Classification of Edge-dependent Labels of Nodes in Hypergraphs

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ABSTRACT

A hypergraph is a data structure composed of nodes and hyperedges, where each hyperedge is an any-sized subset of nodes. Due to the flexibility in hyperedge size, hypergraphs represent group interactions (e.g., co-authorship by more than two authors) more naturally and accurately than ordinary graphs. Interestingly, many real-world systems modeled as hypergraphs contain edge-dependent node labels, i.e., node labels that vary depending on hyperedges. For example, on co-authorship datasets, the same author (i.e., a node) can be the primary author in a paper (i.e., a hyperedge) but the corresponding author in another paper (i.e., another hyperedge).

In this work, we introduce a classification of edge-dependent node labels as a new problem. This problem can be used as a benchmark task for hypergraph neural networks, which recently have attracted great attention, and also the usefulness of edge-dependent node labels has been verified in various applications. To tackle this problem, we propose WHATSNET, a novel hypergraph neural network that represents the same node differently depending on the hyperedges it participates in by reflecting its varying importance in the hyperedges. To this end, WHATSNET models the relations between nodes within each hyperedge, using their relative centrality as positional encodings. In our experiments, we demonstrate that WHATSNET significantly and consistently outperforms ten competitors on six real-world hypergraphs, and we also show successful applications of WHATSNET to (a) ranking aggregation, (b) node clustering, and (c) product return prediction.

CCS CONCEPTS

• Information systems → Data mining; Social networks; • Computing methodologies → Machine learning.

KEYWORDS

Hypergraph, Graph Neural Network, Edge-Dependent Node Label

INTRODUCTION

Real-world relationships are complex and often go beyond pairwise relations. For example, a research paper is usually coauthored by a group of researchers, and an email is often sent to multiple receivers. A *hypergraph* is a natural representation of such group relations [7, 8, 16, 34, 36]. It consists of nodes and hyperedges, and each hyperedge is a set of any number of nodes (see Figure 1). Hypergraph modeling is used in various fields, including recommendation systems [22, 50, 61], and physics [21], leading to better performance than ordinary-graph modeling in node clustering [60], interaction prediction [64], anomaly detection [35], etc.

To leverage the advantages of hypergraph modeling, several hypergraph neural networks [3, 5, 12, 17, 20, 26, 27, 62] have been proposed. They commonly involve propagating node embeddings

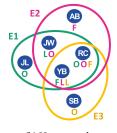
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Authors(Nodes)

Publications (Hyperedges)

- E1: Curriculum learning Y Bengio, J Louradour, R Collobert, J Weston - ICML'09
- E2: Learning structured embeddings of knowledge base A Bordes, J Weston, R Collobert, Y Bengio - AAAI'11
 E3: A parallel mixture of SVMs for very large scale
- R Collobert, S Bengio, Y Bengio NeurIPS'01

 (a) Example data: Coauthors in publications



(b) Hypergraph

Figure 1: The three publications by the six authors in (a) are modeled as the hypergraph with six nodes and three hyperedges in (b). The labels of nodes indicate the orders of the authors (First, Last, or Others) in each publication, and thus they are dependent on hyperedges.

to incident hyperedges for updating, which are subsequently propagated back to the nodes. Most of them have been evaluated on node classification tasks, focusing on the global properties of nodes.

However, in many real-world hypergraphs, node properties vary depending on the hyperedges they are involved in. For instance, in co-authorship, the same researcher can be the primary author in one paper but the corresponding author in another paper, as shown in Figure 1. In emails, the same person can be a receiver or a sender in different emails, and in online Q&A platforms, a person can be a questioner and an answerer in different posts. These edge-dependent node properties have proven useful in various tasks, such as ranking aggregation [13], node clustering [23], product-return prediction [38], and anomaly detection [35].

In this work, we introduce a classification of edge-dependent node labels as a new problem for hypergraphs. The problem works as an effective hypergraph-learning benchmark task that is complementary to common benchmark tasks (e.g., node classification, hyperedge prediction, and clustering) for three reasons. First, it evaluates the capability of models in capturing features unique to hypergraphs. Edge-dependent node labels are unique to hypergraphs and cannot be easily expressed if we decompose hyperedges into pairwise edges between nodes. Second, as shown in our experiments, using node and hyperedge embeddings obtained by existing hypergraph neural networks leads to limited performance for the problem. Lastly and most importantly, it has extensive real-world applications. For example, it can be used to predict the toxicity of chemical compounds (nodes) in specific reactions (hyperedges), offer guidance to students (nodes) who are expected to make limited contributions in group projects (hyperedges), and classify homonyms (nodes) based on the context of sentences (hyperedges). Moreover, the outputs of this problem (i.e., edge-dependent node properties) have proven to be useful in various applications.

In order to tackle the new classification task, we propose WHAT-sNet (Within-Hyperedge Attention Transformer Network). Most existing hypergraph neural networks do not explicitly consider edge-dependent relationships between node pairs within each hyperedge. We design WithinATT, an attention mechanism where the edge-dependent embedding of each node is computed by attending to the other nodes in each hyperedge. Inspired by the usefulness of positional encodings in the attention mechanism, we additionally use the centrality order of nodes within each hyperedge as the positional encoding, which makes attention in WithinATT even more edge-dependent. The effectiveness of WHATsNet on the proposed task is demonstrated through extensive experiments. Our contributions are summarized as follows:

- New Problem: To the best of our knowledge, we are the first to address the problem of classifying edge-dependent node labels. This problem is based on a unique property of hypergraphs and closely related to real-world applications.
- Effective Model: To tackle the problem, we design WHATsNET, a novel hypergraph neural network with attention and positional-encoding schemes that explicitly consider edge-dependent relationships between nodes.
- Extensive Experiments: Using six real-world hypergraphs, we demonstrate the superiority of WHATsNet over 10 competitors on the considered task. We also show the usefulness of WHATsNet in three applications: ranking aggregation, node clustering, and product-return prediction.

For reproducibility, we make the code and data available at [14].

The rest of this paper is organized as follows. In Section 2, we review related works. In Section 3, we introduce preliminaries. In Section 4, we describe our new problem with its applications. In Section 5, we present WHATsNet, a hypergraph neural network for edge-dependent node classification. In Section 6, we provide experimental results. Lastly, we make conclusions in Section 7.

2 RELATED WORK

In this section, we briefly survey related works on hypergraph neural networks and positional encodings.

2.1 Hypergraph Neural Networks

Hypergraph neural networks generalize graph neural networks into higher-order relationships in hypergraphs by allowing propagation between nodes through hyperedges. Early models including HGNN [20] and HyperGCN [62] first transform a given hypergraph into an ordinary graph and then apply graph convolutions, losing high-order relationships embedded in hyperedges. HNHN [17] performs two steps of message passing using a nonlinear function to prevent equivalence to convolutions on the clique-expanded graph ¹. The first step updates hyperedge embeddings and the second updates node embeddings. HNHN can vary weights on the contribution of incident embeddings during aggregation through hyperparameters.

HCHA [5] and HAT [27] apply attention mechanisms to improve the aggregation of the incident node or hyperedge embeddings. The

attention weights are calculated from the concatenation of node and hyperedge embeddings, which change during training.

UniGNN [26] and AllSet [12] generalize graph neural networks to hypergraphs. UniGCNII is a special case of UniGNN that addresses over-smoothing, i.e., the convergence of embeddings of different nodes in deep (hyper)graph neural networks, by extending GC-NII [11] to hypergraphs. AllSet is a framework composed of two multiset functions and generalizes most models, including HGNN, HyperGCN, HNHN, and HCHA. AllSetTransformer replaces the multiset function with SetTransformer [37] and aggregates incident embeddings with attention to global learnable vectors.

A recent study with a similar motivation to ours presents a framework named HNN [3] for jointly learning hyperedge embeddings and a set of hyperedge-dependent node embeddings. But HNN makes the hyperedge-dependent node embeddings by simply concatenating the embeddings of nodes and incident hyperedges.

However, the importance of each node may vary depending on the other nodes it interacts with within each hyperedge, which may not be captured only by the relationship between the node and the hyperedge. Most existing hypergraph neural networks do not explicitly consider edge-dependent relationships between pairs of nodes within each hyperedge. Such relationships have been considered in a few studies in a way different from ours, but none of them directly apply to the considered problem. HyperSAGNN [67] is designed for hyperedge prediction, and it uses two kinds of embeddings: (1) static embeddings, which are obtained from node features independently of hyperedges, and (2) dynamic embeddings, which are calculated by aggregating the embeddings of the other nodes within hyperedges using pairwise attentions. The model is trained to minimize the discrepancy between the static embedding and dynamic embedding of each node. While HyperSAGNN uses pairwise attention, its goal is not to obtain hyperedge-dependent node representations. Higher-order Transformer [29] considers all subsets of nodes in each hyperedge,² and thus, computational and memory cost increases exponentially with the size of hyperedges. The model has been applied only to uniform hypergraphs where the size of every hyperedge is identical, and it is non-trivial to apply it to real-world hypergraphs with hyperedges of varying sizes.

2.2 Positional Encodings

It is known that many graph neural networks (GNNs) have difficulty in discriminating the positions of different nodes if the nodes share similar local structures [65]. To improve the representation power, various positional encodings for graphs have been proposed. Such positional encodings, which we call *absolute positional encodings*, are often added or concatenated to the node features, and they are based on random discriminating features [1, 52], Weisfeiler–Lehman [66], Laplacian Eigenvectors [6, 18, 33], random walk [2, 19, 39], etc. Alternatively, GNNs that are able to capture positional information of nodes [19, 58, 65] can be used.

In Transformer-based GNNs, such positional encodings are usually used to calculate attention. Graph Transformer [18] and SAN [33] use Laplacian eigenvectors, while Graph-Bert [66] uses the Weisfeiler algorithm [46]. Graphormer [63] adds the global degree centrality to node features to capture both semantic correlations

 $^{^1}$ A clique-expanded graph is an ordinary graph obtained by replacing each hyperedge with the clique composed by the constituent nodes.

 $^{^{2}2^{}e}$ for each hyperedge $e\subseteq\mathcal{V}$, where \mathcal{V} is the set of nodes

and node centrality differences. Its performance supports the effectiveness of employing node centrality as the positional encoding, which we also use in a different way for positional encoding.

Besides the absolute positional encodings, relative positional encodings [51, 53] are also used in Transformer-based GNNs to affect attention mechanisms based on the relative distance between a node pair (e.g., between a query and a key). The relative distance can be computed based on positive definite kernels on graphs [42], learnable positional embeddings [41], shortest path distance [49, 63], multi-step transition probability [68], etc. To the best of our knowledge, positional encodings specialized to hypergraphs have not been studied. In this work, we propose WITHINORDERPE, where the centrality order (i.e., ranking) of nodes within each hyperedge is used to encode the relative position within each hyperedge.

3 PRELIMINARIES

In this section, we introduce concepts necessary to describe our method. The frequently-used symbols are summarized in Table 1.

3.1 Hypergraphs

A hypergraph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ consists of a set of nodes $\mathcal{V} = \{v_1, \dots, v_N\}$ and a set of hyperedges $\mathcal{E} = \{e_1, \dots, e_M\} \subseteq 2^{\mathcal{V}}$. Each hyperedge $e \in \mathcal{E}$ is a non-empty subset of \mathcal{V} . We use $\mathcal{N}_v = \{e \in \mathcal{E} : v \in e\}$ to denote the set of hyperedges incident to the node v, i.e., the set of hyperedges that contain v.

3.2 Attention Functions

Scaled Dot-Product Attention. For n_q query vectors $\mathbf{Q} \in \mathbb{R}^{n_q \times d_k}$ and n_k key-value vector pairs $\mathbf{K} \in \mathbb{R}^{n_k \times d_k}$ and $\mathbf{V} \in \mathbb{R}^{n_k \times d_v}$, where d_k and d_v represent vector sizes, the scaled dot-product attention computes the weighted sum of value vectors as follows:

$$Attention(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = softmax(\frac{\mathbf{Q}\mathbf{K}^{\top}}{\sqrt{d_k}})\mathbf{V},$$

where $\sqrt{d_k}$ is typically used to avoid exploding gradients [57]. Note that the more similar a query vector and a key vector are (i.e., the larger their dot product is), the larger the corresponding weight is. **Multihead Attention**. The multihead attention [57] of dimension d_k consists of h attention modules of dimension d_k/h , whose outputs are concatenated for the final output, as follows:

$$MultiheadAttention(Q, K, V) = Concat(O_1, \dots, O_h)W^O,$$

where $O_i = Attention(Q_i, K_i, V_i) = Attention(QW_i^Q, KW_i^K, VW_i^V)$. That is, Q, K, and V are mapped into subspaces $Q_i \in \mathbb{R}^{n_q \times (d_k/h)}$, $K_i \in \mathbb{R}^{n_k \times (d_k/h)}$, and $V_i \in \mathbb{R}^{n_k \times (d_v/h)}$, respectively, by learnable parameters $W_i^Q \in \mathbb{R}^{d_k \times (d_k/h)}$, $W_i^K \in \mathbb{R}^{d_k \times (d_k/h)}$, and $W_i^V \in \mathbb{R}^{d_v \times (d_v/h)}$. In our experiments, the matrix $W^O \in \mathbb{R}^{d_v \times d_v}$ is fixed to the identity matrix, and the number of heads h is fixed to 4.

Multihead Attention Block. We use the multihead attention block (MAB) [57] as a component of our model. It consists of a multihead attention module, a feed-forward layer, residual connections [25], and layer normalization [4], as follows:

$$MAB(Q, K) = LayerNorm(H + FeedForward(H))),$$

Table 1: Frequently-used symbols.

Notation	Definition
$\mathcal{G} = (\mathcal{V}, \mathcal{E})$	a hypergraph with nodes ${\mathcal V}$ and hyperedges ${\mathcal E}$
N, M	the number of nodes and hyperedges
C	the number of (unique) edge-dependent node labels
v, e	a node $v \in \mathcal{V}$ and a hyperedge $e \in \mathcal{E}$
$y_{v,e}$	the edge-dependent label of node v in hyperedge e .
\mathcal{N}_v	the set of hyperedges incident to a node \boldsymbol{v}
l, m	the number of layers and inducing points
d_l	the hidden dimension at l -th layer
d_f	the dimension of WithinOrderPE
F	a node centrality feature matrix
I_w	trainable inducing points in WithinATT
$X^{(l)}, H^{(l)}$	a node/hyperedge embedding matrix at layer l
V_e, E_v	an embedding matrix of e and \mathcal{N}_v

where $\mathbf{H} = LayerNorm(\mathbf{Q} + MultiheadAttention(\mathbf{Q}, \mathbf{K}, \mathbf{K}))$. Note that the feed-forward layer does not change the dimensionality of the input matrix.

Attention with Inducing Points. The scaled dot-product attention module requires all-pair dot-products between the query vectors and key vectors, making its time complexity quadratic, specifically $O(n_q n_k)$. SetTransformer [37] introduces an attention scheme that reduces the complexity to be linear. With $m \ll \min(n_q, n_k)$ trainable inducing points, denoted by I, the all-pair dot-product MAB(\mathbf{Q} , \mathbf{K}) is approximated by MAB(\mathbf{Q} , MAB(\mathbf{I} , \mathbf{K})) whose time complexity is $O(m(n_q+n_k))$. We adopt this strategy in our model for efficiency.

4 PROBLEM DEFINITION: EDGE-DEPENDENT NODE CLASSIFICATION IN A HYPERGRAPH

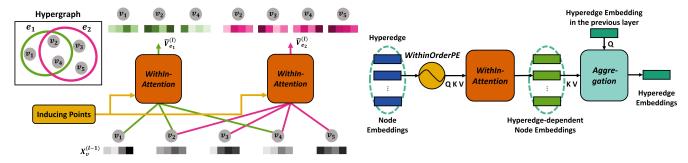
We formally define the edge-dependent node classification problem and introduce its direct applications to real-world tasks.

4.1 Problem Formulation

In classical node classification, a single label is assigned to a node. However, in hypergraphs, the labels of nodes can vary depending on the hyperedges that the nodes belong to. For example, in a co-authorship hypergraph, the role of a researcher is categorized into the first, the last, and the middle author, and the position is likely to change in other publications. In this work, we introduce the edge-dependent node classification problem, formalized as follows.

PROBLEM 1 (EDGE-DEPENDENT NODE CLASSIFICATION). Given (a) a hypergraph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, (b) a set of edge-dependent node labels in $\mathcal{E}' \subset \mathcal{E}$ (i.e., $y_{v,e}, \forall v \in e, \forall e \in \mathcal{E}'$), and optionally (c) a node feature matrix X, the problem is to correctly predict the unknown edge-dependent node labels in $\mathcal{E} \setminus \mathcal{E}'$ (i.e., $y_{v,e}, \forall v \in e, \forall e \in \mathcal{E} \setminus \mathcal{E}'$).

This problem serves as an effective benchmark task and complements common hypergraph learning benchmarks for the following reasons: First, the edge-dependent node labels are unique to hypergraphs and cannot be reduced to node labels in the clique-expanded graphs (see Footnote 1). Thus, we can evaluate the capability of methods in capturing these unique characteristics of hypergraphs. Second, as demonstrated in the experiment section 6, existing hypergraph neural networks have limitations in perfectly addressing



(a) Illustration of WITHINATT

(b) Architecture of WHATsNET in Hyperedge Embedding Update

Figure 2: (a) In the given hypergraph, which consists of $e_1 = \{v_1, v_2, v_4\}, e_2 = \{v_2, v_3, v_4, v_5\}$, WithinATT is applied to e_1 and e_2 independently. Even though the input feature of the node v_2 is the same, the output is different within e_1 and e_2 . The inducing points for efficiently calculating pairwise relations are used globally. (b) The embeddings of the nodes in the target hyperedge are fed into WithinATT after WithinOrderPE is added to each. Then, the outputs (i.e., edge-dependent node embeddings) are aggregated to update the embedding of the target hyperedge.

this problem. Lastly, the predictive outputs (i.e., edge-dependent node labels) can directly be applied to various applications.

4.2 Applications

Predicted edge-dependent node labels give information about the importance of nodes within each hyperedge, and leveraging this information has proven useful in a variety of applications.

Ranking Aggregation. The task is to predict the overall (global) ranking of entities based on partial (local) rankings. For example, in a multiplayer game where participants compete in matches, the aim of the task is to determine the global ranking of players using their local rankings from matches, enabling fair and competitive matches. For this task, we can construct a hypergraph where (a) each node is a player, (b) each hyperedge is a match, (c) and the participants of a match are labeled based on their contribution levels during the match, as described in [13]. A similar task can be considered for a co-authorship dataset. When the contribution level of each author in each publication is given, which is determined by the order of authors in each publication, the objective is to infer meaningful rankings for all authors.

Clustering. Clustering refers to the problem of grouping similar elements, and the problem is commonly considered for data analysis. Hayashi et al. [23] designed a node clustering algorithm that leverages edge-dependent node weights, demonstrating its high-quality clusters for real-world hypergraphs. Edge-dependent node labels, inferred by resolving Problem 1, can be directly transformed into node weights for clustering purposes. For example, in a co-authorship dataset, the weights of authors (nodes), determined by their positions (e.g., first, last, or others) within each publication (hyperedge), can be utilized to enhance clustering results.

Product Return Prediction. In E-commerce, predicting customers' intention to return products is helpful to take proactive actions. Li et al. [38] showed that the product return probability of each target basket can be accurately estimated by using hypergraphs where nodes and hyperedges are baskets and products, respectively, and baskets are labeled based on the number of each product they contain. The authors showed that these edge-dependent node labels are informative in predicting product returns. For instance, multiple purchases of the same product within a basket may indicate that

the customer purchases the same product with different colors or sizes, increasing the likelihood of product return.

5 PROPOSED MODEL: WHATSNET

We propose WHATsNet (Within-Hyperedge Attention Transformer Network) for edge-dependent node classification, with each layer consisting of two message passing steps: (1) updating hyperedge embeddings by aggregating node embeddings belonging to each hyperedge, and (2) updating node embeddings by aggregating hyperedge embeddings that include the corresponding node. In each step, input embeddings of nodes (or hyperedges) are adapted using an attention module called WithinATT, and then aggregated into hyperedge (or node) embeddings. WithinATT considers edgedependent (or node-dependent) relations between adjacent nodes (or hyperedges) by incorporating edge-dependent positional encodings named WithinOrderPE. The embeddings generated from the final layer are utilized to predict edge-dependent node labels.

5.1 WITHINATT: Attention to Other Nodes within Hyperedges

In many real-world hypergraphs, the importance or role of a node is shaped by the other nodes within the same hyperedge. For instance, if a grown-up researcher co-authors a paper only with students, she is likely to be the last author of the paper. Conversely, if she co-authors with other grown-up researchers, then the probability of her being the last author of that paper is relatively low.

Motivated by this observation, we devise WITHINATT based on Transformer [57], and it adapts a node embedding by attending to the other nodes in the same hyperedge. Specifically, it uses a set of node embeddings as queries, keys, and values in the attention mechanism. It, thereby, models and utilizes relations between nodes by taking the dot-product of all node pairs within the hyperedge.

However, calculating the dot-product for every node pair has computational complexity quadratic in the hyperedge size, making it challenging to use in large-scale real-world hypergraphs. To overcome this issue, we adopt the inducing point method (described in Section 3.2) in SetTransformer [37], which performs comparably to all-pair attention while being significantly more efficient.

Let $\mathbf{V}_e^{(l)} = \{\mathbf{X}_u^{(l)}: u \in e\}$ denote the set of the embeddings of nodes in a hyperedge e in the l-th layer, which are in the form of a matrix in $\mathbb{R}^{|e| \times d_l}$. Along with $\mathbf{V}_e^{(l)}$, WITHINATT uses m number of d_l -dimensional trainable inducing points $I_w \in \mathbb{R}^{m \times d_l}$, where m is typically much smaller than $\max_{e \in \mathcal{E}} |e|$. In our experiments, m is fixed to 4. Then, WITHINATT is formally expressed as follows:

WITHINATT(
$$\mathbf{V}_e^{(l)}; \mathbf{I}_w$$
) = MAB($\mathbf{V}_e^{(l)}, \text{MAB}(\mathbf{I}_w, \mathbf{V}_e^{(l)})$). (1)

Even though I_w is shared across all hyperedges, training the inducing points can be seen as finding a proper projection function for any input onto a lower-dimensional space. Additionally, the inner MAB (defined in Section 3.2) would summarize the node embeddings in e using the well-trained I_w . Through these outputs, the outer MAB would generate edge-dependent representations of nodes within e, leveraging the attention between the input node embeddings and the summary of them. Consequently, the resulting representations serve as an approximation of the attention between all node pairs while avoiding the quadratic complexity.

WITHINORDERPE: Using Centrality for **Positional Encoding**

We expect that edge-dependent node labels are closely related to the relative positions of nodes within each hyperedge, which can be measured, for example, by centrality relative to the other nodes in each hyperedge. For instance, in co-authorship datasets, degree centrality indicates the number of papers authored by each researcher. Hence, the author with the highest centrality among all authors of a paper is more likely to be the last author.

Based on this reasoning, we devise WITHINORDERPE, a positional encoding that facilitates edge-dependent attention between nodes within each hyperedge. Specifically, we use the relative order of node centrality within the hyperedge for WITHINORDERPE. We define the *order* of each element *a* in a set *A* as follows:

$$Order(a, A) = \sum_{a' \in A} \mathbb{1}(a' \le a). \tag{2}$$

Then, given node centralities $\mathbf{F} \in \mathbb{R}^{N \times d_f}$ where d_f is the number of centrality measures, corresponding to the dimensionality of positional encodings, we define WithinOrderPE of a node v within a hyperedge *e* as follows:

$$\text{WITHINORDERPE}(v,e;\mathbf{F}) = \mid\mid_{i=1}^{d_f} \frac{1}{|e|} Order(\mathbf{F}_{v,i}, \{\mathbf{F}_{u,i}: \forall u \in e\}),$$
 (3

where || represents the concatenation of the orders with respect to different centrality measures. We simply add WITHINORDERPE to the node embeddings and feed them into WITHINATT. In our experiments, we leverage four types of node centrality: degree, eigenvector centrality, PageRank, and coreness. Details of them are provided in Appendix B.2.

Similarly, for the message passing from hyperedges to nodes, we explicitly give the target node's order within the source hyperedge. In other words, the same position encoding is used for each hyperedge-node pair in both directions of message passing. This is because the role of a hyperedge e with respect to the target node $v \in e$ is also affected by the importance of node v in e.

WHATsNET: Our Final Model

We introduce WHATsNET, a hypergraph neural network that integrates the afore-described modules. In each layer, hyperedge embeddings are first updated and then node embeddings are updated. Before updating hyperedge embeddings, edge-dependent node embeddings are computed by incorporating edge-dependent relationships between nodes within each hyperedge via WITHI-NATT (Eq. (5)) and WITHINORDERPE (Eq. (4)). The hyperedge embedding is then updated by aggregating these edge-dependent node embeddings with weights determined by the dot-product with the hyperedge embedding from the previous layer. This process can be simplified using MAB (defined in Section 3.2) (Eq. (6)). Specifically, a hyperedge e's embedding $\mathbf{H}_{e}^{(l)}$ is updated as follows:

$$\mathbf{V}_{e, \boxplus}^{(l)} = \{\mathbf{X}_v^{(l-1)} \boxplus \mathbf{WithinOrderPE}(v, e)) : v \in e\}, \tag{4}$$

$$\tilde{\mathbf{V}}_{e}^{(l)} = \text{WithinATT}(\mathbf{V}_{e, \mathbb{H}}^{(l)}), \tag{5}$$

$$\mathbf{H}_{e}^{(l)} = \text{MAB}(\mathbf{H}_{e}^{(l-1)}, \tilde{\mathbf{V}}_{e}^{(l)})$$
 (6)

embeddings, after matching the dimension of the former with that of the latter through a learnable weight matrix, $\mathbf{W} \in \mathbb{R}^{d_f \times d_{l-1} \ 3}$.

Similarly, node embeddings are updated by aggregating (Eq. (9)) node-dependent hyperedge embeddings from WITHINATT (Eq. (8)) and WITHINORDERPE (Eq. (7)). Specifically, a node v's embedding $\mathbf{X}_{n}^{(l)}$ is updated as follows:

$$\mathbf{E}_{v,\mathbb{H}}^{(l)} = \{\mathbf{H}_{e}^{(l)} \boxplus \text{WithinOrderPE}(v,e)) : e \in \mathcal{N}_{v}\}, \tag{7}$$

$$\tilde{\mathbf{E}}_{n}^{(l)} = \text{WithinATT}(\mathbf{E}_{n}^{(l)}), \tag{8}$$

$$\mathbf{X}_{v}^{(l)} = \text{MAB}(\mathbf{X}_{v}^{(l-1)}, \tilde{\mathbf{E}}_{v}^{(l)})$$
 (9)

One can stack more than one WITHINATT module before aggregation to make attention between nodes within each hyperedge even more edge-dependent. We stack two WITHINATT modules in our experiments.

Application to Edge-Dependent Node Classification

Given node and hyperedge embeddings, we predict edge-dependent node labels with a single-layer perceptron classifier, denoted as ψ , which takes the concatenation of node and hyperedge embeddings as its input. Let $X^{(L)}$ and $H^{(L)}$ be the node and hyperedge embeddings generated from the last *L*-th layer of WHATsNET respectively. Then, the label of a node v in a hyperedge e is predicted as follows:

$$\hat{y}_{(v,e)} = \arg\max(\psi([\mathbf{X}_v^{(L)} \parallel \mathbf{H}_e^{(L)}])). \tag{10}$$

Eq. (10) can readily be applied to other hypergraph neural networks, such as HNHN [17], that generate separate node and hyperedge embeddings as their outputs. Thus, any accuracy gain of WHATsNET with Eq. (10), compared to such models, is attributed to its ability to generate more informative node and hyperedge embeddings.

Alternatively, one can utilize intermediate edge-dependent node embeddings $\tilde{\mathbf{V}}_e^{(L)} \in \mathbb{R}^{|e| \times d_L}$ in Eq. (5), which are generated inside a WHATsNет layer:

$$\frac{\bar{y}_{(v,e)} = \arg\max(\psi(\tilde{\mathbf{V}}_e^{(L)}[v]))}{{}^3\text{Formally, }\mathbf{A} \boxplus \mathbf{B} = \mathbf{A} + \mathbf{B}\mathbf{W} \text{ where }\mathbf{A} \in \mathbb{R}^{n \times d_A}, \, \mathbf{B} \in \mathbb{R}^{n \times d_B} \text{ and } \mathbf{W} \in \mathbb{R}^{d_B \times d_A}.$$

Dataset	Num. of Nodes	Num. of Hyperedges	Max. of Node Deg.	Max. of Hyperedge Size	Sum of Hyperedge Size	Num. of Class 0	Num. of Class 1	Num. of Class 2	Corr. w/ Centrality	Avg. Entropy
Coauth-DBLP	108,484	91,266	236	36	321,011	91,266	138,479	91,266	0.19	0.13
Coauth-AMiner	1,712,433	2,037,605	752	115	5,129,998	2,037,605	1,652,332	1,503,061	0.24	0.13
Email-Enron	21,251	101,124	18,168	948	1,186,521	635,268	450,129	101,124	0.10	0.28
Email-Eu	986	209,508	8,659	59	541,842	209,508	332,334	-	0.24	0.48
Stack-Biology	15,490	26,823	1,318	12	56,257	26,290	18,444	11,523	0.29	0.10
Stack-Physics	80,936	200,811	6,332	48	479,809	194,575	201,121	84,113	0.30	0.12

Table 2: Summary of real-world hypergraphs with edge-dependent labels.

where [v] means indexing the vector corresponding to node v. In this way, one can avoid conducting the explicit concatenation with hyperedge embeddings, since $\tilde{\mathbf{V}}_e^{(L)}$ already has such information.

Table 11 in Appendix B compares the two approaches of Eq. (10) and (11).⁴ There is no clear superiority between the two choices, and both of them consistently outperform the best competitor. Still, we choose the first approach as our default choice because it is more general and memory-efficient: we can store the node and hyperedge embeddings separately and then concatenate them for any downstream task utilizing edge-dependent node embeddings.⁵

5.5 Complexity Analysis

We analyze the time and space complexities of WHATsNET.

Time Complexity. WithinATT requires dot products between the input embeddings and inducing points, and the aggregation involves dot products between the input embeddings and a single query. Thus, the total time complexity of the inference step of WHATSNET without WithinOrderPE is $O(\sum_{l=1}^L (\sum_{e \in \mathcal{E}} (|e|md_l) + \sum_{v \in \mathcal{V}} (|N_v|md_l))) = O(m \sum_{l=1}^L d_l \sum_{e \in \mathcal{E}} |e|)$, where the last equality is from $\sum_{v \in \mathcal{V}} |N_v| = \sum_{e \in \mathcal{E}} |e|$. As for WithinOrderPE, we first compute four node centralities of each node (spec., degree, coreness, eigenvector centrality, and PageRank), whose complexity is $O(\sum_{e \in \mathcal{E}} |e|)$ (see Appendix C for details). Next, we compute the order of nodes within hyperedges by sorting nodes based on each centrality value, whose time complexity is $O(\sum_{e \in \mathcal{E}} |e| \log |e|)$. Thus, the complexity of computing WithinOrderPE is $O(\sum_{e \in \mathcal{E}} |e| \log |e|)$, and the total time complexity of WHATsNet with WithinOrderPE is $O(m \sum_{l=1}^L d_l \sum_{e \in \mathcal{E}} |e| + \sum_{e \in \mathcal{E}} |e| \log |e|)$.

Space Complexity. We consider full-batch training. Storing the input hypergraph $\mathcal{G}=(\mathcal{V},\mathcal{E})$ and the d_f -dimensional positional encodings obtained by WithinorderPE requires $O(d_f\sum_{e\in\mathcal{E}}|e|)$ space. We first consider the message passing from nodes to hyperedges at the l-th layer. Withinatt requires (a) node embeddings, whose size $O(|V|d_l)$, (b) a weight matrix for adjusting the dimension of positional encodings, whose size is $O(d_fd_l)$, and (c) m inducing points of d_l dimension, whose size is $O(md_l)$. It also requires two attention matrices between the inputs and m inducing points, whose sizes are |e| by m and m by |e| for each hyperedge e. Thus, the additional space required for the node-to-hyperedge message passing is $O(md_l + d_fd_l + |V|d_l + m\sum_{e\in\mathcal{E}}|e|)$.

Similarly, the message passing from hyperedges to nodes at the l-th layer requires $O(md_l + d_f d_l + |E|d_l + m \sum_{v \in V} |\mathcal{N}_v|)$. Since

 $\sum_{v \in \mathcal{V}} |\mathcal{N}_v| = \sum_{e \in \mathcal{E}} |e|, \text{ the total space complexity of WHATsNet}$ with L layers is $O((m+d_f+|\mathcal{V}|+|\mathcal{E}|) \sum_{l=1}^{L} d_l + (Lm+d_f) \sum_{e \in \mathcal{E}} |e|)$.

5.6 Comparison to Existing Models

To efficiently capture the edge-dependent relationships between node pairs within hyperedges, we incorporate the encoder part of SetTransformer [37] as a component of the message passing in our model. It is important to note that SetTransformer is primarily designed to obtain proper representations of sets, and its primary focus is not on hypergraph representation learning.

While both WHATsNet and SetTransformer aggregate input embeddings using a weighted sum, there are notable differences in the aggregation methods. SetTransformer uses weights obtained by attending to a global learnable parameter, whereas WHATsNet attends to the previous embedding of the target. Additionally, WHATsNet incorporates WithinOrderPE into attention, enhancing its ability to capture edge-dependent relationships within hyperedges.

There is another approach, called AllSetTransformer [12], which integrates SetTransformer into hypergraph neural networks. However, it should be noted that AllSetTransformer does not adopt the encoder part of SetTransformer but instead adopts its decoder with modifications to the number of stacking feed-forward layers in the multi-head attention block. Therefore, the usage of SetTransformer in AllSetTransformer differs from how WHATSNET utilizes it.

6 EXPERIMENTAL RESULTS

We evaluate WHATsNET by answering the following questions:

- Q1. Does WHATsNet accurately predict the edge-dependent labels of nodes?
- Q2. Does WHATsNET classify the same node differently depending on hyperedges?
- Q3. Does each component of WHATsNET make a meaningful contribution to the performance?
- Q4. How can we apply WHATsNET to real-world downstream tasks? Does WHATsNET show usefulness in these tasks?

6.1 Experimental settings

<u>Datasets.</u> We use six real-world hypergraphs from three domains:

Co-authorship (DBLP [54] and AMinerAuthor⁶): Each hyperedge indicates a publication, and the nodes in it are the authors of the publication. Edge-dependent node labels indicate the orders of authors (first, last, or others) in each publication. We exclude publications where the authors are in alphabetical order, which may not reflect the difference in the authors' contributions.

 $^{^4\}mathrm{We}$ remove WithinorderPE from the last layer of WHATsNet when applying the approach of Eq. (11), because if not, the node centralities affect the classification performance too much.

⁵which is O(N+M) instead of O(NM) when N nodes and M hyperedges exist.

⁶https://www.aminer.org/aminernetwork

Dataset	Metric	BaselineU	BaselineP	HNHN	HGNN	HCHA	HAT	UniGCNII	HNN	HST	AST	WHATsNet
Coauth- DBLP	MicroF1 MacroF1	0.333 ± 0.001 0.330 ± 0.001	$\begin{array}{c} 0.346 \pm 0.001 \\ 0.332 \pm 0.001 \end{array}$	$0.486 \pm 0.004 \\ 0.478 \pm 0.008$	$0.540 \pm 0.004 \\ 0.519 \pm 0.002$	$0.451 \pm 0.007 \\ 0.334 \pm 0.048$	$0.503 \pm 0.004 \\ 0.483 \pm 0.006$	0.497 ± 0.003 0.476 ± 0.002	0.488 ± 0.006 0.482 ± 0.006	$ \begin{vmatrix} 0.564 \pm 0.004 \\ 0.549 \pm 0.003 \end{vmatrix} $	0.495 ± 0.038 0.487 ± 0.040	$\begin{array}{c} \textbf{0.605} \pm 0.002 \\ \textbf{0.595} \pm 0.002 \end{array}$
Coauth- AMiner	MicroF1 MacroF1	$\begin{vmatrix} 0.334 \pm 0.000 \\ 0.332 \pm 0.000 \end{vmatrix}$	0.339 ± 0.000 0.333 ± 0.000	$0.520 \pm 0.002 \\ 0.514 \pm 0.002$	$0.566 \pm 0.002 \\ 0.551 \pm 0.004$	$0.468 \pm 0.020 \\ 0.447 \pm 0.040$	$0.543 \pm 0.002 \\ 0.533 \pm 0.003$	$0.520 \pm 0.001 \\ 0.507 \pm 0.001$	$0.543 \pm 0.002 \\ 0.533 \pm 0.002$	$ \begin{vmatrix} 0.596 \pm 0.007 \\ 0.583 \pm 0.008 \end{vmatrix} $	0.577 ± 0.005 0.570 ± 0.002	$\begin{array}{c} \textbf{0.630} \pm 0.005 \\ \textbf{0.623} \pm 0.007 \end{array}$
Email- Enron	MicroF1 MacroF1	$ \begin{vmatrix} 0.334 \pm 0.001 \\ 0.300 \pm 0.001 \end{vmatrix} $	0.439 ± 0.001 0.333 ± 0.001	0.738 ± 0.028 0.637 ± 0.023	$0.725 \pm 0.004 \\ 0.674 \pm 0.003$	0.666 ± 0.010 0.464 ± 0.002	$0.817 \pm 0.001 \\ 0.753 \pm 0.004$	$0.734 \pm 0.010 \\ 0.656 \pm 0.010$	0.763 ± 0.003 0.679 ± 0.007	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	0.796 ± 0.014 0.719 ± 0.020	$\begin{array}{c} \textbf{0.826} \pm 0.001 \\ \textbf{0.760} \pm 0.004 \end{array}$
Email- Eu	MicroF1 MacroF1	$\begin{array}{c} 0.500 \pm 0.001 \\ 0.493 \pm 0.001 \end{array}$	0.525 ± 0.001 0.499 ± 0.001	$0.643 \pm 0.004 \\ 0.552 \pm 0.014$	$0.633 \pm 0.001 \\ 0.533 \pm 0.008$	$0.620 \pm 0.000 \\ 0.497 \pm 0.001$	$0.669 \pm 0.001 \\ 0.638 \pm 0.002$	$0.630 \pm 0.005 \\ 0.565 \pm 0.013$	OutOfMemory OutOfMemory	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	0.666 ± 0.005 0.624 ± 0.021	$\begin{array}{c} \textbf{0.671} \pm 0.000 \\ \textbf{0.646} \pm 0.003 \end{array}$
Stack- Biology	MicroF1 MacroF1	0.335 ± 0.000 0.326 ± 0.000	$0.368 \pm 0.001 \\ 0.334 \pm 0.003$	0.640 ± 0.005 0.592 ± 0.006	0.689 ± 0.002 0.624 ± 0.007	0.589 ± 0.007 0.465 ± 0.060	0.661 ± 0.005 0.606 ± 0.005	0.610 ± 0.004 0.433 ± 0.007	0.618 ± 0.015 0.568 ± 0.013	0.694 ± 0.002 0.631 ± 0.006	0.571 ± 0.054 0.446 ± 0.081	0.742 ± 0.003 0.686 ± 0.004
Stack-	MicroF1	0.333 ± 0.001	0.370 ± 0.000	0.506 ± 0.053	0.686 ± 0.004	0.622 ± 0.003	0.708 ± 0.005	0.671 ± 0.022	0.683 ± 0.005	0.755 ± 0.010	0.728 ± 0.039	0.770 ± 0.003

 $MacroF1 \quad 0.322 \pm 0.001 \quad 0.332 \pm 0.000 \quad 0.422 \pm 0.043 \quad 0.630 \pm 0.002 \quad 0.481 \pm 0.007 \quad 0.643 \pm 0.009 \quad 0.492 \pm 0.016 \quad 0.617 \pm 0.005 \quad 0.666 \pm 0.013 \quad 0.646 \pm 0.046 \quad 0.707 \pm 0.004 \quad 0.$

Table 3: Results of Edge-Dependent Node Classification: Mean and standard deviation of Micro-F1 and Macro-F1 scores over five independent runs are reported. Best scores are in bold. Note that WHATSNET performs best in all datasets.

- Email (Enron⁷ and Eu [48]): Each hyperedge represents an email, and the nodes in it represent the people involved in the email. Edge-dependent labels distinguish (1) the sender, (2) the receivers, and (3) the CC'ed.
- StackOverflow (Biology⁸ and Physics⁸): Each hyperedge represents a post, and the nodes in it are the users contributing to this post. Edge-dependent labels distinguish (1) the questioner, (2) answerers chosen by the questioner, and (3) the other answerers.

Table 2 shows some statistics for the datasets. We measure the correlation coefficient between within-edge node-centrality orders and edge-dependent node labels, using the average of Cramer's coefficient matrix [15]. We also report the average entropy in each node's label distribution. Note that the average entropy is non-zero in all datasets, implying that node labels do vary across hyperedges. Competitors. We implemented all models using Deep Graph Library (DGL) [59]. In all competitors, edge-dependent labels are predicted by a single-layer perceptron from the concatenation of the global embeddings of nodes and hyperedges, as in ours (Eq. (10)). As competitors, we use seven hypergraph neural networks that generate both hyperedge and node embeddings and thus can be used for edge-dependent node classification: HNHN [17], HGNN [20], HCHA [5], HNN [3], HAT [27], UniGCNII [26], and AllSetTransformer (AST) [12]. We do not include HyperGCN [62] as a competitor because it does not provide hyperedge embeddings. In addition, we consider HypergraphSetTransformer (HST), which extends SetTransformer [37] to hypergraphs by applying it to obtain the representations of sets of incident nodes and hyperedges in the two stages of message passing. Lastly, we consider two simple approaches for comparison: (a) BaselineU, which predicts node labels uniformly at random, and (b) BaselineP, which randomly assigns labels proportionally to their global distribution.

Other Settings. Since external features are absent, we create initial node features by adopting 2nd-order random walks on hypergraphs as in [67]. Specifically, we construct fixed-length random walks for each node and obtain embeddings using a skip-gram model [43, 44]. All parameters are initialized via Xavier initialization [24] and trained with Adam optimizer [30]. WITHINORDERPE incorporates four centrality measures: degree, coreness, eigenvector centrality, and PageRank (refer to Appendix B.2). We randomly divide all hyperedges in each hypergraph into training (60%), validation (20%),

and test (20%) sets. For the edge-dependent node classification task, we stop training when the number of epochs reaches 100 or the accuracy on the validation set no longer improves for 25 epochs. Whereas, for downstream tasks, we stop training when the number of epochs reaches 300 or the mean of Micro-F1 and Macro-F1 scores does not change for 10 epochs. We use the search space described in Appendix A for hyperparameter tuning. We select the hyperparameter values that maximize the mean of Micro-F1 and Macro-F1 scores on the validation set and report its performance on the test set over five independent runs.

6.2 Q1. Edge-Dependent Node Classification

To evaluate the performance of WHATsNET for the edge-dependent node classification, we measure the predictive performances using Micro-F1 and Macro-F1 scores on test data, averaged over five runs. Table 3 shows that WHATsNET *consistently* achieves the highest scores in terms of both Micro-F1 and Macro-F1. While HST performs well overall and ranks second, the statistical analysis using the Wilcoxon signed-rank test indicates that WHATsNET is significantly better than HST with a p-value less than 0.05 in almost all cases (only except for Macro-F1 in Email-Enron and Micro-F1 in Email-Eu). Some other models, including HGNN and HAT, perform well on specific datasets but fail to achieve overall success. HNN runs out of memory on the email-Eu dataset due to the large size of the random-walk hyperedge transition matrix.⁹

We would like to emphasize that HST, AST, and WHATSNET utilize different aggregation methods, and relationships among nodes within each hyperedge (or among hyperedges incident to each node) are explicitly considered only in HST and WHATSNET. Additionally, positional encoding is used only in WHATSNET (see Section 5.6). Thus, the fact that AST underperforms HST and WHATSNET supports the effectiveness of WITHINATT, and the fact that WHATSNET outperforms HST supports the usefulness of WITHINORDERPE and our aggregation method.

Figure 3 visually demonstrates the effectiveness of WHATSNET using the Coauthorship-DBLP dataset. The visualization showcases (a) the embeddings of hyperedges containing a specific node and (b) the concatenated embeddings of all incident pairs of nodes and hyperedges in the test set. Notably, the embeddings exhibit clear distinctions based on the edge-dependent labels.

⁷https://www.cs.cmu.edu/ enron/

⁸https://archive.org/download/stackexchange

 $^{^9}$ Implementation details of HNN can be found in [14].

Table 4: <u>Jensen-Shannon divergence (JSD)</u> between Ground-truth and <u>Predicted Node Label Distributions</u>: The average and standard deviation of the average JSD over five independent runs are reported. The lower JSD is, the better a model preserves node-level label distributions. Best scores are in bold. WHATSNET yields the lowest JSD in all datasets.

Dataset	BaselineU	BaselineP	HNHN	HGNN	НСНА	HAT	UniGCNII	HNN	HST	AST	WHATsNet
Coauth-DBLP	0.532 ± 0.002	0.518 ± 0.002	0.450 ± 0.002	0.394 ± 0.005	0.450 ± 0.002	0.429 ± 0.004	0.449 ± 0.006	0.450 ± 0.003	0.388 ± 0.006	0.453 ± 0.038	0.350 ± 0.002
Coauth-AMiner	0.529 ± 0.000	0.523 ± 0.000	0.440 ± 0.003	0.372 ± 0.002	0.462 ± 0.002	0.414 ± 0.003	0.424 ± 0.002	0.411 ± 0.003	0.356 ± 0.005	0.382 ± 0.009	0.328 ± 0.004
Email-Enron	0.486 ± 0.002	0.395 ± 0.001	0.162 ± 0.003	0.212 ± 0.007	0.291 ± 0.007	0.157 ± 0.004	0.187 ± 0.002	0.205 ± 0.002	0.302 ± 0.233	0.178 ± 0.019	0.136 ± 0.001
Email-Eu	0.199 ± 0.006	0.164 ± 0.004	0.232 ± 0.009	0.291 ± 0.001	0.268 ± 0.002	0.154 ± 0.004	0.300 ± 0.004	OutOfMemory	0.158 ± 0.005	0.168 ± 0.015	0.151 ± 0.009
Stack-Biology	0.536 ± 0.001	0.467 ± 0.003	0.266 ± 0.007	0.202 ± 0.003	0.237 ± 0.016	0.235 ± 0.006	0.263 ± 0.004	0.311 ± 0.026	0.200 ± 0.002	0.259 ± 0.022	0.152 ± 0.002
Stack-Physics	0.532 ± 0.001	0.482 ± 0.001	0.286 ± 0.036	0.219 ± 0.008	0.289 ± 0.004	0.227 ± 0.006	0.285 ± 0.050	0.292 ± 0.005	0.162 ± 0.008	0.185 ± 0.021	0.141 ± 0.003

Table 5: Real-World Applications of WHATSNET: In the three considered applications, utilizing hypergraphs with edge-dependent node labels predicted by WHATSNET (1) consistently outperforms using hypergraphs without such labels, (2) tends to outperform using edge-dependent node labels obtained by AST or HST (especially for clustering), and (3) performs comparably to and sometimes even better (especially for ranking aggregation) than using ground-truth labels.

(a) Ranking Aggregation (Accuracy)

Method Halo H-Index RW [13] w/ Ground Truth 0.711 0.675 RW [13] w/ WHATsNet 0.714 0.693 RW [13] w/ HST 0.707 0.695 RW [13] w/ AST 0.706 0.696 RW [13] w/o Labels 0.532 0.654

(b) Clustering (NMI: The higher, the better)

Method	DBLP	AMiner
RDC-Spec [23] w/ GroundTruth	0.221	0.359
RDC-Spec [23] w/ WHATsNET RDC-Spec [23] w/ HST RDC-Spec [23] w/ AST	0.184 0.166 0.168	0.352 0.339 0.332
RDC-Spec [23] w/o Labels	0.163	0.338

(c) Product Return Prediction (F1)

Method	Synthetic E-tail
HyperGO [38] w/ GroundTruth	0.738
HyperGO [38] w/ WHATsNET HyperGO [38] w/ HST HyperGO [38] w/ AST	0.723 <u>0.724</u> 0.721
HyperGO [38] w/o Labels	0.718

Table 6: <u>Ablation Study of WHATsNet</u>: The performance of WHATsNet is largely improved by WITHINATT and WITHINORDERPE, as shown in the average rankings of models.

Dataset	Metric	w/o WithinATT	w/o WithinOrderPE	WHATsNET
Coauth-	MicroF1	$ 0.581 \pm 0.004 \\ 0.577 \pm 0.003 $	0.591 ± 0.003	0.605 ± 0.002
DBLP	MacroF1		0.584 ± 0.003	0.595 ± 0.002
Coauth-	MicroF1		0.583 ± 0.095	0.630 ± 0.005
AMiner	MacroF1		0.536 ± 0.174	0.623 ± 0.007
Email-	MicroF1	$ \begin{vmatrix} 0.812 \pm 0.008 \\ 0.747 \pm 0.014 \end{vmatrix} $	0.825 ± 0.001	0.826 ± 0.001
Enron	MacroF1		0.762 ± 0.004	0.760 ± 0.004
Email-	MicroF1	$\begin{array}{c c} 0.651 \pm 0.019 \\ 0.630 \pm 0.018 \end{array}$	0.670 ± 0.000	0.671 ± 0.000
Eu	MacroF1		0.638 ± 0.002	0.646 ± 0.003
Stack- Biology	MicroF1 MacroF1	$\begin{array}{c c} 0.723 \pm 0.002 \\ 0.656 \pm 0.005 \end{array}$	0.732 ± 0.002 0.672 ± 0.004	0.742 ± 0.003 0.686 ± 0.004
Stack-	MicroF1	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	0.765 ± 0.002	0.770 ± 0.003
Physics	MacroF1		0.688 ± 0.008	0.707 ± 0.004
AVG.	MicroF1	2.83	2.17	1.00
Ranking	MacroF1	2.83	2.00	1.17

6.3 Q2. Node Label Distribution Preservation

In the task of edge-dependent node classification, each node may have different labels for different edges. That is, each node has its own ground-truth label distribution (node-level label distribution), which describes how many times it has each label. In this experiment, we aim to check how well WHATsNet preserves such node-level label distributions compared to the other baseline approaches. To this end, we measure the Jensen-Shannon divergence (JSD) [40] between the ground-truth and the predicted node-level label distribution for each node in the test data. The average JSD over all nodes is used as a metric to evaluate how well the model captures the ground-truth node-level label distributions. As shown in Table 4, WHATsNet outperforms all other models, with the lowest JSD in all datasets. This result suggests that WHATsNet preserves well the ground-truth node-level label distributions.

6.4 Q3. Ablation Study of WHATsNET

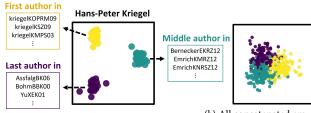
For an ablation study, we compare the performance of WHATsNET with two variants of it in Table 6: (a) WHATsNET w/o WITHINATT, where WITHINATT is removed and only the aggregation is used for message passing, and (b) WHATsNET w/o WITHINORDERPE, which computes WITHINATT without positional encodings.

Importance of WITHINATT. As shown in Table 6, WHATSNET consistently outperforms the variant without WITHINATT. This result demonstrates the importance of WITHINATT in achieving accurate edge-dependent node label classification. That is, considering relationships among nodes within each hyperedge is crucial for precise classification. In Appendix B.3, we also empirically confirm that the improvement is also contributed by WITHINATT among hyperedges containing each node, by using a variant without it. Figure 4 visually illustrates the effectiveness of WITHINATT by demonstrating WITHINATT makes node embeddings better distinguished based on edge-dependent labels.

Usefulness of WithinOrderPE. Table 6 also indicates that WHAT-sNet also performs better than the variant without WithinOrderPE in terms of both Micro F1 and Macro F1 scores across most datasets. This result supports that WithinOrderPE contributes to the improvement in performance. However, in the Email-Enron dataset, WithinOrderPE does not have a significant impact, which aligns with the lowest correlation between node labels and node centrality orders in Table 2. In Appendix B.1, we show that WithinOrderPE outperforms several positional encoding schemes, including global node-centrality ranks.

6.5 Q4. Usefulness in Downstream Tasks

To evaluate the usefulness of WHATsNET, we conduct experiments on three downstream tasks: ranking aggregation, clustering, and product return prediction (see Section 4.2). We compare the performance of the tasks using three different types of inputs: hypergraphs with (a) ground-truth edge-dependent node labels, (b)



- (a) Embeddings of publications containing "Hans-Peter Kriegel"
- (b) All concatenated embeddings of incident hyperedges and nodes

Figure 3: <u>Visualization of embeddings from WHATSNET.</u> (a) The embeddings of all publications of "Hans-Peter Kriegel" visualized using LDA. (b) The concatenated embeddings of all incident pairs of nodes and hyperedges in the test set, visualized in the same manner. Note that they are clearly clustered based on the edge-dependent labels.

labels predicted by hypergraph neural networks (spec., WHATsNet, HST, and AST) trained for our problem (i.e., edge-dependent node classification problem), and (c) no labels, respectively. We aim to demonstrate that even imperfect edge-dependent node labels predicted by the trained model (especially, by WHATsNET) lead to better performances, compared to those without labels. Refer to [14] for details of the edge-dependent node labels used in each task. Ranking Aggregation. This task aims to correctly predict the global node ranks using local node ranks in subsets (hyperedges). We use a recent random-walk-based method [13], where a random walker selects a node in each hyperedge proportionally to its rank within it, and the global node ranking is determined by the stationary distribution. We use two real-world datasets: (1) the Halo 2 game dataset, where scores (edge-dependent node labels) of players (nodes) in matches (hyperedges) of up to 8 players are given, and the global rankings of players need to be inferred; (2) the AMiner dataset, where the order of authorship (i.e., edge-dependent labels) in each publication is given to predict the rankings of all authors in terms of their H-index. For evaluation, we measure the accuracy in identifying the node with a higher rank for each node pair.

<u>Clustering.</u> From two co-authorship datasets, (1) DBLP and (2) AMiner, we group publications by venues as their ground-truth clusters. We use RDC-Spec [23], a well-performing method that uses spectral clustering and weighs authors differently according to their order (edge-dependent label) in each publication, as the backbone hypergraph clustering algorithm. For evaluation, we measure Normalized mutual information (NMI).

Product Return Prediction. We use a state-of-the-art method,

HyperGo [38], as the predictor for the returned product. It utilizes the information about the count of products in each basket, which corresponds to edge-dependent labels. We evaluate by F1 score of the predicted return probability of products in each target basket.

Results. As shown in Table 5, across all the examined applications, the utilization of imperfect edge-dependent node labels predicted by WHATsNet consistently leads to performance improvements compared to the results obtained without labels. Furthermore, these enhancements generally surpass those achieved by HST and AST. Surprisingly, in ranking aggregation, the performance is even higher than what is achieved by using ground-truth labels. We would like to emphasize that WHATsNet can be applied to any algorithm that

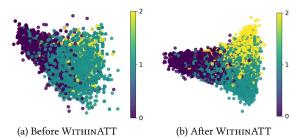


Figure 4: <u>Visualization of the effect of WITHINATT</u>. Node embeddings in StackOverflow-Biology (a) before and (b) after the WITHINATT module are visualized using LDA. WITHINATT makes node embeddings better distinguished based on edge-dependent labels, represented by different colors.

utilizes edge-dependent labels, and WHATSNET is not specialized to any of the methods considered for the tasks. The three application tasks are described in greater detail in [14].

7 CONCLUSIONS

In this work, we propose the edge-dependent node classification problem, which is a new benchmark task for hypergraph neural networks with various real-life applications. In order to tackle this problem, we devise WHATsNet, a hypergraph neural network for considering edge-dependent relationships between node pairs within each hyperedge. In our experiments with 6 real-world hypergraphs, WHATsNet consistently outperformed 10 competitors. Our contributions are summarized as follows:

- New Problem: We formulate the edge-dependent node classification problem with six real-world datasets and three applications.
- Effective Model: We propose WHATsNet, a novel hypergraph neural network equipped with the WITHINATT module and WITHINORDERPE. They are designed to capture edge-dependent relationships between node pairs within each hyperedge.
- Extensive Experiment: We empirically show the advantage of WHATsNeT over 10 competitors and the effectiveness of each component of it. We also demonstrated the usefulness of WHATsNeT in three applications.

For reproducibility, we make the code and data available at [14]. Acknowledgements. This work was supported by National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. NRF-2020R1C1C1008296) and Institute of Information & Communications Technology Planning & Evaluation (IITP) grant funded by the Korea government (MSIT) (No. 2022-0-00157, Robust, Fair, Extensible Data-Centric Continual Learning) (No. 2019-0-00075, Artificial Intelligence Graduate School Program (KAIST)).

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Hyperparameter	Datasets for Problem 1		Datasets for Downstream Tasks						
Tryperparameter	Coauth-AMiner	The others	Ranking Halo	Ranking H-Index	Clustering DBLP	Clustering AMiner	Synthetic E-tail		
Learning rate	0.001, 0.0001	0.001, 0.0001	0.0001, 0.001	0.0001, 0.0005	0.0001, 0.0005, 0.005	0.0001, 0.0005	0.001, 0.003, 0.005, 0.01, 0.03, 0.05		
Size of batch	256, 512	64, 128	128, 256	32, 64, 128	32, 64, 128	32, 64, 128	64, 128, 256, 512		
Number of layers	1, 2*	1, 2	1	1, 2	1, 2	1, 2	1, 2		

Table 7: Search spaces of hyperparameters.

PARAMETER SETTING

The search spaces of hyperparameters are given in Table 7. For all models, we fix the hidden dimension to 64, the final embedding dimension to 128, the number of the inducing points to 4, the number of attention layers to 2, and the dropout ratio to 0.7.

We employ sampling for efficiency in hyperedge-to-node message passing (but not in node-to-hyperedge message passing) and set the size of sampling (i.e. a set of hyperedges sampled among those incidents to each node) as follows: (a) All methods do not use sampling in Coauthorship-DBLP, (b) HST, AST, and WHATsNET sample 40 hyperedges in the other datasets, and (c) HNHN, HGNN, HCHA, HAT, and UniGCNII do not sample in StackOverflow-Biology but sample 40 or 100 hyperedges in the other datasets.

Exceptionally, for HCHA [5] and HNN [3], we use full-batch training without sampling. For a fair comparison, we tune their hyperparameters in a larger search space: {0.005, 0, 01, 0.03, 0.05, 0.1} for learning rates, {1, 2} for the number of layers, and {0.3, 0.5, 0.7} for dropout ratios, while we fix the dimension of final node and hyperedge embeddings to 128, the hidden dimension to 64, and the number of epochs to 300 with early stopping.

ADDITIONAL ABLATION STUDIES

Positional Encoding

We examine the usefulness of WITHINORDERPE by replacing it with alternative positional encoding schemes for graph neural networks (see Section 2.2). In our study, we initialize node features using random walks (see Section 6.1) so that they capture global positional information. Thus, we compare WithinOrderPE with two relative positional encodings: Shaw et al. [53] and GraphIT [42], using diffusion kernels [31] (DK) and the p-step random-walk kernel [42] (PRWK) for calculating distances between nodes. We also consider learnable positional encodings called LSPE [19], which are added to node embeddings (as WithinOrderPE is added) and updated together with other parameters. In addition, we consider WholeOrderPE, a variant of WITHINORDERPE that uses the global centrality order among all nodes, instead of the relative order within each hyperedge. Since the relative positional encoding methods pose challenges when used with inducing points, we do not employ inducing points consistently, and for WHATsNET, we consider two versions with and without inducing points. The base model for comparing positional encoding schemes is defined as follows:

$$\tilde{V}_e^{(l)} = MAB(V_e^{(l-1)}, V_e^{(l-1)}; PE)$$
 (12)

$$H_e^{(l)} = \text{MAB}(H_e^{(l-1)}, \tilde{V}_e^{(l)})$$
 (13)

$$\begin{split} H_e^{(l)} &= \text{MAB}(H_e^{(l-1)}, \tilde{V}_e^{(l)}) \\ X_v^{(l)} &= \text{MAB}(X_v^{(l-1)}, \text{WithinATT}(E_v^{(l)})) \end{split} \tag{13}$$

Only Eq. (12) depends on positional encoding schemes PE. To specifically investigate the impact of node positional encoding schemes, we do not employ any positional encodings for hyperedges.

The results are shown in Table 8, where WITHINORDERPE outperforms all other positional encoding methods, particularly surpassing WholeOrderPE. This highlights the effectiveness of incorporating relative order within hyperedges for positional encodings. It is worth noting that WHATsNET with inducing points, which offers improved efficiency, achieves competitive performance compared to WHATsNet without inducing points.

B.2 Node-centrality measures

We investigate the impact of node-centrality measures used in WITHINORDERPE on the performance of WHATsNet. We consider individually the following seven node-centrality measures:

- Degree: The number of hyperedges a node belongs to.
- Coreness [10, 28, 45]: The maximum k such that a node belongs to the *k*-core which is the maximal sub-hypergraph where every node has at least degree k within it.
- Eigenvector Centrality [9] and PageRank [47]: The eigenvector centrality and the PageRank score on a clique-expanded graph where each edge weight $w_{u,v} = |\{e \in \mathcal{E} : v \in e \text{ and } u \in e\}|$.
- H-Coreness [56]: Hypergraph core-periphery scores determining the proximity of nodes to the hypergraph core.
- H-Eigenvector [55]: Node and hyperedge centralities on hypergraphs using the max centrality model. Different positional encodings are used for different message-passing directions.
- Vector Centrality [32]: A vectorial measure of the roles of each node at different orders of interactions. The dimension of this measure is one less than the maximum hyperedge size.

In WHATsNET, we use only four centrality measures (spec., degree, coreness, eigenvector, and PageRank) for computational efficiency (see Appendix C for details). We additionally consider WHATsNETall, which uses all seven centrality measures together. Table 9 shows that the performance of WHATsNET is not highly sensitive to the choice of node centrality measures, and especially it consistently outperforms HST (the strongest baseline approach) regardless of the choice of centrality measures. Moreover, the results indicate that increasing the dimensionality of WITHINORDERPE tends to lead to performance improvement, which is evident from the high performance of vector centrality, WHATsNET, and WHATsNET-all, which utilize higher-dimensional WITHINORDERPE.

Advantage of using WITHINATT for both **B.3** directions

Recall that we devise the WITHINATT with the intention of capturing edge-dependent relationships between nodes within each hyperedge. However, we also utilize this module for the propagation from hyperedges to nodes. To validate the effectiveness of using WITHINATT in both directions, we replace the message passing from hyperedges to nodes with the aggregation methods used in HNHN (WHATsNET + HNHN) and HAT (WHATsNET + HAT).

^{*:} We use 1 layer for WHATsNET, AST, and HST.

Table 8: Comparison of positional encoding schemes. The symbol I_w denotes inducing points.

Da	Dataset Positional Encodings								Within	OrderPE
Da	iasei	w/o PE	GraphIT/DK	GraphIT/PRWK	Shaw/DK	Shaw/PRWK	LSPE	WholeOrderPE	w/o I _w	w/ I _w
Stack	MicroF1	0.732 ± 0.002	0.719 ± 0.006	0.710 ± 0.004	0.731 ± 0.003	0.456 ± 0.014	0.727 ± 0.003	0.732 ± 0.003	0.737 ± 0.006	0.737 ± 0.003
Biology	MacroF1	0.672 ± 0.004	0.645 ± 0.012	0.638 ± 0.012	0.667 ± 0.005	0.338 ± 0.038	0.658 ± 0.010	0.669 ± 0.011	$\textbf{0.680} \pm 0.005$	0.679 ± 0.007

Table 9: Comparison of node-centrality measures that can be used for WITHINORDERPE.

Da	taset	Degree	Coreness	Eigenvector	PageRank	H-Coreness	H-Eigenvector	Vector Centrality	WHATsNet	WHATsNet-all
Stack	MicroF1	0.735 ± 0.001	0.739 ± 0.005	0.738 ± 0.003	0.741 ± 0.003	0.738 ± 0.005	0.738 ± 0.004	0.745 ± 0.002	0.742 ± 0.003	0.745 ± 0.002
Biology	MacroF1	0.678 ± 0.004	0.685 ± 0.010	0.681 ± 0.004	0.681 ± 0.004	0.683 ± 0.008	0.681 ± 0.006	0.687 ± 0.003	0.686 ± 0.004	0.690 ± 0.005

Table 10: Effect of the number of inducing points and comparison of architectures for hyperedge-to-node message passing.

Dataset Number of Inducing Points					MSG. Passing from I	Hyperedge to Node			
Da	lasei	2	4	8	HNHN	HAT	WHATsNet + HNHN	WHATsNet + HAT	WHATsNet
Stack	MicroF1	0.740 ± 0.002	0.742 ± 0.003	0.742 ± 0.003	0.640 ± 0.005	0.661 ± 0.005	0.645 ± 0.023	0.670 ± 0.015	0.742 ± 0.003
Biology	MacroF1	0.682 ± 0.006	0.686 ± 0.004	$\textbf{0.688} \pm 0.002$	0.592 ± 0.006	0.606 ± 0.005	0.583 ± 0.029	0.618 ± 0.010	$\textbf{0.686} \pm 0.004$

Table 11: Effect of inputs to the final classifier

Dataset	Metric	Best Competitor	WHATsNet-IM	WHATsNet
Coauth-	MicroF1	$0.564 \pm 0.004 \\ 0.549 \pm 0.003$	0.602 ± 0.002	0.605 ± 0.002
DBLP	MacroF1		0.592 ± 0.002	0.595 ± 0.002
Coauth-	MicroF1	0.596 ± 0.007	0.637 ± 0.003	0.630 ± 0.005
AMiner	MacroF1	0.583 ± 0.008	0.631 ± 0.003	0.623 ± 0.007
Email-	MicroF1	$\begin{array}{c} 0.779 \pm 0.067 \\ 0.681 \pm 0.123 \end{array}$	0.858 ± 0.001	0.826 ± 0.001
Enron	MacroF1		0.796 ± 0.004	0.760 ± 0.004
Email-	MicroF1	$ \begin{vmatrix} 0.671 \pm 0.001 \\ 0.640 \pm 0.002 \end{vmatrix} $	0.687 ± 0.004	0.671 ± 0.000
Eu	MacroF1		0.660 ± 0.009	0.646 ± 0.003
Stack-	MicroF1	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	0.736 ± 0.003	0.742 ± 0.003
Biology	MacroF1		0.679 ± 0.007	0.686 ± 0.004
Stack-	MicroF1	$0.755 \pm 0.010 \\ 0.666 \pm 0.013$	0.769 ± 0.001	0.770 ± 0.003
Physics	MacroF1		0.692 ± 0.011	0.707 ± 0.004

Table 10 demonstrates that WHATsNET outperforms both WHATsNET + HNHN and WHATsNET + HAT, providing justification for employing the WITHINATT module in both directions. It is also worth noting that WHATsNET + HNHN and WHATsNET + HAT outperform their corresponding vanilla models, HNHN and HAT.

B.4 The number of inducing points

We explore how the performance of WHATsNet changes with respect to the numbers of inducing points (2, 4, and 8). Table 10 shows that the performance improves as more inducing points are employed. However, considering memory constraints, using 4 inducing points is favorable as it requires half the memory while achieving comparable performance to using 8 inducing points.

B.5 Inputs to the final classifier

As discussed in Section 5.4, we consider two possible inputs for a single-layer perceptron classifier: (a) intermediate edge-dependent node embeddings, referred to as WHATsNet-IM, which are generated by WithinATT inside a WHATsNet (Eq. (11)) and (b) the concatenation of final output node and hyperedge embeddings from

WHATsNet (Eq. (10)). Table 11 indicates that one approach does not consistently outperform the other; WHATsNet-IM performs better in Coauth-AMiner, Email-Enron, and Email-Eu datasets, while WHATsNet performs better in the remaining three datasets. It is also worth noting that both approaches are superior to HST, which is overall the best competitor.

C TIME COMPLEXITY OF NODE CENTRALITY MEASURES

We analyze the time complexity of computing each node's centrality using each of the four node measures used for WITHINORDERPE in WHATsNET. We assume $O(|\mathcal{V}| + |\mathcal{E}|) \in O(\sum_{e \in \mathcal{E}} |e|)$ for a hypergraph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ for simplicity.

<u>Degree.</u> The time complexity is $O(\sum_{e \in \mathcal{E}} |e|)$ if we increment the degree of each of |e| members of each hyperedge $e \in \mathcal{E}$.

Coreness. The time complexity is $O(\sum_{e \in \mathcal{E}} |e|)$, as proven in Theorem 1 of [10].

Eigenvector centrality. The time complexity is $O(\sum_{e \in \mathcal{E}} |e|)$. If we let I be the $|\mathcal{V}|$ by $|\mathcal{E}|$ incidence matrix of \mathcal{G} and nnz(I) be the number of non-zero entries (i.e., $nnz(I) = \sum_{e \in \mathcal{E}} |e|$), the eigenvector centralities of all nodes in the clique-expanded graph, whose adjacency matrix is $A = II^T$, are equivalent to the leading left singular vector of I. This can be computed by Power Iteration in O(nnz(I)T) time, where T is the maximum number of iterations. In practice (and in our setting), T is set to a constant, and thus the time complexity is $O(nnz(I)) = O(\sum_{e \in \mathcal{E}} |e|)$, which is even lower than that of materializing the clique-expanded graph.

<u>PageRank.</u> The time complexity is also $O(\sum_{e \in \mathcal{E}} |e|)$ since its calculation is almost the same as that of the eigenvector centrality. We repeat (at most T times) computing $\mathbf{r} \leftarrow \beta II^T\mathbf{r} + (1-\beta)\mathbf{1}$ for a $|\mathcal{V}|$ -dimensional vector \mathbf{r} and a constant β . Note that computing $II^T\mathbf{r}$ can be done in O(nnz(I)) time by two steps: (1) computing $\mathbf{r}' \leftarrow I^T\mathbf{r}$ and (2) computing $I\mathbf{r}'$. Since T is set to a constant in practice (and in our setting), the time complexity is $O(nnz(I)) = O(\sum_{e \in \mathcal{E}} |e|)$.