with exponential negative sampling, the Variant-I with two GNN modules in transductive setting achieves slightly better performance in Cora dataset. Variant-II and Variant-III with different node-level/hyperedge-level pretext task objectives could not improve the performance of HyperGene. Variant-IV with tree expansion could also not achieve improvements over original methods. Further sophisticated model training and variants are left for future work.

| Models       | Cora-noisy | Cora-clean | Pubmed-noisy | Pubmed-clean | Corum  | Disgenet |
|--------------|------------|------------|--------------|--------------|--------|----------|
| Variant-I    | 78.97±3.69 | 84.13±2.65 | 84.72±1.22   | 88.20±0.68   | 84.65±0.05 | 33.00±2.69 |
| Variant-II   | 76.20±2.21 | 81.84±0.65 | 83.25±0.66   | 87.42±1.24   | 82.98±1.81 | 30.72±0.76 |
| Variant-III  | 74.17±1.82 | 82.19±2.16 | 85.09±0.92   | 88.11±0.90   | 83.12±0.31 | 31.54±2.39 |
| Variant-IV   | 76.56±1.43 | 82.64±0.39 | 85.56±0.39   | 87.32±0.97   | 68.24±1.41 | 32.15±2.10 |
| HyperGene (Exp.) | 78.78±1.28 | 83.77±1.62 | 86.94±0.73   | 90.84±0.29   | 85.33±1.09 | 33.90±2.26 |