HGNN*: General Hypergraph Neural Networks

HGNN*: 通用超图神经网络

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Abstract-Graph Neural Networks have attracted increasing attention in recent years. However, existing GNN frameworks are deployed based upon simple graphs, which limits their applications in dealing with complex data correlation of multi-modal/multi-type data in practice. A few hypergraph-based methods have recently been proposed to address the problem of multi-model/multi-type data correlation by directly concatenating the hypergraphs constructed from each single individual modality/type, which is difficult to learn an adaptive weight for each modality/type. In this paper, we extend the original conference version HGNN, and introduce a general high-order multi-modal/multi-type data correlation modeling framework called HGNN $^{+}$ to learn an optimal representation in a single hypergraph based framework. It is achieved by bridging multi-modal/multi-type data and hyperedge with hyperedge groups. Specifically, in our method, hyperedge groups are first constructed to represent latent high-order correlations in each specific modality/ type with explicit or implicit graph structures. An adaptive hyperedge group fusion strategy is then used to effectively fuse the correlations from different modalities/types in a unified hypergraph. After that a new hypergraph convolution scheme performed in spatial domain is used to learn a general data representation for various tasks. We have evaluated this framework on several popular datasets and compared it with recent state-of-the-art methods. The comprehensive evaluations indicate that the proposed HGNN $^{+}$ framework can consistently outperform existing methods with a significant margin, especially when modeling implicit data correlations. We also release a toolbox called THU-DeepHypergraph for the proposed framework, which can be used for various of applications, such as data classification, retrieval and recommendation.

摘要——近年来，图神经网络越来越受到关注。然而，现有的图神经网络框架是基于简单图部署的，这限制了它们在实际处理多模态/多类型数据复杂数据相关性方面的应用。最近提出了一些基于超图的方法，通过直接连接从每个单独模态/类型构建的超图来解决多模型/多类型数据相关性问题，但这种方法难以学习每个模态/类型的自适应权重。在本文中，我们扩展了原始会议版本的 HGNN，并引入了一个通用的高阶多模态/多类型数据相关性建模框架 HGNN $^{+}$，以在基于单个超图的框架中学习最优表示。这是通过超边组将多模态/多类型数据与超边连接起来实现的。具体来说，在我们的方法中，首先构建超边组来用显式或隐式图结构表示每个特定模态/类型中的潜在高阶相关性。然后使用自适应超边组融合策略在统一的超图中有效融合来自不同模态/类型的相关性。之后，使用在空间域中执行的新超图卷积方案来学习各种任务的通用数据表示。我们在几个流行数据集上评估了这个框架，并与最近的最先进方法进行了比较。综合评估表明，所提出的 HGNN $^{+}$ 框架能够始终显著优于现有方法，特别是在对隐式数据相关性进行建模时。我们还为所提出的框架发布了一个名为 THU-DeepHypergraph 的工具箱，可用于各种应用，如数据分类、检索和推荐。

Index Terms—Hypergraph, classification, hypergraph convolution, representation learning

关键词——超图；分类；超图卷积；表示学习

1 INTRODUCTION

1 引言

GRAPH Neural Networks (GNN) [1], [2], [3], [4], [5] have attracted ever-increasing attention in recent years, which is effective in dealing with irregular correlation-based data structures such as social networks, functional networks, and recommendation systems. Despite the exciting progress made by the literature, effectively dealing with multi-modal/multi-type data and capturing high-order data correlation are still the critical problems for GNN networks. On one hand, the data correlation in the real world is far beyond pairwise correlation, which cannot be well modeled with a plain graph. For example, users in social networks may have different properties, and the correlation among those users could be in the manner of group, e.g., several users may share the same hobbies or are involved in the same event, as shown in Fig. 1. Under such circumstances, it is hard to formulate such a correlation in a graph structure. A traditional graph structure is capable of formulating pairwise (i.e., first-order relationship) between two subjects, which would not be powerful enough to deal with high-order correlations and thus limit the capability on high-order correlation modeling.

图神经网络 (GNN)[1,2,3,4,5] 近年来受到了越来越多的关注，它在处理基于不规则相关性的数据结构 (如社交网络、功能网络和推荐系统) 方面很有效。尽管文献取得了令人兴奋的进展，但有效处理多模态/多类型数据和捕获高阶数据相关性仍然是 GNN 网络的关键问题。一方面，现实世界中的数据相关性远远超出了成对相关性，用简单图无法很好地建模。例如，社交网络中的用户可能具有不同的属性，这些用户之间的相关性可能以群组的方式存在，例如，几个用户可能有相同的爱好或参与同一事件，如图 1 所示。在这种情况下，很难在图结构中表述这种相关性。传统的图结构能够表述两个主体之间的成对 (即一阶关系)，但在处理高阶相关性方面不够强大，因此限制了高阶相关性建模的能力。

Another limitation of simple graph is its weak capability in modeling multi-modal/multi-type real-world data. For example, the microblog data in social network may contain time, image, emoticon or even videos, with social connections among them, as shown in Fig. 1. Given such correlations from multi-modal/multi-type data representations, traditional GNN-based methods need to integrate multiple graphs in the learning stage, and the exploration of the correlations among multi-modal/multi-type data becomes a challenging task.

简单图的另一个局限性是其在建模多模态/多类型现实世界数据方面能力较弱。例如，社交网络中的微博数据可能包含时间、图像、表情符号甚至视频，它们之间存在社交联系，如图 1 所示。考虑到来自多模态/多类型数据表示的这种相关性，传统的基于 GNN 的方法需要在学习阶段整合多个图，而探索多模态/多类型数据之间的相关性成为一项具有挑战性的任务。

In this paper, we propose a general hypergraph neural network framework to handle the challenges on representation learning using high-order correlations. This work was first published in AAAI 2019 [6] and this journal version is an extension of HGNN. In our work, we propose hyper-graph-convolution-based representation learning to handle high-order data correlation during representation learning and shows decent performance. This work is an extension of the HGNN, called HGNN+, and the framework is shown in Fig. 3. The proposed HGNN $^+$ can model high-order data correlation and is easy to incorporate with multi-modal/multi-type data. First, to better capture the underlying high-order correlations among data, the hypergraph structure is used for data correlation modeling. Hypergraph, which encodes high-order data correlation with degree-free hyperedges, is a more general structure compared with the simple graph. The illustrative comparison between graph and hypergraph is shown in Fig. 2. Each edge in a graph can only connect two vertices, while in a hypergraph, each hyperedge can connect more than two vertices and thus is more flexible. When handling multi-modal/multi-type data, the hypergraph can generate different types of hyperedges using the multimodal/multi-type data and then directly concatenates these hyperedges into one hypergraph.

在本文中，我们提出了一个通用的超图神经网络框架，以应对使用高阶相关性进行表示学习的挑战。这项工作首次发表于 2019 年的 AAAI [6]，本期刊版本是 HGNN 的扩展。在我们的工作中，我们提出基于超图卷积的表示学习，以在表示学习过程中处理高阶数据相关性，并表现出良好的性能。这项工作是 HGNN 的扩展，称为 HGNN+，其框架如图 3 所示。所提出的 HGNN $^+$ 可以对高阶数据相关性进行建模，并且易于与多模态/多类型数据结合。首先，为了更好地捕获数据之间潜在的高阶相关性，使用超图结构进行数据相关性建模。超图用无度超边编码高阶数据相关性，与简单图相比是一种更通用的结构。图 2 展示了图和超图之间的说明性比较。图中的每条边只能连接两个顶点，而在超图中，每个超边可以连接两个以上的顶点，因此更灵活。在处理多模态/多类型数据时，超图可以使用多模态/多类型数据生成不同类型的超边，然后直接将这些超边连接成一个超图。

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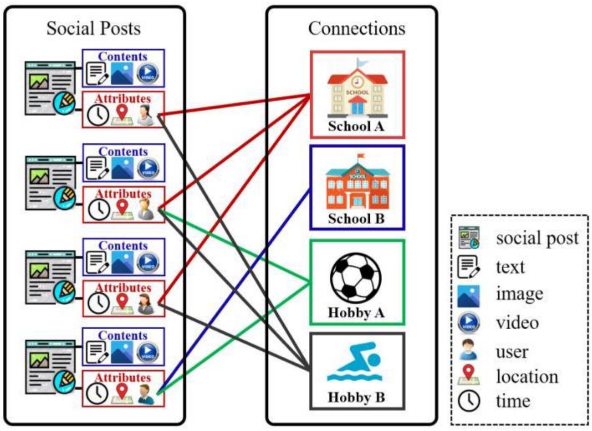

Fig. 1. Examples of high-order correlation and multi-modal data in real world. In social media data, the high-order correlation among microblogs can contain connections from the geo-locations, tags and relationships among users. For each social post, it may contain different types of data, such as images, videos, texts, and emoticons.

图 1. 现实世界中的高阶关联和多模态数据示例。在社交媒体数据中，微博之间的高阶关联可以包含地理位置、标签以及用户之间关系的连接。对于每一条社交帖子，它可能包含不同类型的数据，如图像、视频、文本和表情符号。

Compared with the conference version, we further generalize the "hyperedge group" conception. Mathematically speaking, a hyperedge group can be defined as a set family upon the vertex set. On the vertex set, there may exist multi-type relationships among vertices. One hyperedge group can be constructed based on one type of relationship, indicating different characteristics of multifarious information. We then systematically divide hypergraph modeling into two steps: hyperedge groups construction and fusion. Given the data with/without graph structure, four types of hyperedge groups are introduced to generate the hyper-graph, i.e., using pairwise edge, attribute, k -Hop and neighbors in the feature space, respectively.

与会议版本相比，我们进一步推广了“超边组”的概念。从数学上讲，超边组可以定义为顶点集上的一个集族。在顶点集上，顶点之间可能存在多种类型的关系。可以基于一种关系构建一个超边组，以表示各种信息的不同特征。然后，我们将超图建模系统地分为两个步骤：超边组构建和融合。对于有/无图结构的数据，引入了四种类型的超边组来生成超图，即分别使用成对边、属性、k -跳和特征空间中的邻居。

After generating multiple hyperedge groups, compared with the conference version, we further introduce two solutions for constructing the overall hypergraph structures. The first strategy, as adopted in the conference version [6], directly concatenates different hyperedge group incidence matrices (namely Coequal Fusion). Here, we want to highlight the second fusion strategy: Adaptive Fusion. It associates each hyperedge group with a learnable parameter, thus adaptively identifying the importance of different hyper-edge groups to the overall hypergraph representation learning and better exploiting the complementary representation of multi-modal/multi-type information.

生成多个超边组后，与会议版本相比，我们进一步介绍了两种构建整体超图结构的解决方案。第一种策略，如会议版本 [6] 中所采用的，直接连接不同超边组的关联矩阵 (即同等融合)。在此，我们想强调第二种融合策略：自适应融合。它为每个超边组关联一个可学习参数，从而自适应地确定不同超边组对整体超图表示学习的重要性，并更好地利用多模态/多类型信息的互补表示。

Drawing inspiration from the information flow path (vertex sequence) [10] in spatial graph convolution, we take a step forward on the basis of HGNN and develop a general two-stage hypergraph convolution in the spatial domain. By specifying four task-dependent message aggregation and updating functions, it can be flexibly applied to different scenarios. We further provide a specific spatial-domain hypergraph convolution operator that employs simple average aggregation in both two stages. An example is also discussed to show that HGNN$^+$ can be naturally extended to the directed hypergraph, which cannot be realized by HGNN as it is defined in the spectral domain.

借鉴空间图卷积中信息流路径 (顶点序列)[10] 的灵感，我们在 HGNN 的基础上更进一步，在空间域中开发了一种通用的两阶段超图卷积。通过指定四个依赖于任务的消息聚合和更新函数，它可以灵活地应用于不同场景。我们进一步提供了一个特定的空间域超图卷积算子，该算子在两个阶段都采用简单平均聚合。还讨论了一个示例，以表明 HGNN$^+$ 可以自然地扩展到有向超图，而这是 HGNN 在谱域中定义时无法实现的。

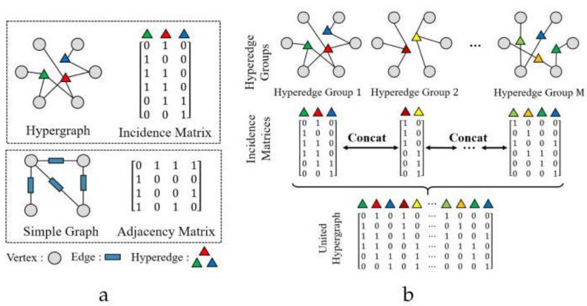

Fig. 2. The comparison between graph and hypergraph. (a) The example and representation of graph and hypergraph. (b) The general strategy of the hypergraph for multi-modal/multi-type data.

图 2. 图与超图的比较。(a) 图和超图的示例及表示。(b) 超图处理多模态/多类型数据的一般策略。

To evaluate the performance of our HGNN$^+$ framework, comprehensive experiments on five public benchmarks with graph structure for the vertex classification task are conducted. We further conduct experiments on two datasets that contain view-based 3D objects to investigate the effectiveness of our proposed method on data without explicit graph structure. Besides, two natural hypergraph datasets are employed to demonstrate the superiority of the proposed HGNN and HGNN $^+$ in learning high-order data correlations compared with graph-based neural networks. The results have demonstrated the effectiveness of the proposed method compared with the state-of-the-art methods. In this paper, we also release a toolbox called THU-DeepHyper-graph for the HGNN$^+$ framework.

为了评估我们的 HGNN$^+$ 框架的性能，针对顶点分类任务，在五个具有图结构的公共基准上进行了全面实验。我们还在两个包含基于视图的 3D 对象的数据集上进行了实验，以研究我们提出的方法在没有显式图结构的数据上的有效性。此外，使用了两个自然超图数据集来证明所提出的 HGNN 和 HGNN $^+$ 在学习高阶数据相关性方面相对于基于图的神经网络的优越性。结果表明，与现有最先进的方法相比，所提出的方法是有效的。在本文中，我们还为 HGNN$^+$ 框架发布了一个名为 THU-DeepHyper-graph 的工具箱。

In the conference version [6], we introduce the hyper-graph neural networks, i.e., HGNN, for representation learning using hypergraph structure. HGNN is able to formulate complex and high-order data correlation through its hyper-graph structure and can also be efficient using hyperedge convolution operations. This work was firstly published on AAAI 2019. Compared with the conference version, we have the following extensions in this journal version:

在会议版本 [6] 中，我们介绍了用于使用超图结构进行表示学习的超图神经网络，即 HGNN。HGNN 能够通过其超图结构来构建复杂的高阶数据相关性，并且还能通过超边卷积操作实现高效性。这项工作首次发表于 2019 年的 AAAI。与会议版本相比，本期刊版本有以下扩展:

1) We complete the modeling framework and systematically introduce a general hypergraph neural network framework HGNN $^+$, which includes two main procedures, i.e., hyperedge modeling and hyper-graph convolution. In hypergraph modeling, we conceptually introduce "hyperedge group" and further define four ways to generate hyperedge groups. An adaptive hyperedge groups fusion strategy is also proposed to optimally generate the hypergraph and better exploit the complementary information of multifarious correlations.

1) 我们完善了建模框架，并系统地介绍了一个通用的超图神经网络框架 HGNN $^+$，它包括两个主要过程，即超边建模和超图卷积。在超图建模中，我们从概念上引入了“超边组”，并进一步定义了生成超边组的四种方式。还提出了一种自适应超边组融合策略，以最优地生成超图并更好地利用多种相关性的互补信息。

2) The original convolution strategy HGNNConv is extended to a general two-stage hypergraph convolution operation from the spatial domain. A specific variant of it is also defined (namely HGNNConv+), which is much more scalable compared with the hypergraph convolution in HGNN.

2) 原始的卷积策略 HGNNConv 从空间域扩展为通用的两阶段超图卷积操作。还定义了它的一个特定变体 (即 HGNNConv+)，与 HGNN 中的超图卷积相比，它具有更高的可扩展性。

3) Extensive experiments on the data with/without graph structure as well as that with hypergraph structure are conducted to demonstrate the effectiveness of the proposed method. Besides, detailed mathematical discussions are provided to offer a deeper understanding of the hypergraph structure and the proposed

3) 针对有无图结构以及超图结构的数据进行了广泛实验，以证明所提方法的有效性。此外，还提供了详细的数学讨论，以更深入地理解超图结构和所提方法。

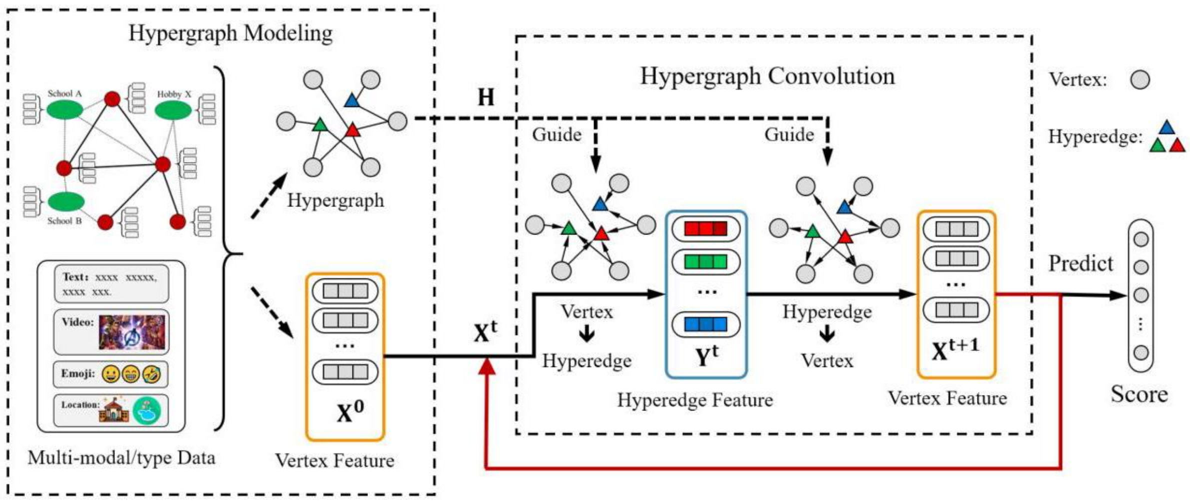

Fig. 3. The proposed hypergraph neural network framework (HGNN*). In the left part, a hypergraph is employed to model raw multi-modal/type data. H is generated to indicate hypergraph structure and **X** denotes the vertex feature extracted from raw data. In the right part, Hypergraph Convolution Module shows one hypergraph convolution process and the red line from the module allows stacking multiple hypergraph convolution layers for deeper vertex embedding extraction.

图 3. 所提的超图神经网络框架 (HGNN*)。在左半部分，使用超图对原始多模态/类型数据进行建模。生成 H 以表示超图结构，**X** 表示从原始数据中提取的顶点特征。在右半部分，超图卷积模块展示了一个超图卷积过程，该模块的红线允许堆叠多个超图卷积层以进行更深层次的顶点嵌入提取。

HGNN^+ . A toolbox for the HGNN^+ framework, called THU-DeepHypergraph [1] , is released for public use.

HGNN^+ 。发布了一个用于 HGNN^+ 框架的工具箱，名为 THU-DeepHypergraph [1] ，供公众使用。

The remainder of the paper is organized as follows. First, we briefly review related work on GNN and hypergraph learning in Section 2. Section 3 presents the preliminaries of hypergraphs. In Section 4, we introduce the proposed general hypergraph neural network HGNN^+ , including hypergraph modeling and hypergraph convolution. In Section 5, we first mathematically compare the hypergraph structure with the graph structure, and then discuss the relationships among GCN, HGNN, and HGNN^+ . Experimental results and discussions are provided in Section 6. The THU-DeepHypergraph toolbox is introduced in Section 7. We conclude this paper in Section 8.

本文的其余部分组织如下。首先，我们在第 2 节简要回顾关于 GNN 和超图学习的相关工作。第 3 节介绍超图的预备知识。在第 4 节，我们介绍所提的通用超图神经网络 $HGNN^+$，包括超图建模和超图卷积。在第 5 节，我们首先从数学上比较超图结构和图结构，然后讨论 GCN、HGNN 和 $HGNN^+$ 之间的关系。第 6 节给出实验结果和讨论。第 7 节介绍 THU-DeepHypergraph 工具箱。我们在第 8 节总结本文。

2 RELATED WORK

2 相关工作

2.1 Graph Neural Networks

2.1 图神经网络

Recent years have witnessed the rapid progress of GNN [1], [2], [3], [4], [5]. GNN is designed for fixing the gap between deep convolution and irregular data processing, which can be directly applied on arbitrary graph structures. Generally, GNN can be mainly divided into two categories: spectral-based and spatial-based methods.

近年来，GNN[1,2,3,4,5] 取得了快速进展。GNN 旨在解决深度卷积与不规则数据处理之间的差距，它可以直接应用于任意的图结构。一般来说，GNN 主要可分为两类: 基于谱的方法和基于空间的方法。

Spectral-based approaches [2], [5], [11], [12], [13] define graph convolution from the perspective of graph signal processing [11], where the graph convolution operation is interpreted as removing noise from graph signals, or smoothing the information among the linked vertices via graph Laplacian normalization. In [12], Bruna et al. introduced the first GNN, which adopted the graph Laplacian eigen basis as an analogy of the Fourier transform. In [14], the spectral filters can be parameterized with smooth coefficients to make them spatial-localized. In [2], the Chebyshev polynomials were simplified into 1-order polynomials to form an efficient layer-wise propagation.

基于谱的方法 [2,5,11,12,13] 从图信号处理 [11] 的角度定义图卷积，其中图卷积操作被解释为从图信号中去除噪声，或通过图拉普拉斯归一化来平滑相连顶点之间的信息。在 [12] 中，布鲁纳等人引入了第一个 GNN，它采用图拉普拉斯特征基作为傅里叶变换的类比。在 [14] 中，谱滤波器可以用平滑系数进行参数化，使其具有空间局部性。在 [2] 中，切比雪夫多项式被简化为一阶多项式以形成高效的逐层传播。

Spatial-based approaches [1], [3], [15], [16] are formulated as aggregating messages from neighbor vertices, and the convolution operation is defined in groups of spatially closed vertices. In [16], the powers of a transition matrix

基于空间的方法 [1,3,15,16] 被表述为聚合来自相邻顶点的消息，并且卷积操作在空间上封闭的顶点组中定义。在 [16] 中，使用转移矩阵的幂来定义顶点的邻域。在 [3] 中，注意力机制被引入到图中以构建基于注意力的架构，从而在图上进行节点分类。为了在魏斯费勒 - 莱曼 (WL) 图同构测试中实现更强大的表达，凯尤鲁等人 [17] 在邻居消息聚合中利用了求和聚合器，它可以区分更多类型的局部图结构。

1. https://github.com/iMoonLab/THU-DeepHypergraph were employed to define the neighborhood of vertices. In [3], the attention mechanisms were introduced into the graph to build attention-based architecture to perform node classification on the graph. To achieve a more powerful expression in Weisfeiler-Lehman (WL) graph isomorphism test, Keyulu et al. [17] leveraged a sum aggregator in neighbor message aggregation that can discriminate more types of local graph structure.

1. https://github.com/iMoonLab/THU-DeepHypergraph 被用于定义顶点邻域。在 [3] 中，注意力机制被引入到图中以构建基于注意力的架构，从而在图上进行节点分类。为了在魏斯费勒 - 莱曼 (WL) 图同构测试中实现更强大的表达，凯尤鲁等人 [17] 在邻居消息聚合中利用了求和聚合器，它可以区分更多类型的局部图结构。

Both spectral-based and spatial-based GNNs perform representation learning on the graph structure and show decent performance. GNN has been used in various applications, such as drug-target interaction (DTI) prediction, collaborative filtering, community detection and brain functional network. For DTI prediction task, in [18] Manoochehri et al. adopted WL-GNN to learn the latent pattern of DTIs. For collaborative filtering task, in [19] Wang et al. proposed Neural Graph Collaborative Filtering (NGCF) to learn the latent collaborative signal in user-item interaction graph.

基于频谱和基于空间的图神经网络 (Graph Neural Networks，GNN) 都在图结构上进行表示学习，并展现出不错的性能。GNN 已被应用于各种领域，如药物-靶点相互作用 (Drug-Target Interaction, DTI) 预测、协同过滤、社区检测和脑功能网络。对于 DTI 预测任务，在 [18] 中，Manoochehri 等人采用了 WL-GNN 来学习 DTIs 的潜在模式。对于协同过滤任务，在 [19] 中，Wang 等人提出了神经图协同过滤 (Neural Graph Collaborative Filtering，NGCF) 来学习用户-项目交互图中的潜在协同信号。

2.2 Hypergraph Learning

2.2 超图学习

In recent years, hypergraph has shown strong capability of modeling and learning complex correlations.

近年来，超图在建模和学习复杂相关性方面展现出强大的能力。

Hypergraph learning was first introduced in [20], which conducts transductive learning and can be seen as a propagation process on the hypergraph structure. The transduc-tive inference on hypergraph aims to minimize the label difference among vertices with stronger connections on the hypergraph. For the past few years, hypergraph learning has been extensively developed and applied in many areas. Wang et al. [21] constructed a complex hypergraph including global, local visual feature and tag information to learn the relevance of image in the task of tag-based image retrieval. To model brain functional connectivity networks (FCN), Xiao et al. [22] proposed weighted hypergraph learning, which is capable of capturing the relations among brain regions than the traditional graph based methods and the existing unweighted hypergraph based method.

超图学习最早在 [20] 中被引入，它进行直推式学习，可以看作是超图结构上的传播过程。超图上的直推式推理旨在最小化超图上连接更强的顶点之间的标签差异。在过去的几年里，超图学习得到了广泛的发展，并应用于许多领域。Wang 等人 [21] 构建了一个包含全局、局部视觉特征和标签信息的复杂超图，以学习基于标签的图像检索任务中图像的相关性。为了对脑功能连接网络 (Functional Connectivity Networks， FCN) 进行建模，Xiao 等人 [22] 提出了加权超图学习，它比传统的基于图的方法和现有的基于非加权超图的方法更能捕捉脑区之间的关系。

Inspired by the recent immense success of deep learning, some researchers have developed deep hypergraph learning methods. For example, in our conference version Feng et al. [6] proposed hypergraph neural networks (HGNN)

受深度学习近期巨大成功的启发，一些研究人员开发了深度超图学习方法。例如，在我们的会议版本中，Feng 等人 [6] 提出了超图神经网络 (Hypergraph Neural Networks， HGNN)

 towards modeling and learning beyond-pairwise complex correlations. Unlike GNN, HGNN designs a vertex-hyper-edge-vertex information propagating pattern to iteratively learn the data representation. Besides, in this literature, the hypergraph Laplacian is first approximated and introduced into the deep hypergraph learning method to accelerate learning. Built on our conference version [6], Bai et al. [7] further focused on attention module on hypergraph (Hyper-Atten), which follows the hypergraph convolution patterns defined in HGNN. Enlightened by [3], Hyper-Atten introduces a hyperedge-vertex attention learning module to adaptively identify the importance of different vertices in the same hyperedge and thus revealing the intrinsic correlation between vertices. Besides, Yadati et al. [8] proposed a method of training a GCN on hypergraphs (HyperGCN) for semi-supervised learning. HyperGCN is designed based on the spectral theory of hypergraphs. Given a hypergraph, HyperGCN first translates it into a simple weighted graph through a specific strategy and then performs standard GCN on the graph to learn data representations. All the above-mentioned methods are conducted on the fixed hypergraph structure. However, the initial hypergraph constructed from raw data may not be optimal.

用于建模和学习超越成对的复杂相关性。与 GNN 不同，HGNN 设计了一种顶点-超边-顶点信息传播模式来迭代学习数据表示。此外，在这篇文献中，超图拉普拉斯算子首先被近似并引入到深度超图学习方法中以加速学习。基于我们的会议版本 [6]，Bai 等人 [7] 进一步关注超图上的注意力模块 (Hyper-Atten)，它遵循 HGNN 中定义的超图卷积模式。受 [3] 的启发，Hyper-Atten 引入了一个超边-顶点注意力学习模块，以自适应地识别同一超边中不同顶点的重要性，从而揭示顶点之间的内在相关性。此外，Yadati 等人 [8] 提出了一种在超图上训练图卷积网络 (Graph Convolutional Network, GCN) 用于半监督学习的方法 (HyperGCN)。HyperGCN 是基于超图的谱理论设计的。给定一个超图，HyperGCN 首先通过特定策略将其转换为一个简单的加权图，然后在该图上执行标准的 GCN 以学习数据表示。上述所有方法都是在固定的超图结构上进行的。然而，从原始数据构建的初始超图可能不是最优的。

TABLE 1

Notations and Definitions

符号和定义

Notation	Definition
G	$\mathcal{G}=(\mathcal{V},\mathcal{E},\mathbf{W})$ indicates a hypergraph, and $\mathcal{V},\mathcal{E}$
	and $\mathbf{W}$ indicate the set of vertices, the set of
	edges, and the weights of the edges,
	respectively.
V	The set of vertices of $\mathcal{G}$.
E	The set of hyperedges of $\mathcal{G}$.
N	The number of vertices on $\mathcal{G}$, i.e., $\|\mathcal{V}\|$.
M	The number of edges on $\mathcal{G}$, i.e., $\|\mathcal{E}\|$.
x_i^0	The initial feature for the i -th vertex on $\mathcal{G}$.
$\mathbf{X}^0$	The initial feature for all the vertices on $\mathcal{G}$.
$\mathbf{X}^t$	The input feature of convolution layer t .
X_i^t	The embedding for vertex i in layer t .
W	The diagonal matrix of the hyperedge weights.
$d(v)$	The degree of vertex v .
$\delta(e)$	The degree of hyperedge e .
$\mathbf{D}_v$	The diagonal matrix of vertex degrees. $\mathbf{D}_v \in \mathbb{R}^{N\times N}$
$\mathbf{D}_e$	The diagonal matrix of hyperedge degrees.
	$\mathbf{D}_v \in \mathbb{R}^{M\times M}$.

符号表示	定义
G	$\mathcal{G}=(\mathcal{V},\mathcal{E},\mathbf{W})$ 表示一个超图，且 $\mathcal{V},\mathcal{E}$
	而 $\mathbf{W}$ 分别表示顶点集、
	边集和边的权重,
	依次类推。
V	$\mathcal{G}$ 的顶点集。
E	$\mathcal{G}$ 的超边集。
N	$\mathcal{G}$ 上的顶点数量，即 $\|\mathcal{V}\|$ 。
M	$\mathcal{G}$ 上的边数量，即 $\|\mathcal{E}\|$ 。
x_i^0	$\mathcal{G}$ 上第 i 个顶点的初始特征。
$\mathbf{X}^0$	$\mathcal{G}$ 上所有顶点的初始特征。
$\mathbf{X}^t$	卷积层 t 的输入特征。
X_i^t	第 t 层中顶点 i 的嵌入。
W	超边权重的对角矩阵。
$d(v)$	顶点 v 的度。
$\delta(e)$	超边 e 的度。
$\mathbf{D}_v$	顶点度的对角矩阵。$\mathbf{D}_v \in \mathbb{R}^{N\times N}$
$\mathbf{D}_e$	超边度的对角矩阵。
	$\mathbf{D}_v \in \mathbb{R}^{M\times M}$.

As discussed above, most existing deep hypergraph learning methods are derived from the spectral theory of hyper-graphs. Therefore, these methods are usually defined on undirected hypergraphs, which limits their applications. Besides, some methods also suffer from structural over-simplification or over-parametrization. For example, HyperGCN only considers one simple edge for each hyperedge. Even though it introduces mediators, such irreversible simplification will certainly lose key information. Hyper-Atten leverages a hyperedge-vertex attention module, which introduces a large number of parameters and may lead to overfitting problem.

如上文所述，大多数现有的深度超图学习方法源自超图的谱理论。因此，这些方法通常是在无向超图上定义的，这限制了它们的应用。此外，一些方法还存在结构过度简化或参数过多的问题。例如，HyperGCN 对于每个超边仅考虑一条简单边。尽管它引入了中介节点，但这种不可逆转的简化肯定会丢失关键信息。Hyper-Atten 利用了一个超边-顶点注意力模块，这引入了大量参数，可能会导致过拟合问题。

3 PRELIMINARIES OF HYPERGRAPHS

3 超图的预备知识

The hypergraph is a generalization of the graph. Different from the graph, an edge in the hypergraph, called

超图是图的一种推广。与图不同，超图中的边称为超边，是超图中所有顶点的一个子集。为便于说明，我们首先在表 1 中总结本文中使用的重要符号和定义。一个超图定义为 <b0></b0>，它包括一个顶点集 <b1></b1>、一个超边集 <b2></b2> 和一个超边权重矩阵 <b3></b3>。一个超图 <b4></b4> 可以用一个 <b5></b5> 关联矩阵 <b6></b6> 来描述，其元素定义为 <b7></b7>，其顶点度定义为 <b8></b8>。对于一个超边 <b9></b9>，其边度定义为 <b10></b10>。<b11></b11> 和 <b12></b12> 分别表示顶点度和边度的对角矩阵。每个顶点的初始特征集表示为 <b13></b13>，其中 <b14></b14> 是特征的维度。

 hyperedge, is a subset of all vertices in the hypergraph. For clarification, we first summarize important notations and definitions throughout this paper in Table 1. A hypergraph is defined as $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{W})$, which includes a vertex set $\mathcal{V}$, a hyperedge set $\mathcal{E}$, and a hyperedge weight matrix $\mathbf{W}$. A hypergraph $\mathcal{G}$ can be described by an $|\mathcal{V}| \times |\mathcal{E}|$ incidence matrix $\mathbf{H}$, whose entries are defined as $\mathbf{H}(v,e) = \begin{cases} 1, & \text{if } v \in e \\ 0, & \text{otherwise} \end{cases}$. For a vertex $v \in \mathcal{V}$, its vertex degree is defined as $d(v) = \sum_{e \in \mathcal{E}} \omega(e) \mathbf{H}(v,e)$. For a hyperedge $e \in \mathcal{E}$, its edge degree is defined as $\delta(e) = \sum_{v \in \mathcal{V}} \mathbf{H}(v,e)$. $\mathbf{D}_v$ and $\mathbf{D}_e$ denote the diagonal matrices of vertex degrees and edge degrees, respectively. The initial feature set for each vertex is denoted as $\mathbf{X}^0 = \{x_1^0, x_2^0, \cdots, x_N^0\}, x_i^0 \in \mathbb{R}^{C_0}$, where C_0 is the dimension of the feature.

Given a hypergraph, the classification task turns to classify the vertices on the hypergraph, where the labels on the hypergraph are required to be smoothed through the hyper-graph structure. The task can be formulated as a regularization as introduced in [20]:

给定一个超图，分类任务就是对超图上的顶点进行分类，其中超图上的标签需要通过超图结构进行平滑处理。该任务可以如 [20] 中所介绍的那样表述为一个正则化问题:

$$\arg\min_{f}\left\{\mathcal{R}_{emp}(f)+\Omega(f)\right\} \tag{1}$$

where $\Omega(f)$ is a regularizer on hypergraph, $\mathcal{R}_{emp}(f)$ denotes the supervised empirical loss and $f(\cdot)$ is a classification function. The regularizer $\Omega(f)$ can be defined as:

其中 $\Omega(f)$ 是超图上的正则化项, $\mathcal{R}_{emp}(f)$ 表示监督经验损失, $f(\cdot)$ 是一个分类函数。正则化项 $\Omega(f)$ 可以定义为:

$$\Omega(f)=\frac{1}{2}\sum_{e\in\mathcal{E}}\sum_{\{u,v\}\in\mathcal{V}}\frac{w(e)\,\mathbf{H}(u,e)\,\mathbf{H}(v,e)}{\delta(e)}\left(\frac{f(u)}{\sqrt{d(u)}}-\frac{f(v)}{\sqrt{d(v)}}\right)^{2},$$

(2)

Here we let $\Theta=\mathbf{D}_v^{-1/2}\mathbf{H}\mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^{\top}\mathbf{D}_v^{-1/2}$ and $\Delta=\mathbf{I}-\Theta$, and the normalized $\Omega(f)$ can be rewritten as $\Omega(f)=f^{\top}\Delta f$, where Δ is positive semi-definite and usually called the hypergraph Laplacian.

在此我们令 $\Theta=\mathbf{D}_v^{-1/2}\mathbf{H}\mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^{\top}\mathbf{D}_v^{-1/2}$ 和 $\Delta=\mathbf{I}-\Theta$，并且归一化后的 $\Omega(f)$ 可以重写为 $\Omega(f)=f^{\top}\Delta f$，其中 Δ 是半正定的，通常称为超图拉普拉斯矩阵 (hypergraph Laplacian)。

4 The Framework of Hypergraph Neural NETWORK HGNN $^+$

4 超图神经网络 HGNN $^+$ 的框架

In this section, we briefly introduce the framework of hypergraph neural network (HGNN $^+$), which aims to provide a general framework for representation learning on a given raw data. It is composed of two procedures, as shown in Fig. 3, i.e., hypergraph modeling and hyper-graph convolution. In the step of hypergraph modeling, the available data are used to generate high-order correlations which are represented by a hypergraph. There are three types of hyperedge groups, using pairwise edge, k -Hop and neighbors in the feature space, respectively. In this procedure, all these types of hyperedge groups (if available) are generated and concatenated in a hypergraph for data correlation modeling. In the step of hypergraph convolution, a set of hypergraph convolution family, i.e., spectral hypergraph convolution and spatial hypergraph convolution, is conducted for representation learning. These convolution procedures can utilize the information from high-order correlation and multi-modal data to generate better representations.

在本节中，我们简要介绍超图神经网络 (HGNN $^+$) 的框架，其目的是为给定原始数据的表示学习提供一个通用框架。它由两个过程组成，如图 3 所示，即超图建模和超图卷积。在超图建模步骤中，可用数据用于生成由超图表示的高阶相关性。有三种类型的超边组，分别使用成对边、k -跳和特征空间中的邻居。在这个过程中，所有这些类型的超边组 (如果可用) 都会被生成并连接在一个超图中用于数据相关性建模。在超图卷积步骤中，进行一组超图卷积族，即谱超图卷积和空间超图卷积，用于表示学习。这些卷积过程可以利用来自高阶相关性和多模态数据的信息来生成更好的表示。

有图结构的数据，直接把普通边转化为超边

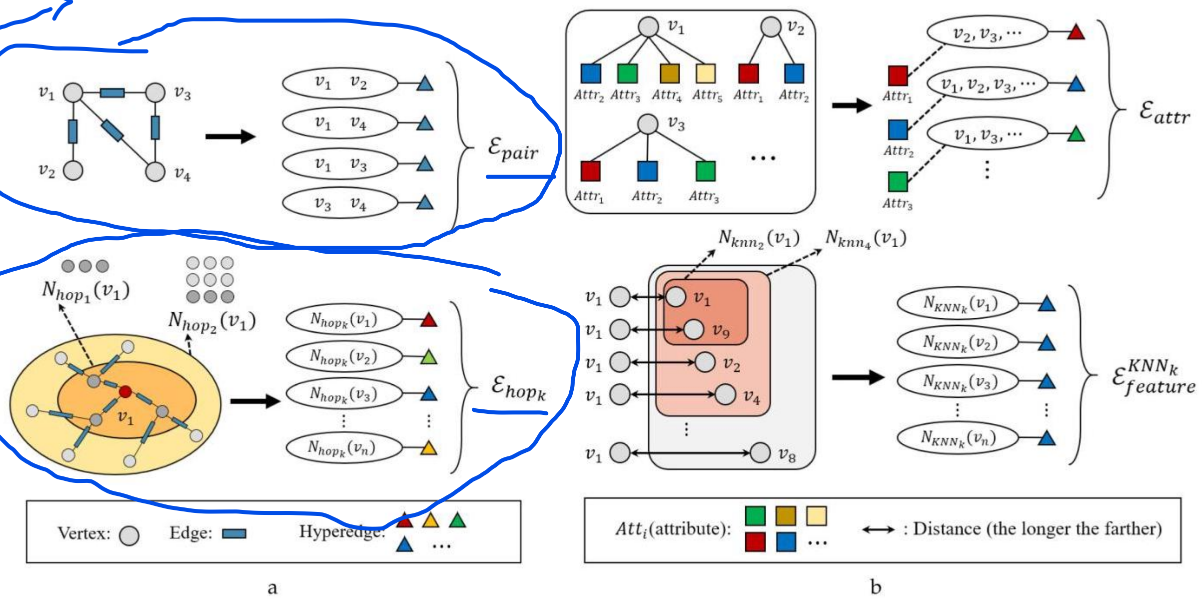

Fig. 4. Illustration for hyperedge group generation.

图 4. 超边组生成的示意图。

4.1 Hypergraph Modeling

4.1 超图建模

In this section, we introduce how to construct a flexible hypergraph from the raw data if there is no natural hyper-graph structure. The hypergraph structure is used to model data correlation. To better exploit the high-order correlation among the data, how to generate a good hypergraph structure is important. It is noted that there is no explicit hyper-graph structure in most cases. Therefore, we need to generate the hypergraph using different strategies. Usually, the situation for hypergraph generation from scratch can be divided into three scenarios, i.e., the data with graph structure, the data without graph structure, and the data with multi-modal/multi-type representations. Given the data, three hyperedge generation strategies, which employ pairwise edge, k -Hop and neighbors in the feature space respectively, are introduced here. The strategies of using pairwise edge and k -Hop are utilized for hyperedge group generation from the data with graph structure, and that of using neighbors in feature space is employed for hyperedge group generation from the data without graph structure. Finally, all the hyperedge groups will be further concatenated to generate the overall hypergraph. We will introduce the hyperedge group generation first, and then introduce the combination of these hyperedges groups and the method to deal with multi-modal/multi-type data. Compared with the conference version, we have extended from two aspects in this journal version: 1) we systematically introduce four typical hyperedge group construction strategies toward complex applications including graph-based representation, feature-based representation, and attribute-based representation. 2) We further propose an adaptive hyperedge group fusion strategy to balance the contribution of hyperedge groups that constructed from different aspects.

在本节中，我们介绍如果没有自然超图结构，如何从原始数据构建一个灵活的超图。超图结构用于对数据相关性进行建模。为了更好地利用数据之间的高阶相关性，如何生成一个好的超图结构很重要。需要注意的是，在大多数情况下没有明确的超图结构。因此，我们需要使用不同的策略来生成超图。通常，从头开始生成超图的情况可以分为三种场景，即具有图结构的数据、不具有图结构的数据以及具有多模态/多类型表示的数据。给定数据，这里介绍三种超边生成策略，它们分别采用成对边、k -跳和特征空间中的邻居。使用成对边和 k -跳的策略用于从具有图结构的数据生成超边组，而使用特征空间中的邻居的策略用于从没有图结构的数据生成超边组。最后，所有超边组将进一步连接以生成整体超图。我们将首先介绍超边组生成，然后介绍这些超边组与处理多模态/多类型数据的方法的组合。与会议版本相比，我们在本期刊版本中从两个方面进行了扩展:1) 我们系统地介绍了四种典型的超边组构建策略，用于复杂应用，包括基于图的表示、基于特征的表示和基于属性的表示。2) 我们进一步提出了一种自适应超边组融合策略，以平衡从不同方面构建的超边组的贡献。

4.1.1 Hyperedge Group Generation

4.1.1 超边组生成

When the data correlation is with graph structure. In some scenarios, there are available pairwise data correlations, such as existing graph structure for the data. Here we let $\mathcal{G}_s = (\mathcal{V}_s, \mathcal{E}_s)$ indicate the graph structure, where $v_i \in \mathcal{V}_s$ is a vertex and $e_{s_{ij}} \in \mathcal{E}_s$ is an edge in the graph connecting v_i and v_j . Let $\mathbf{A}$ denotes the adjacency matrix of $\mathcal{G}_s$. Given such graph structure, two types of hyperedge groups can be generated as follows:

当数据相关性具有图结构时。在某些场景中，存在可用的成对数据相关性，例如数据现有的图结构。在此我们令 $\mathcal{G}_s = (\mathcal{V}_s, \mathcal{E}_s)$ 表示图结构，其中 $v_i \in \mathcal{V}_s$ 是一个顶点，$e_{s_{ij}} \in \mathcal{E}_s$ 是图中连接 v_i 和 v_j 的一条边。令 $\mathbf{A}$ 表示 $\mathcal{G}_s$ 的邻接矩阵。给定这样的图结构，可以如下生成两种类型的超边组:

- Hyperedge group using pairwise edge $\left(\mathcal{E}_{\text{pair}}\right)$.$\mathcal{E}_{\text{pair}}$ targets on directly transforming the graph structure to a group of 2-uniform hyperedges, as shown in the top of Fig. 4a, in which each hyperedge e_{ij} in this group just connects the two vertices v_i and v_j in the corresponding edge in the graph $\mathcal{G}_J$:

- 使用成对边 $\left(\mathcal{E}_{\text{pair}}\right)$.$\mathcal{E}_{\text{pair}}$ 目标的超边组直接将图结构转换为一组 2-均匀超边，如图 4a 顶部所示，其中该组中的每个超边 e_{ij} 仅连接图 $\mathcal{G}_J$ 中相应边的两个顶点 v_i 和 v_j :

$$\mathcal{E}_{\text{pair}} = \left\{\{v_i, v_j\} \mid (v_i, v_j) \in \mathcal{E}_s\right\}. \tag{3}$$

$\mathcal{E}_{\text{pair}}$ is able to fully cover the low-order (pairwise) correlation in the graph structure, which is the basic information needed in the high-order correlation modeling.

$\mathcal{E}_{\text{pair}}$ 能够完全覆盖图结构中的低阶 (成对) 相关性，这是高阶相关性建模所需的基本信息。

- Hyperedge group using k -Hop neighbors $\left(\mathcal{E}_{\text{hop}}\right)$.

- 使用 k -跳邻居 ($\mathcal{E}_{\text{hop}}$) 的超边组。

$\mathcal{E}_{\text{hop}}$ aims to find the related vertices for a central one through the k -Hop reachable positions in the graph structure, as shown in the bottom of Fig. 4a. The k -Hop neighborhoods of a vertex v in graph $\mathcal{G}_s$ is defined as: $N_{\text{hop}_k}(v) = \{u \mid \mathbf{A}^k_{uv} \neq 0, u \in \mathcal{V}_s\}$. Here k can be vary from $[2, n_v]$, where n_v is the number of vertices in $\mathcal{G}_s$. The hyperedge group $\mathcal{E}_{\text{hop}}$ with k -Hop can be written as:

$\mathcal{E}_{\text{hop}}$ 旨在通过图结构中的 k -跳可达位置找到中心顶点的相关顶点，如图 4a 底部所示。图 $\mathcal{G}_s$ 中顶点 v 的 k -跳邻域定义为: $N_{\text{hop}_k}(v) = \{u \mid \mathbf{A}^k_{uv} \neq 0, u \in \mathcal{V}_s\}$。这里，$k$ 可以从 $[2, n_v]$ 变化到，其中 n_v 是 $\mathcal{G}_s$ 中的顶点数。具有 k -跳的超边组 $\mathcal{E}_{\text{hop}}$ 可以写成:

$$\mathcal{E}_{\text{hop}_k} = \{N_{\text{hop}_k}(v) \mid v \in \mathcal{V}\}. \tag{4}$$

$\mathcal{E}_{\text{hop}}$ is able to exploit external correlated vertices for the central one by extending the search radius in the graph structure, which also leads to groups of vertices, instead of two vertices, for the hyperedge. It can provide richer correlation information compared with just the pairwise one in $\mathcal{E}_{\text{pair}}$.

$\mathcal{E}_{\text{hop}}$ 能够通过在图结构中扩展搜索半径为中心顶点利用外部相关顶点，这也导致超边的顶点组而不是两个顶点。与 $\mathcal{E}_{\text{pair}}$ 中仅成对的情况相比，它可以提供更丰富的相关信息。

When the data correlation is without graph structure. When there is no available graph structure for the data, we need to build it following different methods. Usually, there could be two types of data for each subject: one is the attribute-like data, and the other one is the feature(s) associated with each vertex.

当数据相关性没有图结构时。当数据没有可用的图结构时，我们需要按照不同的方法来构建它。通常，每个主题可能有两种类型的数据: 一种是类似属性的数据，另一种是与每个顶点相关联的特征。

- Hyperedge group using attributes ($\varepsilon_{\text{attribute}}$). Given the attribute-like data, such as geo-locations, time and other specific information shared by different subjects, a group of hyperedges using neighbors in the attribute space can be generated, as shown in the top of Fig. 4b, where each hyperedge represents one attribute a (or one subtype of the attribute if available) and connects all the subjects sharing the same attribute. Vertex subset that shares the attribute a can be denoted as $N_{\text{att}}(a)$.$\mathcal{A}$ is a set that contains all attributes or subtypes of the attribute. This group of hyperedges from the attribute can be written as:

- 使用属性 ($\varepsilon_{\text{attribute}}$) 的超边组。给定类似属性的数据，如地理位置、时间和不同主题共享的其他特定信息，可以生成一组使用属性空间中邻居的超边，如图 4b 顶部所示，其中每个超边代表一个属性 a (如果可用，是该属性的一个子类型) 并连接共享相同属性的所有主题。共享属性 a 的顶点子集可以表示为 $N_{\text{att}}(a)$.$\mathcal{A}$ 是包含该属性的所有属性或子类型的集合。来自属性的这组超边可以写成:

$$\mathcal{E}_{\text{attribute}} = \{N_{\text{att}}(a) \mid a \in \mathcal{A}\}. \tag{5}$$

Here, $\mathcal{E}_{\text{attribute}}$ can model the correlation in the attribute space from the group level.

这里，$\mathcal{E}_{\text{attribute}}$ 可以从组级别对属性空间中的相关性进行建模。

- Hyperedge group using features ($\mathcal{E}_{\text{feature}}$). Given the feature for each vertex, the second type of $\mathcal{E}_{\text{feature}}$ can be generated by finding the neighbors of each vertex in the feature space. Here different strategies can be employed. Given a vertex as the centroid, its k -nearest neighbors in the feature space can be connected by a hyperedge, or all the neighbors within a distance d to the centroid (including the centroid) can be selected, as shown in the bottom of Fig. 4b.

- 使用特征 ($\mathcal{E}_{\text{feature}}$) 的超边组。给定每个顶点的特征，可以通过在特征空间中找到每个顶点的邻居来生成第二种类型的 $\mathcal{E}_{\text{feature}}$ 。这里可以采用不同的策略。给定一个顶点作为质心，可以通过超边连接其在特征空间中的 k -最近邻，或者可以选择到质心距离 d 内的所有邻居 (包括质心)，如图 4b 底部所示。

$$\begin{cases} \mathcal{E}_{\text{feature}}^{\text{KNN}_k} = \{N_{\text{KNN}_k}(v) \mid v \in \mathcal{V}\} \\ \mathcal{E}_{\text{feature}}^{\text{distance } d} = \{N_{\text{dis } d}(v) \mid v \in \mathcal{V}\} \end{cases}. \tag{6}$$

This type of hyperedges aims to find the relationship behind the feature of the vertices. It can be set in multi-scales, such as different k or d values in the neighbor finding procedure.

这种类型的超边旨在找到顶点特征背后的关系。它可以设置为多尺度，例如在邻居查找过程中不同的 k 或 d 值。

4.1.2 Combination of Hyperedge Groups

4.1.2 超边组的组合

Here, several hyperedge groups can be generated using above strategies. Given generated hyperedge groups or natural hyperedge groups, we need to further combine them to generate the final hypergraph. Supposing there are K hyperedge groups $\{\mathcal{E}_1, \mathcal{E}_2, \cdots, \mathcal{E}_K\}$, we can have K incidence matrices $\mathbf{H}_k \in \{0,1\}^{N \times M_k}$ respectively. The simplest fusion way to construct the incidence matrix for the hypergraph $\mathcal{G}$ is directly concatenating all the hyper-edge groups as: $\mathbf{H} = \mathbf{H}_1 \left\| \mathbf{H}_2 \right\| \cdots \| \mathbf{H}_K$, where $\cdot \| \cdot$ is matrix concatenation operation. The hyperedge weight matrix of the hypergraph can be assigned with value 1 for treating it equally. We call the simplest fusion way as Coequal Fusion.

在这里，可以使用上述策略生成多个超边组。给定生成的超边组或自然超边组后，我们需要进一步将它们组合起来以生成最终的超图。假设存在 K 个超边组 $\{\mathcal{E}_1, \mathcal{E}_2, \cdots, \mathcal{E}_K\}$，我们可以分别得到 K 个关联矩阵 $\mathbf{H}_k \in \{0,1\}^{N \times M_k}$ 。构建超图 $\mathcal{G}$ 的关联矩阵的最简单融合方法是直接将所有超边组连接起来，如下所示: $\mathbf{H} = \mathbf{H}_1 \left\| \mathbf{H}_2 \right\| \cdots \| \mathbf{H}_K$ ，其中 $\cdot \| \cdot$ 是矩阵连接操作。超图的超边权重矩阵可以赋值为 1 以平等对待它。我们将最简单的融合方法称为"同等融合"。

However, considering that the information richness of different hyperedge groups varies a lot, such a simple Coequal Fusion cannot make full use of the multi-modal hybrid high-order correlations. Therefore, in this paper, we propose an adaptive strategy for the fusion of hyper-edge groups, namely Adaptive Fusion. More specifically, each hyperedge group is associated with a trainable parameter, which can adaptively adjust the effect of multiple hyperedge groups on the final vertex embed-dings. It is defined as:

然而，考虑到不同超边组的信息丰富度差异很大，这样简单的同等融合无法充分利用多模态混合高阶相关性。因此，在本文中，我们提出了一种超边组融合的自适应策略，即自适应融合。更具体地说，每个超边组都与一个可训练参数相关联，该参数可以自适应地调整多个超边组对最终顶点嵌入的影响。其定义如下:

$$
\left\{
\begin{array}{l}
\mathbf{w}_k = \operatorname{copy}\left(\operatorname{sigmoid}\left(w_k\right), M_k\right) \\
\mathbf{W} = \operatorname{diag}\left(\mathbf{w}_1^1, \cdots, \mathbf{w}_1^{M_1}, \cdots, \mathbf{w}_K^1, \cdots, \mathbf{w}_K^{M_K}\right), \\
\mathbf{H} = \mathbf{H}_1 \,||\, \mathbf{H}_2 \,||\, \cdots \,||\, \mathbf{H}_K
\end{array}
\right.
\tag{7}
$$

where $\mathbf{w}_k \in \mathbb{R}$ is a trainable parameter shared by all hyper-edges inside a specified hyperedge group k . sigmoid $(\cdot)$ is an element-wise normalization function. Vector $\mathbf{w}_k = \left(\mathbf{w}_k^1, \cdots, \mathbf{w}_k^{M_k}\right) \in \mathbb{R}^{M_k}$ denotes the generated weight vector for hyperedge group k . copy (a, b) function returns a vector of size b , and the value of which is padded by copying ab times. Let $M = M_1 + M_2 + \cdots + M_K$ denotes the summation of the hyperedges in all hyperedge groups. $\mathbf{W} \in \mathbb{R}^{M \times M}$ is a diagonal matrix that indicates the weight matrix of hypergraph, with each entry $\mathbf{W}^{ii}$ denoting the weight of the corresponding hyperedge e_i.$\mathbf{H} \in \{0,1\}^{N \times M}$ indicates the incidence matrix of the hypergraph generated by concatenating $(\cdot \,||\, \cdot)$ the incidence matrices of multiple hyper-edge groups.

其中 $\mathbf{w}_k \in \mathbb{R}$ 是指定超边组 k 内所有超边共享的可训练参数。Sigmoid $(\cdot)$ 是一个逐元素归一化函数。向量 $\mathbf{w}_k = \left(\mathbf{w}_k^1, \cdots, \mathbf{w}_k^{M_k}\right) \in \mathbb{R}^{M_k}$ 表示超边组 k 生成的权重向量。复制 (a, b) 函数返回一个大小为 b 的向量，其值通过复制 ab 次进行填充。设 $M = M_1 + M_2 + \cdots + M_K$ 表示所有超边组中超边的总和。$\mathbf{W} \in \mathbb{R}^{M \times M}$ 是一个对角矩阵，它表示超图的权重矩阵，每个条目 $\mathbf{W}^{ii}$ 表示相应超边的权重 e_i.$\mathbf{H} \in \{0,1\}^{N \times M}$ 表示通过连接 $(\cdot \,||\, \cdot)$ 多个超边组的关联矩阵生成的超图的关联矩阵。

Given the multi-model/multi-type data, multiple hyper-edge groups can be generated accordingly. Hypergraph incidence matrix $\mathbf{H}$ and hyperedge weight matrix $\mathbf{W}$ will be generated from the constructed hyperedge groups, which can then be fed into Hypergraph Convolution Layer for further computation.

给定多模型/多类型数据，可以相应地生成多个超边组。将从构建的超边组中生成超图关联矩阵 $\mathbf{H}$ 和超边权重矩阵 $\mathbf{W}$ ，然后将它们输入到超图卷积层进行进一步计算。

4.2 Hypergraph Convolution

4.2 超图卷积

In this subsection, we define two hypergraph convolution HGNNConv and HGNNConv+ from the spectral aspect and the spatial aspect, respectively. The former is proposed in the conference version, and the later is proposed in this journal version. As for the spatial convolution on hyper-graph, we first define a general spatial hypergraph convolution layer, a two stage message passing framework. In the following, HGNNConv+ is proposed by specifying aggregation function in the two stages. Compared with the conference version, the extended HGNNConv+ exhibits more salability, which can be easily generalized into various applications such as the directed hypergraph in future work.

在本小节中，我们分别从谱域和空域两个方面定义了两种超图卷积 HGNNConv 和 HGNNConv+。前者是在会议版本中提出的，后者是在本期刊版本中提出的。至于超图上的空域卷积，我们首先定义了一个通用的空域超图卷积层，即一个两阶段消息传递框架。接下来，通过在两个阶段指定聚合函数来提出 HGNNConv+。与会议版本相比，扩展后的 HGNNConv+ 具有更强的可扩展性，在未来的工作中可以很容易地推广到各种应用中，比如有向超图。

4.2.1 Spectral Convolution on Hypergraph

4.2.1 超图上的谱卷积

Given a hypergraph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \Delta)$ with N vertices, since the hypergraph Laplacian $\square$ is a $N \times N$ positive semi-definite matrix, the eigen decomposition $\Delta = \Phi\Lambda\Phi^\top$ can be employed to get the orthonormal eigen vectors $\square = \operatorname{diag}(\phi_1, \ldots, \phi_N)$ and a diagonal matrix $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_\mathrm{N})$ containing corresponding non-negative eigenvalues. Then, the Fourier transform for a signal $\mathbf{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_\mathrm{N})$ in hyper-graph is defined as $\hat{\mathbf{x}} = \square^\top \mathbf{x}$, where the eigen vectors are regarded as the Fourier bases and the eigenvalues are interpreted as frequencies. The spectral convolution of signal $\mathbf{x}$ and filter $\mathbf{g}$ can be denoted as

给定一个具有 N 个顶点的超图 $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \Delta)$，由于超图拉普拉斯矩阵 $\square$ 是一个 $N \times N$ 半正定矩阵，因此可以采用特征分解 $\Delta = \Phi\Lambda\Phi^\top$ 来得到正交特征向量 $\square = \operatorname{diag}(\phi_1, \ldots, \phi_N)$ 和一个包含相应非负特征值的对角矩阵 $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_\mathrm{N})$。然后，超图中信号 $\mathbf{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_\mathrm{N})$ 的傅里叶变换定义为 $\hat{\mathbf{x}} = \square^\top \mathbf{x}$，其中特征向量被视为傅里叶基，特征值被解释为频率。信号 $\mathbf{x}$ 和滤波器 $\mathbf{g}$ 的谱卷积可以表示为

$$\mathbf{g} \star \mathbf{x} = \Phi\left(\left(\Phi^\top \mathbf{g}\right) \odot \left(\Phi^\top \mathbf{x}\right)\right) = \square g\left(\square\right) \square^\top \mathbf{x}, \tag{8}$$

where $\odot$ denotes the element-wise Hadamard product and $g(\Lambda) = \operatorname{diag}(\mathbf{g}(\lambda_1), \ldots, \mathbf{g}(\lambda_\mathrm{n}))$ is a function of the Fourier coefficients. However, the computation cost in forward and inverse Fourier transform is $\mathcal{O}\left(n^2\right)$. To solve the problem, we can follow [49] to parametrize $g(\Lambda)$ with K order polynomials. Furthermore, we use the truncated Chebyshev expansion as one such polynomial. Chebyshv polynomials $T_k(x)$ is recursively computed by $T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$, with $T_0(x) = 1$ and $T_1(x) = x$. Thus, the $g(\square)$ can be parametried as

其中 $\odot$ 表示按元素的哈达玛积，$g(\Lambda) = \operatorname{diag}(\mathbf{g}(\lambda_1), \ldots, \mathbf{g}(\lambda_\mathrm{n}))$ 是傅里叶系数的函数。然而，傅里叶变换的正向和反向计算成本为 $\mathcal{O}\left(n^2\right)$。为了解决这个问题，我们可以按照 [49] 的方法，用 K 阶多项式对 $g(\Lambda)$ 进行参数化。此外，我们使用截断切比雪夫展开作为这样的一个多项式。切比雪夫多项式 $T_k(x)$ 通过 $T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$ 递归计算，其中 $T_0(x) = 1$ 和 $T_1(x) = x$。因此，$g(\square)$ 可以参数化为

$$\mathbf{g} \star \mathbf{x} \approx \sum_{k=0}^{K} \theta_k T_k\left(\tilde{\square}\right) \mathbf{x}, \tag{9}$$

where $T_k\left(\tilde{\square}\right)$ is the Chebyshev polynomial of order k with scaled Laplacian $\tilde{\square} = \frac{2}{\lambda_{\max}} \square - \mathbf{I}$. In Eq. (9), the expansive computation of Laplacian Eigen vectors is excluded and only matrix powers, additions and multiplications are included, which brings further improvement in computation complexity. We can further let $K = 1$ to limit the order of convolution operation due to that the Laplacian in hyper-graph can already well represent the high-order correlation between nodes. It is also suggested in [2] that $\lambda_{\max} \approx 2$ because of the scale adaptability of neural networks. Then, the convolution operation can be further simplified to

其中 $T_k\left(\tilde{⍰}\right)$ 是具有缩放拉普拉斯矩阵 $\tilde{⍰} = \frac{2}{\lambda_{\max}}⍰ - \mathbf{I}$ 的 k 阶切比雪夫多项式。在式 (9) 中，排除了拉普拉斯特征向量的扩展计算，只包括矩阵幂、加法和乘法，这在计算复杂度上带来了进一步的改进。由于超图中的拉普拉斯矩阵已经能够很好地表示节点之间的高阶相关性，我们可以进一步令 $K = 1$ 来限制卷积操作的阶数。[2] 中也建议 $\lambda_{\max} \approx 2$，这是由于神经网络的尺度适应性。然后，卷积操作可以进一步简化为

$$\mathbf{g} \star \mathbf{x} \approx \theta_0 \mathbf{x} - \theta_1 \mathbf{D}_v^{-1/2} \mathbf{H} \mathbf{W} \mathbf{D}_e^{-1} \mathbf{H}^\top \mathbf{D}_v^{-1/2} \mathbf{x}, \tag{10}$$

where θ_0 and θ_1 is parameters of filters over all nodes. We further use a single parameter θ to avoid the overfitting problem, which is defined as

其中 θ_0 和 θ_1 是所有节点上滤波器的参数。我们进一步使用单个参数 θ 来避免过拟合问题，其定义为

$$\begin{cases} \theta_1 = -\frac{1}{2}\theta \\ \theta_0 = \frac{1}{2}\theta \mathbf{D}_v^{-1/2} \mathbf{H} \mathbf{D}_e^{-1} \mathbf{H}^\top \mathbf{D}_v^{-1/2} \end{cases} \tag{11}$$

Then, the convolution operation can be simplified to the following expression

然后，卷积操作可以简化为以下表达式

$$\mathbf{g} \star \mathbf{x} \approx \frac{1}{2}\theta \mathbf{D}_v^{-1/2} \mathbf{H} \left(\mathbf{W} + \mathbf{I}\right) \mathbf{D}_e^{-1} \mathbf{H}^\top \mathbf{D}_v^{-1/2} \mathbf{x} \approx \theta \mathbf{D}_v^{-1/2} \mathbf{H} \mathbf{W} \mathbf{D}_e^{-1} \mathbf{H}^\top \mathbf{D}_v^{-1/2} \mathbf{x}, \tag{12}$$

where $(\mathbf{W} + \mathbf{I})$ can be regarded as the weight of the hyper-edges. $\mathbf{W}$ is initialized as an identity matrix, which means equal weights for all hyperedges.

其中 $(\mathbf{W} + \mathbf{I})$ 可以被视为超边的权重。$\mathbf{W}$ 初始化为单位矩阵，这意味着所有超边的权重相等。

When we have a hypergraph signal $\mathbf{X}^t$ for t -th layer, our hyperedge convolution layer HGNNConv can be formulated by

当我们有第 t 层的超图信号 $\mathbf{X}^t$ 时，我们的超边卷积层 HGNNConv 可以表示为

$$\mathbf{X}^{t+1} = \sigma\left(\mathbf{D}_v^{-1/2} \mathbf{H} \mathbf{W} \mathbf{D}_e^{-1} \mathbf{H}^\top \mathbf{D}_v^{-1/2} \mathbf{X}^t ⍰\right), \tag{13}$$

where ⍰ is the parameter to be learned during the training process. The filter ⍰ is applied over the nodes in hyper-graph to extract features. After convolution, we can obtain $\mathbf{X}^{t+1}$, which can be used for further learning.

其中 ⍰ 是在训练过程中要学习的参数。滤波器 ⍰ 应用于超图中的节点以提取特征。卷积之后，我们可以得到 $\mathbf{X}^{t+1}$ ，其可用于进一步学习。

4.2.2 General Spatial Convolution on Hypergraph

4.2.2 超图上的通用空间卷积

In this subsection, we introduce the hypergraph convolution from spatial domain. First, let's briefly review the definition of a typical spatial-based graph convolution. An image can be considered as a grid graph where each pixel represents a vertex and each vertex only connects its surrounding neighborhood vertices. Each vertex (pixel) in image owns a C -channel feature. Filtering on image can be regarded as a process that central vertex aggregates its neighbors' feature with average aggregation after transforming their feature. Similarly, for a simple graph, spatial-based graph convolution takes the aggregation of its neighbor vertices to get a new representation of the central vertex. Messages in spatial graph convolution run from neighbor vertices to center vertex, which is following the definition of ”Path” in simple graph. A path in graph is defined as $P(v_1, v_k) = (v_1, v_2, \cdots, v_k)$. It is a sequence of vertices with the property that each vertex in the sequence is adjacent to the vertex next to it, which means that all the vertex pairs of i and $i+1\,(1 \leq i \leq k-1)$ have Neighbor Relation.

在本小节中，我们从空间域引入超图卷积。首先，让我们简要回顾一下典型的基于空间的图卷积的定义。一幅图像可以被视为一个网格图，其中每个像素代表一个顶点，并且每个顶点仅连接其周围的邻域顶点。图像中的每个顶点 (像素) 都拥有一个 C 通道的特征。对图像进行滤波可以看作是一个过程，即中心顶点在变换其邻居的特征后通过平均聚合来聚合它们的特征。类似地，对于一个简单图，基于空间的图卷积通过聚合其邻居顶点来获得中心顶点的新表示。空间图卷积中的消息从邻居顶点流向中心顶点，这遵循简单图中“路径”的定义。图中的路径定义为 $P(v_1, v_k) = (v_1, v_2, \cdots, v_k)$ 。它是一个顶点序列，具有这样的属性: 序列中的每个顶点都与它旁边的顶点相邻，这意味着 i 和 $i+1\,(1 \leq i \leq k-1)$ 的所有顶点对都具有邻居关系。

Here, we can define the spatial convolution on hypergraph. For each vertex in hypergraph, we aggregate its neighbor vertex messages to update itself according to the ”path” between the central vertex and each vertex in its neighborhood. The path in hypergraph, named hyperpath [10], between two distinct vertices v_1 and v_k is defined as a sequence:

在这里，我们可以定义超图上的空间卷积。对于超图中的每个顶点，我们根据中心顶点与其邻域中每个顶点之间的“路径”来聚合其邻居顶点的消息以更新自身。超图中两个不同顶点 v_1 和 v_k 之间的路径，称为超路径 [10]，定义为一个序列:

$$P(v_1, v_k) = (v_1, e_1, v_2, e_2, \ldots, v_{k-1}, e_k, v_k), \tag{14}$$

in which v_j and v_{j+1} belong to the same vertex subset that indicated by a hyperedge e_j . Obviously, each two neighbor vertices in a hyperpath is separated by a hyperedge. Message in hypergraph between two vertices is propagated through related hyperedges, which can take the advantage of high-order relationship through hyperedge compared with that in graph. For the message propagation from vertex to hyperedge and that from hyperedge to vertex using hyperpath, we first extend the Neighbor Relation definition among vertices to the Inter-neighbor Relation N over vertex set $\mathcal{V}$ and hyperedge set $\mathcal{E}$.

其中 v_j 和 v_{j+1} 属于由超边 e_j 指示的同一个顶点子集。显然，超路径中的每两个相邻顶点都由一条超边隔开。超图中两个顶点之间的消息通过相关超边传播，与图相比，这可以利用超边的高阶关系。对于使用超路径从顶点到超边以及从超边到顶点的消息传播，我们首先将顶点之间的邻居关系定义扩展到顶点集 $\mathcal{V}$ 和超边集 $\mathcal{E}$ 上的邻域间关系 N 。

Definition 1. The Inter-Neighbor Relation $N \subseteq \mathcal{V} \times \mathcal{E}$ on a hypergraph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{W})$ with incidence matrix $\mathbf{H} \in \{0,1\}^{|\mathcal{V}|\times|\mathcal{E}|}$ is defined as:

定义 1. 具有关联矩阵 $\mathbf{H} \in \{0,1\}^{|\mathcal{V}|\times|\mathcal{E}|}$ 的超图 $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{W})$ 上的邻域间关系 $N \subseteq \mathcal{V} \times \mathcal{E}$ 定义为:

$$N = \{(v, e) \mid \mathbf{H}(v, e) = 1, v \in \mathcal{V} \text{ and } e \in \mathcal{E}\} \tag{15}$$

Then, we define the vertex inter-neighbor set $N_v(e)$ of hyperedge e and the hyperedge inter-neighbor set $N_e(v)$ of vertex v based on the Inter-Neighbor Relation.

然后，我们基于邻域间关系定义超边 e 的顶点邻域间集合 $N_v(e)$ 和顶点 v 的超边邻域间集合 $N_e(v)$ 。

Definition 2. The vertex inter-neighbor set of hyperedge $e \in \mathcal{E}$ is defined as:

定义 2. 超边 $e \in \mathcal{E}$ 的顶点邻域间集合定义为:

$$\mathcal{N}_v(e) = \{v \mid vNe, v \in \mathcal{V} \text{ and } e \in \mathcal{E}\} \tag{16}$$

Definition 3. The hyperedge inter-neighbor set of vertex $v \in \mathcal{V}$ is defined as:

定义 3. 顶点 $v \in \mathcal{V}$ 的超边邻域间集合定义为:

$$\mathcal{N}_e(v) = \{e \mid vNe, v \in \mathcal{V} \text{ and } e \in \mathcal{E}\} \tag{17}$$

Following Definition 1, 2, and 3, we introduce the message passing of neighbor vertex message aggregation via hyper-path for one spatial hypergraph convolution layer. Given a vertex $\alpha \in \mathcal{V}$ of hypergraph $\mathcal{G} = \{\mathcal{V}, \mathcal{E}, \mathbf{W}\}$, we aim to aggregate messages from its hyperedge inter-neighbor set $N_e(\alpha)$. To obtain those hyperedge messages for each hyperedge β in the hyperedge inter-neighbor set $\mathcal{N}_e(\alpha)$, we aggregate messages from its vertex inter-neighbor set $\mathcal{N}_v(\beta)$. Then, the two steps of hypergraph convolution make a closed message passing loop from vertex feature set X^t to X^{t+1} . A

根据定义 1、2 和 3，我们介绍了用于一个空间超图卷积层的通过超路径进行邻居顶点消息聚合的消息传递。给定超图 $\mathcal{G} = \{\mathcal{V}, \mathcal{E}, \mathbf{W}\}$ 中的一个顶点 $\alpha \in \mathcal{V}$ ，我们旨在聚合来自其超边内部邻居集 $N_e(\alpha)$ 的消息。为了获得超边内部邻居集 $\mathcal{N}_e(\alpha)$ 中每个超边 β 的那些超边消息，我们聚合来自其顶点内部邻居集 $\mathcal{N}_v(\beta)$ 的消息。然后，超图卷积的这两个步骤形成了一个从顶点特征集 X^t 到 X^{t+1} 的封闭消息传递循环。A general spatial hypergraph convolution in the t -th layer can be defined as:

第 t 层的一般空间超图卷积可定义为:

$$\left.\begin{cases} m_\beta^t & = \sum\limits_{\alpha \in \mathcal{N}_v(\beta)} M_v^t\left(x_\alpha^t\right) \\ y_\beta^t & = U_e^t\left(w_\beta, m_\beta^t\right) \\ m_\alpha^{t+1} & = \sum\limits_{\beta \in \mathcal{N}_e(\alpha)} M_e^t\left(x_\alpha^t, y_\beta^t\right) \\ x_\alpha^{t+1} & = U_v^t\left(x_\alpha^t, m_\alpha^{t+1}\right) \end{cases}\right\} \text{Stage 1} \tag{18}$$

where $x_\alpha^t \in \mathbf{X}^t$ is the input feature vector of vertex $\alpha \in \mathcal{V}$ in layer $t = 1, 2, \cdots, T$, and x_α^{t+1} is the updated feature of vertex $\alpha . m_\beta^t$ is the message of hyperedge $\beta \in \mathcal{E}$, and w_β is a weight associated to hyperedge $\beta . m_\alpha^{t+1}$ denotes the message of vertex $\alpha . y_\beta^t$ is the hyperedge feature of hyperedge β which is a element of hyperedge feature set $Y^t = \left\{y_1^t, y_2^t, \cdots, y_M^t\right\}, y_i^t \in \mathbb{R}^{C_t}$ in layer $t . M_v^t(\cdot), U_e^t(\cdot), M_e^t(\cdot), U_v^t(\cdot)$ are the vertex message function, hyperedge update functions, hyperedge message function and vertex update function in t_{th} layer, respectively, which can be flexibility defined for specified applications.

其中 $x_\alpha^t \in \mathbf{X}^t$ 是第 $t = 1, 2, \cdots, T$ 层中顶点 $\alpha \in \mathcal{V}$ 的输入特征向量，x_α^{t+1} 是顶点 $\alpha . m_\beta^t$ 的更新特征，$\beta \in \mathcal{E}$ 是超边 $\beta \in \mathcal{E}$ 的消息，w_β 是与超边 $\beta . m_\alpha^{t+1}$ 相关联的权重，$\beta . m_\alpha^{t+1}$ 表示顶点 $\alpha . y_\beta^t$ 的消息，β 是超边 β 的超边特征，它是第 $t . M_v^t(\cdot), U_e^t(\cdot), M_e^t(\cdot), U_v^t(\cdot)$ 层中超边特征集 $Y^t = \left\{y_1^t, y_2^t, \cdots, y_M^t\right\}, y_i^t \in \mathbb{R}^{C_t}$ 的一个元素，t_{th} 分别是第 t_{th} 层中的顶点消息函数、超边更新函数、超边消息函数和顶点更新函数，它们可以针对特定应用灵活定义。

The spatial hypergraph convolution layer is designed for high-level representation learning via the high-order relationship in hypergraph structure. Compared with the one-stage message passing in graph convolution, the two-stage spatial hypergraph convolution is composed of four flexible operations with learned differentiable functions. Similar to the neighbor relation defined in graph, a vertex's hyperedge inter-neighbors and a hyperedge's vertex inter-neighbors have no natural ordering. Therefore, a summation operation is used to aggregate vertex/hyperedge messages from $M_v^t(\cdot) / M_e^t(\cdot)$ operation.

空间超图卷积层旨在通过超图结构中的高阶关系进行高级表示学习。与图卷积中的单阶段消息传递相比，两阶段空间超图卷积由四个具有可学习可微函数的灵活操作组成。类似于图中定义的邻居关系，一个顶点的超边内部邻居和一个超边的顶点内部邻居没有自然顺序。因此，使用求和操作从 $M_v^t(\cdot) / M_e^t(\cdot)$ 操作中聚合顶点/超边消息。

4.2.3 HGNN $^+$ Convolution Layer Configurations

4.2.3 HGNN $^+$ 卷积层配置

A simple spatial hypergraph convolution layer (named HGNNConv+) via specifying the message-update functions (vertex message function $M_v^t(\cdot)$, hyperedge update function $U_e^t(\cdot)$, hyperedge message function $M_e^t(\cdot)$ and vertex update function $U_v^t(\cdot)$) are introduced as:

通过指定消息更新函数 (顶点消息函数 $M_v^t(\cdot)$ 、超边更新函数 $U_e^t(\cdot)$ 、超边消息函数 $M_e^t(\cdot)$ 和顶点更新函数 $U_v^t(\cdot)$) 引入一个简单的空间超图卷积层 (名为 HGNNConv+)，定义如下:

$$
\begin{cases}
M_v^t\left(x_\alpha^t\right) & = \frac{x_\alpha^t}{|\mathcal{N}_v(\beta)|} \\
U_e^t\left(w_\beta, m_\beta^t\right) & = w_\beta \cdot m_\beta^t \\
M_e^t\left(x_\alpha^t, y_\beta^t\right) & = \frac{y_\beta^t}{|\mathcal{N}_e(\alpha)|} \\
U_e^t\left(x_\alpha^t, m_\alpha^{t+1}\right) & = \sigma\left(m_\alpha^{t+1} \cdot \square^t\right)
\end{cases}, \tag{19}
$$

where $\square^t \in \mathbb{R}^{C^t \times C^{t+1}}$ is a trainable parameter of layer t , which can be learned in training phase. $\sigma(\cdot)$ is an arbitrary non-linear activation function like ReLU $(\cdot)$ etc. Note that in Eq. (19), $x_\alpha^t / |\mathcal{N}_v(\beta)|$ and $y_\beta^t / |\mathcal{N}_e(\alpha)|$ denote the normalized vertex/hyperedge feature, which is adopted to accumulate convergence and prevent jittering in some degree.

其中 $\square^t \in \mathbb{R}^{C^t \times C^{t+1}}$ 是层 t 的一个可训练参数，它可以在训练阶段学习得到。$\sigma(\cdot)$ 是一个任意的非线性激活函数，如 ReLU $(\cdot)$ 等。注意，在式 (19) 中，$x_\alpha^t / |\mathcal{N}_v(\beta)|$ 和 $y_\beta^t / |\mathcal{N}_e(\alpha)|$ 表示归一化的顶点/超边特征，它被用于积累收敛并在一定程度上防止抖动。

For faster forward propagation of HGNNConv+ in GPU/CPU devices, we rewrite it in the matrix format. Considering X^t is the input vertex feature set of layer t . From Definition 1 and 2, $\mathbf{H}^\top \in \{0,1\}^{M \times N}$ can control the hyper-edge inter-neighbor of each vertex feature in X^t . Hence, we use it to guide each vertex to aggregate and generate the hyperedge feature set Y^t , which can be formulated as $\mathbf{Y}^t = \mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^\top\mathbf{X}^t$. In a similar way, the process that updating vertex feature set $\mathbf{X}^{t+1}$ from hyperedge feature set $\mathbf{Y}^t$ can be formulated as $\mathbf{X}^{t+1} = \sigma\left(\mathbf{D}_v^{-1}\mathbf{H}\mathbf{Y}^t\square^t\right)$. Thus, the matrix format of HGNNConv+ can be written as:

为了在 GPU/CPU 设备中更快地进行 HGNNConv+ 的前向传播，我们将其重写为矩阵形式。考虑到 X^t 是层 t 的输入顶点特征集。根据定义 1 和 2, $\mathbf{H}^\top \in \{0,1\}^{M \times N}$ 可以控制 X^t 中每个顶点特征的超边邻域。因此,我们用它来引导每个顶点进行聚合并生成超边特征集 Y^t ,其可以表示为 $\mathbf{Y}^t = \mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^\top\mathbf{X}^t$ 。以类似的方式，从超边特征集 $\mathbf{Y}^t$ 更新顶点特征集 $\mathbf{X}^{t+1}$ 的过程可以表示为 $\mathbf{X}^{t+1} = \sigma\left(\mathbf{D}_v^{-1}\mathbf{H}\mathbf{Y}^t\square^t\right)$ 。因此，HGNNConv+ 的矩阵形式可以写成:

$$
\mathbf{X}^{t+1} = \sigma\left(\mathbf{D}_v^{-1}\mathbf{H}\mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^\top\mathbf{X}^t\square^t\right). \tag{20}
$$

5 DISCUSSIONS

5 讨论

In this section, we provide comprehensive analyses and comparisons of the hypergraph structure and the proposed methods for a deeper understanding.

在本节中，我们对超图结构和所提出的方法进行全面的分析和比较，以便更深入地理解。

5.1 Hypergraph vs. Graph

5.1 超图与图

Here, we provide a mathematical comparison of hyper-graphs and graphs via the random walks [36] and the Markov chain [35]. The proof concludes that: from the random walks' aspect, a hypergraph with edge-independent vertex weights is equivalent to a weighted graph, and a hypergraph with edge-dependent vertex weights cannot be reduced to a weighted graph.

在这里，我们通过随机游走 [36] 和马尔可夫链 [35] 对超图和图进行数学比较。证明得出: 从随机游走的角度来看，具有边独立顶点权重的超图等同于加权图，而具有边相关顶点权重的超图不能简化为加权图。

In general, to accurate describe the real-world correlations, two types of hypergraphs can be constructed, i.e., hypergraphs with edge-independent vertex weights and hypergraphs with edge-dependent vertex weights. The hypergraph with edge-independent vertex weights ($\mathcal{G}_{\text{in}} = \{\mathcal{V}, \mathcal{E}, \mathbf{W}\}$) can model the beyond pair-wise correlations, which can be denoted by the binary hypergraph incidence matrix $\mathbf{H} \in \{0,1\}^{|\mathcal{V}| \times |\mathcal{E}|}$, in which vertices in each hyperedge share the same weight. In contrast, the hypergraph with edge-dependent vertex weights ($\mathcal{G}_{\text{de}} = \{\mathcal{V}, \mathcal{E}, \mathbf{W}, \gamma\}$) can further model the variable correlation intensity in each hyper-edge, which can be denoted by the weighted hypergraph incidence matrix $\mathbf{R} \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{E}|}$. Assuming that the hyperedge e includes the vertex v , then we use $\gamma_e(v)$ to denote the connection intensity between e and v and $w(e)$ to denote the weight of hyperedge e . The definition of binary hypergraph incidence matrix $\mathbf{H}$, vertex degree $d(v)$ and the hyperedge degree $\delta(e)$ in hypergraphs with edge-independent vertex weights is similar to Section 3, In hypergraphs with edge-dependent vertex weights, the $d(v)$, and $\delta(e)$ can be defined as follows:

一般来说，为了准确描述现实世界中的相关性，可以构建两种类型的超图，即具有边独立顶点权重的超图和具有边依赖顶点权重的超图。具有边独立顶点权重的超图 ($\mathcal{G}_{\text{in}} = \{\mathcal{V}, \mathcal{E}, \mathbf{W}\}$) 可以对成对之外的相关性进行建模，其可以由二元超图关联矩阵 $\mathbf{H} \in \{0,1\}^{|\mathcal{V}| \times |\mathcal{E}|}$ 表示，其中每个超边中的顶点具有相同的权重。相比之下，具有边依赖顶点权重的超图 ($\mathcal{G}_{\text{de}} = \{\mathcal{V}, \mathcal{E}, \mathbf{W}, \gamma\}$) 可以进一步对每个超边中的可变相关强度进行建模，其可以由加权超图关联矩阵 $\mathbf{R} \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{E}|}$ 表示。假设超边 e 包含顶点 v ，那么我们使用 $\gamma_e(v)$ 来表示 e 和 v 之间的连接强度，使用 $w(e)$ 来表示超边 e 的权重。具有边独立顶点权重的超图中二元超图关联矩阵 $\mathbf{H}$ 、顶点度 $d(v)$ 和超边度 $\delta(e)$ 的定义与第 3 节类似。在具有边依赖顶点权重的超图中，$d(v)$ 和 $\delta(e)$ 可以如下定义:

$$
\begin{cases}
d(v) = \sum\limits_{\beta \in \mathcal{N}_e(v)} w(\beta) \\
\delta(e) = \sum\limits_{\alpha \in \mathcal{N}_v(e)} \gamma_e(\alpha)
\end{cases}, \tag{21}
$$

where $\mathcal{N}_v(\cdot)$ and $\mathcal{N}_e(\cdot)$ are defined in Eq. (17) and (16), respectively.

其中 $\mathcal{N}_v(\cdot)$ 和 $\mathcal{N}_e(\cdot)$ 分别在式 (17) 和 (16) 中定义。

Random walks and the Markov chain in hypergraphs. We first define the random walk in a hypergraph following [20], [34],[35],[36]. At time t , a random walker at vertex v_t will do the following:

超图中的随机游走和马尔可夫链。我们首先按照 [20]、[34]、[35]、[36] 定义超图中的随机游走。在时间 t ， 位于顶点 v_t 的随机游走者将执行以下操作:

- Pick an edge e containing vertex $v_t = v$, with probability $p_{v \to e}$.

  - 以概率 $p_{v \to e}$ 选择包含顶点 $v_t = v$ 的边 e 。

- Pick vertex u from e , with probability $p_{e \to u}$.

  - 以概率 $p_{e \to u}$ 从 e 中选择顶点 u 。

- Move to vertex $v_{t+1} = u$, at time $t + 1$.

  - 在时间 $t + 1$ 移动到顶点 $v_{t+1} = u$ 。

Then, the transition probability $p_{v,u}$ of the corresponding Markov chain on $\mathcal{V}$ can be defined as $p_{v,u} = \sum_{e \in \mathcal{N}_e(v,u)} p_{v \to e} p_{e \to u}$, where $\mathcal{N}_e(v,u) = \mathcal{N}_e(v) \cap \mathcal{N}_e(u)$ denotes the hyperedge $\beta \in \mathcal{N}_e(v,u)$ containing vertices v and u , simultaneously. In hypergraphs with edge-independent vertex weights, we have $p_{v \to e} = w(e)/d(v)$ and $p_{e \to u} = 1/\delta(e)$. Then, the transition probability $p_{v,u}$ can be defined as: $p_{v,u} = \sum_{\beta \in \mathcal{N}_e(v,u)} \frac{w(\beta)}{d(v)} \cdot \frac{1}{\delta(\beta)}$. In hypergraphs with edge-dependent vertex weights, we have $p_{v \to e} = w(e)/d(v)$ and $p_{e \to u} = \gamma_e(u)/\delta(e)$, Then, the transition probability $p_{v,u}$ can be defined as $p_{v,u} = \sum_{\beta \in \mathcal{N}_e(v,u)} \frac{w(\beta)}{d(v)} \cdot \frac{\gamma_\beta(u)}{\delta(\beta)}$.

然后，在 $\mathcal{V}$ 上相应马尔可夫链的转移概率 $p_{v,u}$ 可定义为 $p_{v,u} = \sum_{e \in \mathcal{N}_e(v,u)} p_{v \to e} p_{e \to u}$ ，其中 $\mathcal{N}_e(v,u) = \mathcal{N}_e(v) \cap \mathcal{N}_e(u)$ 表示同时包含顶点 v 和 u 的超边 $\beta \in \mathcal{N}_e(v,u)$ 。在具有边独立顶点权重的超图中，我们有 $p_{v \to e} = w(e)/d(v)$ 和 $p_{e \to u} = 1/\delta(e)$ 。然后，转移概率 $p_{v,u}$ 可定义为: $p_{v,u} = \sum_{\beta \in \mathcal{N}_e(v,u)} \frac{w(\beta)}{d(v)} \cdot \frac{1}{\delta(\beta)}$ 。在具有边相关顶点权重的超图中，我们有 $p_{v \to e} = w(e)/d(v)$ 和 $p_{e \to u} = \gamma_e(u)/\delta(e)$ ，那么，转移概率 $p_{v,u}$ 可定义为 $p_{v,u} = \sum_{\beta \in \mathcal{N}_e(v,u)} \frac{w(\beta)}{d(v)} \cdot \frac{\gamma_\beta(u)}{\delta(\beta)}$ 。

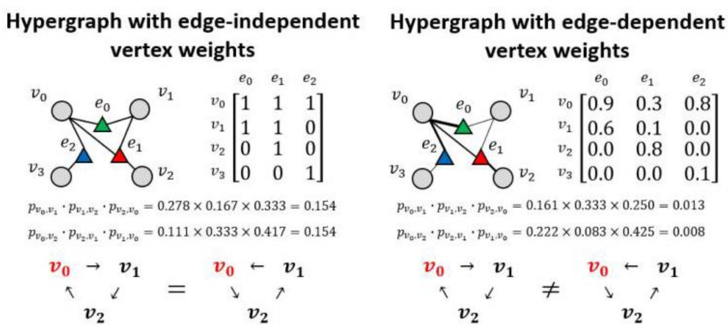

Fig. 5. Examples of two types of hypergraphs.

图 5. 两种超图的示例。

the two reversible paths. In contrast, we will get two different accumulated transition probabilities from two reversible paths in the hypergraph with edge-independent vertex weights.

这两条可逆路径。相比之下，在具有边独立顶点权重的超图中，我们将从两条可逆路径得到两个不同的累积转移概率。

5.2 HGNN/HGNN $^+$ vs. GNN

5.2 HGNN/HGNN $^+$ 与 GNN 的对比

GNN represents the classical convolution operator designed on graphs, such as [1], [2], [3], [4], [5]. In this subsection, we compare the HGNN and HGNN $^+$ with GNN from the spectral perspective and spatial perspective, respectively.

GNN 代表在图上设计的经典卷积算子，如 [1]、[2]、[3]、[4]、[5]。在本小节中，我们分别从谱视角和空间视角将 HGNN 和 HGNN $^+$ 与 GNN 进行比较。

The comparison of HGNN and GNN from the spectral perspective. We prove that the GNN can be a special case of the HGNN mathematically. Assuming that each hyper-edge only connects two nodes and has the same weight as others, the simple hypergraph (2-uniform hypergraph) can also be denoted by a graph with graph adjacency matrix $\mathbf{A}$ and vertex degree matrix $\mathbf{D}$, which can refer to the $\mathcal{E}_{\text{pair}}$ construction in Eq. (3). The corresponding hypergraph can be denoted by hypergraph incidence matrix $\mathbf{H}$, vertex degree matrix $\mathbf{D}_v$, hyperedge degree matrix $\mathbf{D}_e$, and hyper-edge weight matrix $\mathbf{W}$. Under this circumstance, we have the following formulations to reduce the simple hyper-graph:

从谱视角对 HGNN 和 GNN 的比较。我们从数学上证明 GNN 可以是 HGNN 的一种特殊情况。假设每个超边仅连接两个节点且与其他超边具有相同权重，简单超图 (2 - 均匀超图) 也可以用具有图邻接矩阵 $\mathbf{A}$ 和顶点度矩阵 $\mathbf{D}$ 的图表示，这可以参考式 (3) 中的 $\mathcal{E}_{\text{pair}}$ 构造。相应的超图可以用超图关联矩阵 $\mathbf{H}$ 、顶点度矩阵 $\mathbf{D}_v$ 、超边度矩阵 $\mathbf{D}_e$ 和超边权重矩阵 $\mathbf{W}$ 表示。在这种情况下，我们有以下用于简化简单超图的公式:

$$\begin{cases} \mathbf{H}\mathbf{H}^\top &= \mathbf{A} + \mathbf{D} \\ \mathbf{D}_e^{-1} &= 1/2\mathbf{I} \\ \mathbf{W} &= \mathbf{I} \end{cases} \tag{23}$$

Then, the hypergraph convolution defined in the conference version can be reduced as follows:

然后，会议版本中定义的超图卷积可以简化如下:

$$\begin{aligned} \mathbf{X}^{t+1} &= \sigma\left(\mathbf{D}_v^{-1/2}\mathbf{H}\mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^\top\mathbf{D}_v^{-1/2}\mathbf{X}^t\square^t\right) \\ &= \sigma\left(\mathbf{D}_v^{-1/2}\mathbf{H}\left(\frac{1}{2}\mathbf{I}\right)\mathbf{H}^\top\mathbf{D}_v^{-1/2}\mathbf{X}^t\square^t\right) \\ &= \sigma\left(\frac{1}{2}\mathbf{D}^{-1/2}\left(\mathbf{A}+\mathbf{D}\right)\mathbf{D}^{-1/2}\mathbf{X}^t\square^t\right) \\ &= \sigma\left(\frac{1}{2}\left(\mathbf{I}+\mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}\right)\mathbf{X}^t\square^t\right) \end{aligned} \tag{24}$$

$$= \sigma\left(\mathbf{D}^{-1/2}\widehat{\mathbf{A}}\mathbf{D}^{-1/2}\mathbf{X}^t\widehat{\square}^t\right),$$

where $\widehat{\mathbf{A}} = \mathbf{I} + \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$ and $\widehat{\square}^t = \frac{1}{2}\square^t$. The extra $\frac{1}{2}$ can be absorbed by the learnable parameter $\square$. We find that in modeling the simple graph, the spectral-based hypergraph convolution in the conference version has the same formation as the graph convolution in GCN [2]. Therefore, the hypergraph convolution not only inherits the powerful November 03,2025 at 04:07:45 UTC from IEEE Xplore. Restrictions apply.

其中 $\widehat{\mathbf{A}} = \mathbf{I} + \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$ 和 $\widehat{\square}^t = \frac{1}{2}\square^t$ 。额外的 $\frac{1}{2}$ 可以被可学习参数 $\square$ 吸收。我们发现，在对简单图进行建模时，会议版本中基于谱的超图卷积与 GCN [2] 中的图卷积具有相同的形式。因此，超图卷积不仅继承了强大的功能 2025 年 11 月 3 日 04:07:45 协调世界时来自 IEEE Xplore。版权所有。

Following [35] we provide the following Definitions and Lemmas to compare the graph and two types of hypergraphs.

遵循 [35]，我们提供以下定义和引理来比较图和两种类型的超图。

Definition 4. Let M be a Markov chain with state space X and transition probability $p_{x,y}$, for $x, y \in S$. We say M is reversible if there exists a probability distribution π over S such that $\pi_x p_{x,y} = \pi_y p_{y,x}$.

定义 4。设 M 是一个状态空间为 X 且转移概率为 $p_{x,y}$ 的马尔可夫链，其中 $x, y \in S$ 。如果存在一个在 S 上的概率分布 π 使得 $\pi_x p_{x,y} = \pi_y p_{y,x}$. ，我们就说 M 是可逆的。

Lemma 5. Let M be an irreducible Markov chain with finite state space S and transition probability $p_{x,y}$ for $x, y \in S$. M is reversible if and only if there exists a weighted, undirected graph G with vertex set S such that a random walk on G and M are equivalent.

引理 5。设 M 是一个具有有限状态空间 S 且转移概率为 $p_{x,y}$ 的不可约马尔可夫链，其中 $x, y \in S$ 。当且仅当存在一个顶点集为 S 的加权无向图 G 使得在 G 上的随机游走与 M 等价时，M 是可逆的。

Definition 6. A Markov chain is reversible if and only if its transition probability satisfies

定义 6。一个马尔可夫链是可逆的，当且仅当它的转移概率满足

$$p_{v_1,v_2} p_{v_2,v_3} \cdots p_{v_n,v_1} = p_{v_1,v_n} p_{v_n,v_{n-1}} \cdots p_{v_2,v_1}, \tag{22}$$

for any finite sequence of states $v_1, v_2, \cdots v_n \in S$. This definition is also known as Kolmogorov's criterion. The proof can be found in [39].

对于任何有限状态序列 $v_1, v_2, \cdots v_n \in S$ 。这个定义也被称为柯尔莫哥洛夫准则。证明可在 [39] 中找到。

Theorem 1. Let $\mathcal{G}_{\text{in}} = \{\mathcal{V}, \mathcal{E}, \mathbf{W}\}$ be a hypergraph with edge-independent weights. Then, there exists a weighted, undirected graph G such that a random walk on G is equivalent to a random walk on $\mathcal{G}_{\text{in}}$.

定理 1。设 $\mathcal{G}_{\text{in}} = \{\mathcal{V}, \mathcal{E}, \mathbf{W}\}$ 是一个具有边独立权重的超图。那么，存在一个加权无向图 G 使得在 <b >1</b1> 上的随机游走与在 $\mathcal{G}_{\text{in}}$ 上的随机游走等价。

The proof of Theorem 1 can follow the process as:

定理 1 的证明过程如下:

1) A random walk on $\mathcal{G}_{\text{in}}$ is equivalent to a random walk on a reversible Markov chain. (According to Definition 6.)

1) 在 $\mathcal{G}_{\text{in}}$ 上的随机游走与在一个可逆马尔可夫链上的随机游走等价。(根据定义 6。)

2) A random walk on a reversible Markov chain is equivalent to a random walk on a weighted, undirected graph G. (According to Lemma 5.) Detailed proofs of Lemma 5 and Theorem 1 can be found in Appendix. A, (available online).

2) 在一个可逆马尔可夫链上的随机游走与在一个加权无向图 G 上的随机游走等价。(根据引理 5。) 引理 5 和定理 1 的详细证明可在附录 A 中找到 (可在线获取)。

Theorem 2. Let $\mathcal{G}_{\text{de}} = \{\mathcal{V}, \mathcal{E}, \mathbf{W}, \gamma\}$ be a hypergraph with edge-dependent weights. Then, there does not exist a weighted, undirected graph G such that a random walk on G is equivalent to a random walk on $\mathcal{G}_{\text{de}}$.

定理 2。设 $\mathcal{G}_{\text{de}} = \{\mathcal{V}, \mathcal{E}, \mathbf{W}, \gamma\}$ 是一个具有边相关权重的超图。那么，不存在一个加权无向图 G 使得在 G 上的随机游走与在 $\mathcal{G}_{\text{de}}$ 上的随机游走等价。

Proof of Theorem 2. Fig. 5 provides an example that a random walk on $\mathcal{G}_{\text{de}}$ is not equivalent to a random walk on a reversible Markov chain. Thus, according to the second step of Theorem 1's proof, Theorem 2 holds.

定理 2 的证明。图 5 给出了一个例子，说明在 $\mathcal{G}_{\text{de}}$ 上的随机游走与在一个可逆马尔可夫链上的随机游走不等价。因此，根据定理 1 证明的第二步，定理 2 成立。

Then, we provide an illustrative example for an easier understanding as shown in Fig. 5. The two hypergraphs have the same connection structure but different connection intensities. At first, the transition probability $p_{v,u}$ can be computed accordingly for two types of hypergraphs. Then, we start two random walks from vertex v_0 : $''v_0 \to v_1 \to v_2 \to v_0$ ” and ” $v_0 \to v_2 \to v_1 \to v_0$ ”. The accumulated transition probability from the two paths can be computed by $p_{v_0,v_1} \cdot p_{v_1,v_2} \cdot p_{v_2,v_0}$ and $p_{v_0,v_2} \cdot p_{v_2,v_1} \cdot p_{v_1,v_0}$, respectively. According to Theorem 1 and Lemma 5, random walks on this hypergraph are reversible. Thus, we can get the same accumulated transition probability from expressive ability from GCN in handling the simple graph but also has the ability to model and learn the high-order correlation in the hypergraph.

然后，我们给出一个示例以便于理解，如图 5 所示。这两个超图具有相同的连接结构，但连接强度不同。首先，可以针对两种类型的超图相应地计算转移概率 $p_{v,u}$。然后，我们从顶点 v_0 开始两个随机游走: "$v_0 \to v_1 \to v_2 \to v_0$ “和” $v_0 \to v_2 \to v_1 \to v_0$ “。两条路径的累积转移概率可以分别通过 $p_{v_0,v_1} \cdot p_{v_1,v_2} \cdot p_{v_2,v_0}$ 和 $p_{v_0,v_2} \cdot p_{v_2,v_1} \cdot p_{v_1,v_0}$ 来计算。根据定理 1 和引理 5，此超图上的随机游走是可逆的。因此，我们可以从 GCN 的表达能力中获得相同的累积转移概率，它不仅能够处理简单图，还能够对超图中的高阶相关性进行建模和学习。

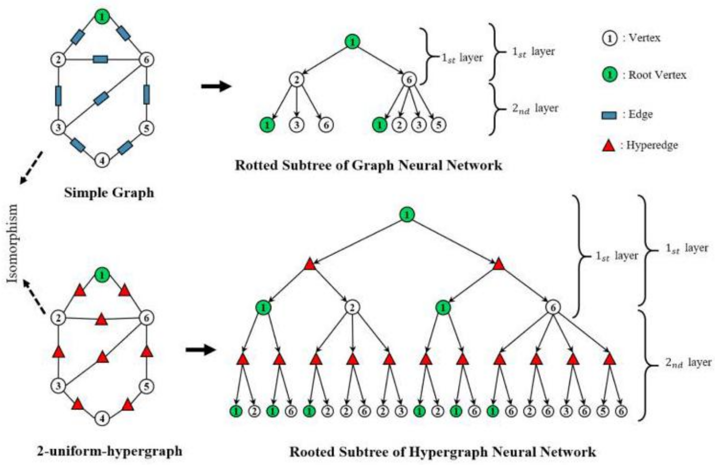

Fig. 6. Rooted subtree of graph and 2-uniform hypergraph. The correlation among six vertices is shown in left, which is represented by graph and two-uniform hypergraph, respectively. Note that for fair comparison the selected graph and two-uniform hypergraph own the same connection structure. In the right part shows the rooted subtree of graph and two-uniform hypergraph from vertex v_1 , which reveals the message passing path in multi-layer GNN/HGNN $^+$.

图 6. 图和 2 - 均匀超图的有根子树。六个顶点之间的相关性如左侧所示，分别由图和 2 - 均匀超图表示。请注意，为了进行公平比较，所选的图和 2 - 均匀超图具有相同的连接结构。右侧部分展示了从顶点 v_1 出发的图和 2 - 均匀超图的有根子树，它揭示了多层 GNN / HGNN $^+$ 中的消息传递路径。

The comparison of HGNN$^+$ and GNN from the spatial perspective. A powerful GNN model can be viewed as learning to embed the rooted subtree to low-dimensional space [17]. Rooted subtree [24] can describe not only the connection of local vertices, but also the message passing path in a graph. Therefore, we use the rooted subtree to compare HGNN $^+$ with GNN. Note that to satisfy the definition of path (also called the message passing path) in hyper-graph, the node in hypergraph's rooted subtree can either be vertex or hyperedge.

从空间角度比较 HGNN$^+$ 和 GNN 。一个强大的 GNN 模型可以被视为学习将有根子树嵌入到低维空间 [17]。有根子树 [24] 不仅可以描述局部顶点的连接，还可以描述图中的消息传递路径。因此，我们使用有根子树来比较 HGNN $^+$ 和 GNN。请注意，为了满足超图中路径 (也称为消息传递路径) 的定义，超图有根子树中的节点可以是顶点或超边。

Isomorphic graph structure can make a more clear comparison. Hence, we select 2-uniform hypergraph (each hyperedge only connects two vertices) for comparison. Fig. 6 depicts the rooted subtree of HGNN$^+$ and GNN for a specified vertex, which can also be expressed as the message path in graph and hyperpath in hypergraph. Obviously, the vertices in graph convolution only consider their neighbors' features, and then aggregate them to update the central vertex feature in one stage. Different from graph convolution layer, the HGNN$^+$ can be described as a hierarchical structure, which endows more powerful expression and modeling ability. HGNN $^+$ performs a two-stage i.e., vertex-hyperedge-vertex, transformation. As formulated in Eq. (18), hyperedge feature is generated according to its vertex inter-neighbor in the first stage. Then, the updated vertices features are obtained by aggregating their hyperedge inter-neighbor's features. Besides, compared with graph convolution, multilayer hypergraph convolution has much more message interaction process. In HGNN $^+$, the rooted vertex appears more frequency in the path of subtree (like a latent extra self-loop), which is the main reason why HGNN$^+$ performs better in Ablation Study (Section 6.2.4 comparison on different convolutional strategies). Therefore, the hypergraph convolution layer can efficiently extract both low-order and high-order correlation on hypergraph by the vertex-hyperedge-vertex transformation compared with graph convolution.

同构图结构可以进行更清晰的比较。因此，我们选择 2 - 均匀超图 (每个超边仅连接两个顶点) 进行比较。图 6 描绘了针对指定顶点的 HGNN$^+$ 和 GNN 的有根子树，它也可以表示为图中的消息路径和超图中的超路径。显然，图卷积中的顶点仅考虑其邻居的特征，然后在一个阶段中将它们聚合以更新中心顶点特征。与图卷积层不同，HGNN$^+$ 可以被描述为一种层次结构，它赋予了更强的表达和建模能力。HGNN $^+$ 执行两阶段，即顶点 - 超边 - 顶点的变换。如式 (18) 所示，在第一阶段根据其顶点间邻居生成超边特征。然后，通过聚合其超边间邻居特征来获得更新后的顶点特征。此外，与图卷积相比，多层超图卷积具有更多的消息交互过程。在 HGNN $^+$ 中，有根子树的路径中根顶点出现的频率更高 (就像一个潜在的额外自环)，这就是 HGNN$^+$ 在消融研究 (第 6.2.4 节不同卷积策略的比较) 中表现更好的主要原因。因此，与图卷积相比，超图卷积层可以通过顶点 - 超边 - 顶点变换有效地提取超图上的低阶和高阶相关性。

5.3 HGNN $^+$ vs. HGNN

5.3 HGNN $^+$ 与 HGNN 的比较

In this journal version, we further extend the HGNN from two aspects: hypergraph modeling and hypergraph convolution. Regarding hypergraph modeling, HGNN fuses the correlations within multiple hypergraphs simply by concatenating incidence matrices of them. By contrast, HGNN$^+$ further conceptually propose "hyperedge group" to adapt for multifarious information. Besides, HGNN$^+$ presents an adaptive strategy for the fusion of different hyperedge groups when generating the overall hypergraph representations to better utilize the complementarities among multifarious information features. To sum up, HGNN $^+$ promotes the modeling of complex relationships from hyperedge-by-hyperedge concatenation to group level adaptive fusion, improving not only the extensibility but also the representation capability.

在本期刊版本中，我们从超图建模和超图卷积两个方面进一步扩展了 HGNN。关于超图建模，HGNN 通过简单地拼接多个超图的关联矩阵来融合它们内部的相关性。相比之下，HGNN$^+$ 进一步从概念上提出了“超边组”以适应多样的信息。此外，HGNN$^+$ 在生成整体超图表示时提出了一种针对不同超边组融合的自适应策略，以便更好地利用多样信息特征之间的互补性。综上所述，HGNN $^+$ 将复杂关系的建模从逐个超边拼接提升到组级自适应融合，不仅提高了可扩展性，还提升了表示能力。

With respect to the convolution, HGNN is derived from the spectral theory of hypergraphs, which leads to its monotonous form of expression and limitation in extensibility. Specifically, convolution in the spectral domain does not apply to the directed graph (hypergraph) as the graph Fourier Basis is the eigenvectors of the graph (hypergraph) Laplacian matrix and the Laplacian matrix it uses is defined on the undirected graph. In contrast, HGNN^{+} defines hypergraph convolution in a more flexible way: designing a discrete and two-stage hypergraph convolution based on message passing from spatial domain. In this way, the convolution and aggregation operation in each stage can be defined flexibly and extended to the directed hypergraph naturally.

关于卷积，HGNN 源自超图的谱理论，这导致其表达形式单调且扩展性有限。具体而言，谱域中的卷积不适用于有向图 (超图)，因为图傅里叶基是图 (超图) 拉普拉斯矩阵的特征向量，且它所使用的拉普拉斯矩阵是在无向图上定义的。相比之下，HGNN^{+} 以更灵活的方式定义超图卷积: 基于从空间域进行消息传递设计了一种离散的两阶段超图卷积。通过这种方式，每个阶段的卷积和聚合操作都可以灵活定义，并自然地扩展到有向超图。

Definition 7. Let $\mathcal{F}:\mathbf{X}\rightarrow\mathbf{X}'$ be a graph/hypergraph message passing layer with trainable parameter ⍰ $\in\mathbb{R}^{C\times C'}$, where $\mathbf{X}=\{x_1,x_2,\cdots,x_N\}, x_i\in\mathbb{R}^{C}$ and $\mathbf{X}'=\{x_1',x_2',\cdots,x_N'\}, x_i'\in\mathbb{R}^{C'}$ denotes the input/output vertex feature, respectively. $\mathcal{F}$ is said to be a symmetric message passing layer $\Leftrightarrow$ there exists a symmetric matrix $\mathbf{A}\in\mathbb{R}^{N\times N}$ such that $\mathcal{F}=\mathbf{AX}\Theta$.

定义 7. 设 $\mathcal{F}:\mathbf{X}\rightarrow\mathbf{X}'$ 是一个具有可训练参数 ⍰ $\in\mathbb{R}^{C\times C'}$ 的图/超图消息传递层，其中 $\mathbf{X}=\{x_1,x_2,\cdots,x_N\}, x_i\in\mathbb{R}^{C}$ 和 $\mathbf{X}'=\{x_1',x_2',\cdots,x_N'\}, x_i'\in\mathbb{R}^{C'}$ 分别表示输入/输出顶点特征。$\mathcal{F}$ 被称为对称消息传递层 $\Leftrightarrow$ 存在一个对称矩阵 $\mathbf{A}\in\mathbb{R}^{N\times N}$ 使得 $\mathcal{F}=\mathbf{AX}\Theta$ 。

$$\begin{cases}\mathbf{X}^{t+1}\xleftarrow{\text{HGNNConv}}\sigma\left(\mathbf{D}_v^{-1/2}\mathbf{H}\mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^{\top}\mathbf{D}_v^{-1/2}\mathbf{X}^{t}⍰^{t}\right)\\ \mathbf{X}^{t+1}\xleftarrow{\text{HGNNConv}}\sigma\left(\mathbf{D}_v^{-1}\mathbf{H}\mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^{\top}\mathbf{X}^{t}⍰^{t}\right)\end{cases}$$

(25)

$\mathbf{D}_v^{-1/2}\mathbf{H}\mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^{\top}\mathbf{D}_v^{-1/2}$ and $\mathbf{D}_v^{-1}\mathbf{H}\mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^{\top}$ in Eq. (28) of HGNNConv/HGNNConv+ play a role of "dummy adjacency matrix" to guide the vertex feature self-updating just like the adjacency matrix in graph convolution. However, in HGNNConv, the "dummy adjacency matrix" is symmetric normalized by $\mathbf{D}_v^{-\frac{1}{2}}$, which leads to a symmetric format of matrix $\mathbf{D}_v^{-\frac{1}{2}}\mathbf{H}\mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^{\top}\mathbf{D}_v^{-\frac{1}{2}}$ with Definition 7. Then, the symmetric "dummy adjacency matrix" of a hypergraph guides a symmetric message passing of vertex feature distribution and aggregation. In contrast, HGNNConv+ allows both symmetric and asymmetric processes of passing messages from vertex to hyperedge (Stage 1) and from hyperedge to vertex (Stage 2). That is to say, HGNNConv is the symmetric message passing, while HGNNConv $^{+}$ is the asymmetric message passing.

HGNNConv/HGNNConv+ 中公式 (28) 里的 $\mathbf{D}_v^{-1/2}\mathbf{H}\mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^{\top}\mathbf{D}_v^{-1/2}$ 和 $\mathbf{D}_v^{-1}\mathbf{H}\mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^{\top}$ 起到了“虚拟邻接矩阵”的作用，就像图卷积中的邻接矩阵一样，用于引导顶点特征的自我更新。然而，在 HGNNConv 中，“虚拟邻接矩阵”通过 $\mathbf{D}_v^{-\frac{1}{2}}$ 进行对称归一化，根据定义 7 这导致矩阵 $\mathbf{D}_v^{-\frac{1}{2}}\mathbf{H}\mathbf{W}\mathbf{D}_e^{-1}\mathbf{H}^{\top}\mathbf{D}_v^{-\frac{1}{2}}$ 具有对称形式。然后，超图的对称“虚拟邻接矩阵”引导顶点特征分布和聚合的对称消息传递。相比之下，HGNNConv+ 允许从顶点到超边 (阶段 1) 以及从超边到顶点 (阶段 2) 传递消息的对称和非对称过程。也就是说，HGNNConv 是对称消息传递，而 HGNNConv $^{+}$ 是非对称消息传递。

On Directed Hypergraph. As analyzed above, our proposed HGNN $^{+}$ can be applied to the directed hypergraph, while HGNN is limited to the undirected case. Here we show, using a simple analytical example, how asymmetric message passing is extended to directed hypergraphs. We first give a trivial definition [23] for directed hypergraph $\mathbf{H}$ with entries being defined as:

关于有向超图。如前所述，我们提出的 HGNN $^+$ 可应用于有向超图，而 HGNN 仅限于无向情况。在此，我们通过一个简单的分析示例展示不对称消息传递是如何扩展到有向超图的。我们首先给出有向超图 $\mathbf{H}$ 的一个简单定义 [23]，其元素定义如下:

$$\hat{\mathbf{H}}(v,e) = \begin{cases} -1 & \text{if } v \in T(e) \\ 1 & \text{if } v \in S(e), \\ 0 & \text{otherwise} \end{cases} \tag{26}$$

in which $T(e)$ and $S(e)$ are the set of target and source vertices for hyperedge e , respectively. Before performing HGNNConv+, we split the incidence matrix $\mathbf{H}$ into two matrices, $\hat{\mathbf{H}}_s$ and $\hat{\mathbf{H}}_t$, describing the source and target vertices for all hyperedges, respectively. These two incidence matrices play a crucial role in keeping the directional information during the message passing. Unlike that in the undirected hypergraph, the message passing in the directed hypergraph is guided by different incidence matrix, i.e., $\hat{\mathbf{H}}_s$ and $\hat{\mathbf{H}}_t$, in two stages of HGNNConv $^+$. In this case, an intuitive paradigm to perform HGNNConv+ on the directed hypergraph can be simply denoted as:

其中 $T(e)$ 和 $S(e)$ 分别是超边 e 的目标顶点集和源顶点集。在执行 HGNNConv+ 之前，我们将关联矩阵 $\mathbf{H}$ 拆分为两个矩阵，$\hat{\mathbf{H}}_s$ 和 $\hat{\mathbf{H}}_t$ ，分别描述所有超边的源顶点和目标顶点。这两个关联矩阵在消息传递过程中保持方向信息方面起着关键作用。与无向超图不同，有向超图中的消息传递在 HGNNConv $^+$ 的两个阶段由不同的关联矩阵，即 $\hat{\mathbf{H}}_s$ 和 $\hat{\mathbf{H}}_t$ 引导。在这种情况下，在有向超图上执行 HGNNConv+ 的一个直观范式可简单表示为:

$$\mathbf{X}^{t+1} = \sigma\left(\underline{\mathbf{D}}_t^{-1}\hat{\mathbf{H}}_t\mathbf{W}\mathbf{D}_s^{-1}\hat{\mathbf{H}}_s^{\top}\mathbf{X}^t\boxed{?}^t\right). \tag{27}$$

$\mathbf{D}_s$ and $\mathbf{D}_t$ are two matrices that conduct average aggregation in the message passing of stage 1 and 2, denoted as

$\mathbf{D}_s$ 和 $\mathbf{D}_t$ 是在第 1 阶段和第 2 阶段的消息传递中进行平均聚合的两个矩阵，记为

$$\begin{cases} \mathbf{D}_s = \operatorname{diag}\left(\operatorname{col\_sum}\left(\hat{\mathbf{H}}_s\right)\right) \\ \mathbf{D}_t = \operatorname{diag}\left(\operatorname{col\_sum}\left(\hat{\mathbf{H}}_t\right)\right) \end{cases}, \tag{28}$$

in which $\operatorname{diag}(v)$ converts a vector v to a diagonal matrix and col_sum(A) returns a vector with each element being the sum of the corresponding column in matrix A. HGNNConv+ can be applied to directed hypergraphs without losing directional information, while the HGNNConv that uses symmetric normalization will obviously ignore such key information regarding directed/asymmetric edges and thus limit its learning capacity compared with HGNNConv $^+$.

其中，$\operatorname{diag}(v)$ 将向量 v 转换为对角矩阵，col_sum(A) 返回一个向量，其每个元素是矩阵 A 中对应列的和。HGNNConv+ 可以应用于有向超图，而不会丢失方向信息，而使用对称归一化的 HGNNConv 显然会忽略有关有向/非对称边的此类关键信息，因此与 HGNNConv $^+$ 相比，其学习能力会受到限制。

6 EXPERIMENTS AND DISCUSSIONS

6 实验与讨论

To evaluate the performance of the proposed hypergraph neural network framework, three types of experiments are conducted. The first two experiments are designed for the data with and without the graph structure. The last one is designed for the data with hypergraph structure. In the following, we introduce experimental settings, results, comparisons, and discussions, respectively.

为了评估所提出的超图神经网络框架的性能，进行了三种类型的实验。前两个实验是针对具有和不具有图结构的数据设计的。最后一个实验是针对具有超图结构的数据设计的。下面，我们分别介绍实验设置、结果、比较和讨论。

6.1 Experimental Settings

6.1 实验设置

6.1.1 Compared Methods

6.1.1 比较方法

Seven typical state-of-the-art methods, including spectral-based (GCN [2], GraphConv [28]), non-spectral-based (GraphSAGE [1], GAT [3], and GIN [17]), and hypergraph-based methods (Hyper-Atten[7] and Hyper-GCN[8]), are selected for comparison. HGNN[6] and HGNN^{+} are the proposed methods.

选择了七种典型的最新方法进行比较，包括基于谱的方法 (GCN [2]，GraphConv [28])、非基于谱的方法 (GraphSAGE [1]，GAT [3] 和 GIN [17]) 以及基于超图的方法 (Hyper-Atten[7] 和 HyperGCN[8])。HGNN[6] 和 HGNN^{+} 是所提出的方法。

GCN [2]. As an efficient spectral network, it realizes convolution of irregular data though a spectral representation of graphs, and avoids overfitting on local neighborhood

GCN [2]。作为一种高效的谱网络，它通过图的谱表示实现不规则数据的卷积，并避免在节点度分布广泛的图中的局部邻域上过度拟合

 structures in graphs featuring wide distributions of node degree.

图中具有广泛节点度分布的局部邻域结构。

GraphSAGE [1]. This is a general inductive non-spectral method. Instead of adopting full graph Laplacian to generate embeddings, GraphSAGE utilizes learnable aggregation functions to improve receptive filed expansion and reduce the computing complexity.

GraphSAGE [1]。这是一种通用的归纳非谱方法。GraphSAGE 不是采用全图拉普拉斯来生成嵌入，而是利用可学习的聚合函数来改善感受野扩展并降低计算复杂度。

GAT [3]. GAT introduces a self-attention strategy in the propagation step to improve the efficiency of weight allocation of the nodes in a single neighborhood.

GAT [3]。GAT 在传播步骤中引入了自注意力策略，以提高单个邻域中节点的权重分配效率。

GIN [17]. GIN is a simple yet powerful GNN, which shows superior performance against other GNN variants. It leverages a sum aggregator and further introduces multilayer perceptrons (MLPs) to parameterize universal multi-set functions, generalizing the Weisfeiler-Lehman (WL) graph isomorphism test and achieving maximum discriminative power among GNNs.

GIN [17]。GIN 是一个简单而强大的 GNN，它相对于其他 GNN 变体表现出卓越的性能。它利用求和聚合器，并进一步引入多层感知器 (MLP) 来参数化通用多集函数，推广了魏斯费勒 - 莱曼 (WL) 图同构测试，并在 GNN 中实现了最大判别力。

GraphConv [28]. Based on the k-dimensional Weisfeiler-Leman algorithm, GraphConv proposes k-dimensional GNNs (k-GNNs), and therefore it can capture higher-order graph structures at different scales.

GraphConv [28]。基于 k 维魏斯费勒 - 莱曼算法，GraphConv 提出了 k 维 GNN(k - GNN)，因此它可以在不同尺度上捕获高阶图结构。

HyperGCN [8]. HyperGCN trains a GCN on hyper-graphs for semi-supervised learning based on the spectral theory of hypergraphs.

HyperGCN [8]。HyperGCN 基于超图的谱理论在超图上训练 GCN 进行半监督学习。

Hyper-Atten [7]. It follows the convolution pattern defined in [6] and further introduces a hyperedge-vertex attention mechanism to adaptively learn the importance of different vertices in the same hyperedge.

Hyper-Atten [7]。它遵循 [6] 中定义的卷积模式，并进一步引入超边 - 顶点注意力机制，以自适应地学习同一超边中不同顶点的重要性。

HGNN and HGNN $^{+}$. Our methods of the initial conference version and this extended journal version.

HGNN 和 HGNN $^{+}$ 。我们初始会议版本和此扩展期刊版本的方法。

6.1.2 Other Common Settings

6.1.2 其他常见设置

Training Details. For comparing methods, the reported model configurations are used. The learning rate on three citation network datasets is set as 0.01 and 0.001 on two social media network datasets for all methods. The dropout is set as 0.5 . Adam optimizer is employed to minimize the cross-entropy loss on classification task. The weight decay is set as 0.0005 .

训练细节。为了比较不同方法，使用已报告的模型配置。所有方法在三个引文网络数据集上的学习率设置为 0.01，在两个社交媒体网络数据集上设置为 0.001。随机失活 (Dropout) 设置为 0.5。采用 Adam 优化器来最小化分类任务中的交叉熵损失。权重衰减设置为 0.0005。

Loss Functions. For the single-label classification task, the commonly-used cross entropy loss is used for optimization $\mathcal{L} = -\sum_{v \in V} \sum_{c=1}^{C} Y_{vc} \log(O_{vc})$, where C denotes the number of categories and V is the vertex set with size N . $Y \in \{0,1\}^{N \times C}$ is the ground truth vertex label encoded using a one-hot encoding schema. $O \in \mathbb{R}^{N \times C}$ is the output of the softmax layer. For the multi-label classification task, the binary cross entropy loss function is adopted.

损失函数。对于单标签分类任务，常用交叉熵损失进行优化 $\mathcal{L} = -\sum_{v \in V} \sum_{c=1}^{C} Y_{vc} \log(O_{vc})$，其中 C 表示类别数量，V 是大小为 N 的顶点集。$Y \in \{0,1\}^{N \times C}$ 是使用独热编码模式编码的真实顶点标签。$O \in \mathbb{R}^{N \times C}$ 是 softmax 层的输出。对于多标签分类任务，采用二元交叉熵损失函数。

Evaluation Metrics. For evaluation, four widely-used metrics, including accuracy (Acc), macro f1 score (F1_ma), exact match ratio (EMR), and example-based accuracy (EB-Acc) are calculated to comprehensively compare the performance of different methods. The former two metrics are used in single-label classification task, and the latter two are adopted for multi-label classification task.

评估指标。为了进行评估，计算四个广泛使用的指标，包括准确率 (Acc)、宏 F1 分数 (F1_ma)、精确匹配率 (EMR) 和基于示例的准确率 (EB - Acc)，以全面比较不同方法的性能。前两个指标用于单标签分类任务，后两个指标用于多标签分类任务。

6.2 Vertex Classification on the Data With Graph Structure

6.2 具有图结构的数据上的顶点分类

6.2.1 Datasets

6.2.1 数据集

Five public benchmarks are selected in this experiment, which belong to two categories, i.e., publication citation network (Cora [25], Citeseer and Pubmed [26]) and social media network (Github Web ML and Facebook [27]). In citation network dataset, each paper is indicated with a vertex associated with an initial feature, which corresponds to a bag of words. The task is to predict which category each paper belongs to. Social media dataset contains relations among web sites, and vertex features are extracted from words of each site. The statistical characteristics of datasets with graph structure are shown in Table 2.

本实验选择了五个公共基准数据集，它们属于两类，即出版物引文网络 (科拉数据集 [25]、Citeseer 和 PubMed[26]) 和社交媒体网络 (Github Web ML 和 Facebook[27])。在引文网络数据集中，每篇论文由一个与初始特征相关联的顶点表示，该特征对应于一个词袋。任务是预测每篇论文属于哪个类别。社交媒体数据集包含网站之间的关系，顶点特征从每个网站的单词中提取。具有图结构的数据集的统计特征如表 2 所示。

TABLE 2

Detailed Information of Five Datasets With Graph Structure

五个具有图结构的数据集的详细信息

Dataset	Citation Network			Social Media Network	
	Cora	Citeseer	PubMed	Github Web ML	Facebook Page-Page
Classes	7	6	3	2	4
Nodes	2708	3327	19717	37700	22470
Edges	5429	4732	44338	289003	171002
Features	1433	3703	500	4005	4714

数据集	引用网络			社交媒体网络	
	科拉 (Cora)	科学文献数据库 (Citeseer)	医学文献数据库 (PubMed)	GitHub 网络机器学习	脸书页面-页面
类别	7	6	3	2	4
节点	2708	3327	19717	37700	22470
边	5429	4732	44338	289003	171002
特征	1433	3703	500	4005	4714

Citation Network. The three widely applied citation network datasets, including Cora [25], CiteSeer and PubMed [26], are composed of sparse bag-of-words feature vectors for each scientific publication, with citation relationships among publications represented by corresponding edges, and ground truth topics as their labels.

引文网络。三个广泛应用的引文网络数据集，包括 Cora [25]、CiteSeer 和 PubMed [26]，由每个科学出版物的稀疏词袋特征向量组成，出版物之间的引用关系由相应的边表示，真实主题作为它们的标签。

Social Media Network. The two selected social media network datasets are GitHub Web ML [27] and Facebook Page-Page [27]. The Github Web and Machine Learning Developers Dataset (GitHub Web ML) constructs a graph describing developers who have starred at least 10 repositories and their relationships, with each node in the graph representing a developer, and each edge between two nodes representing the follower relationships between two developers. The node features are extracted with user information including their locations, employers and the repositories stared at. Therefore, the prediction of whether the working field of a developer is web or machine learning is converted into a bi-classification task of graph nodes. The Facebook Page-Page dataset contains 22,470 verified Facebook sites collected with Facebook Graph API and a graph describing inter-site relationships, with each node representing an official Facebook page and labelled one of the four following categories: politicians, governmental organizations, television shows, and companies. The node features are extracted with page owners' generalization of page themes. One edge is established between each two nodes represented by mutual like sites.

社交媒体网络。选择的两个社交媒体网络数据集是 GitHub Web ML [27] 和 Facebook Page-Page [27]。Github Web 和机器学习开发者数据集 (GitHub Web ML) 构建了一个描述至少收藏了 10 个代码库的开发者及其关系的图，图中的每个节点代表一个开发者，两个节点之间的每条边代表两个开发者之间的关注关系。节点特征是通过包括他们的位置、雇主和收藏的代码库等用户信息提取的。因此，预测开发者的工作领域是网络还是机器学习被转化为图节点的二分类任务。Facebook Page-Page 数据集包含通过 Facebook Graph API 收集的 22470 个经过验证的 Facebook 网站以及一个描述网站间关系的图，每个节点代表一个官方 Facebook 页面，并被标记为以下四类之一: 政治家、政府组织、电视节目和公司。节点特征是通过页面所有者对页面主题的概括提取的。由相互喜欢的网站表示的每两个节点之间建立一条边。

6.2.2 Settings

6.2.2 设置

Data pre-processing. The raw vertex feature is a binary matrix with dimension $N \times C$. For three citation network datasets, each non-zero entry denotes whether a specified word appears in the publication. Following the setting in [29], the row-wise normalization is applied to the feature of each vertex. For two social media network datasets, each non-zero entry denotes that a specified attribute is associated with the website/user. These attributes can be the location of developers, the same users they follow or other kinds of shared data. Different from the vertex feature in citation network (including that uses only words), the vertex feature in social network is more complex. Under such circumstances, using the row-wise normalization directly may be unfair for different attributes. Therefore, raw vertex feature without row-wise normalization is used for two social network datasets.

数据预处理。原始顶点特征是一个维度为 $N \times C$ 的二进制矩阵。对于三个引文网络数据集，每个非零条目表示指定的词是否出现在出版物中。按照 [29] 中的设置，对每个顶点的特征进行逐行归一化。对于两个社交媒体网络数据集，每个非零条目表示指定的属性与网站/用户相关联。这些属性可以是开发者的位置、他们关注的相同用户或其他类型的共享数据。与引文网络中的顶点特征 (仅使用词) 不同，社交网络中的顶点特征更复杂。在这种情况下，直接使用逐行归一化可能对不同属性不公平。因此，两个社交网络数据集使用未经逐行归一化的原始顶点特征。

Train/validation/test Split. For each dataset, 5/10 samples for each category are randomly selected for training and 5 samples for each category are randomly selected for validation. The rest of the vertices are used for testing for all datasets in our experiments. For each experiment, the validation set is used to select the best model in the training stage. Different from the conference version, the training/ validation/testing data split process repeats 20 times for different methods, and the average performances for each method are reported for a fair comparison.

训练/验证/测试划分。对于每个数据集，为每个类别随机选择 5/10 个样本进行训练，为每个类别随机选择 5 个样本进行验证。在我们的实验中，其余的顶点用于所有数据集的测试。对于每个实验，验证集用于在训练阶段选择最佳模型。与会议版本不同，对于不同的方法，训练/验证/测试数据划分过程重复 20 次，并报告每种方法的平均性能以进行公平比较。

Hypergraph Construction. For our proposed method HGNN $^+$, three types of hyperedge groups $\mathcal{E}_{\text{pair}}$

(Eq. (3)), $\mathcal{E}_{\text{hop}_1}$ (Eq. (4)), and $\mathcal{E}_{\text{hop}_2}$ (Eq. (4)) are used for hypergraph generation and Adaptive Fusion strategy is adopted for hyperedge groups fusion. Here, two convolutional layers are adopted for generating the refined embeddings, and then the output is fed into a softmax layer to predict the probability distribution over all categories for each vertex. The hidden dimension is fixed to 64 for all datasets.

超图构建。对于我们提出的方法 HGNN$^+$，使用三种类型的超边组 $\mathcal{E}_{\text{pair}}$ (式 (3))、$\mathcal{E}_{\text{hop}_1}$ (式 (4)) 和 $\mathcal{E}_{\text{hop}_2}$ (式 (4)) 进行超图生成，并采用自适应融合策略进行超边组融合。这里，采用两个卷积层生成精细的嵌入，然后将输出输入到 softmax 层以预测每个顶点在所有类别上的概率分布。所有数据集的隐藏维度固定为 64。

6.2.3 Experimental Results and Discussions

6.2.3 实验结果与讨论

Experimental results on all five datasets are provided in Tables 3 and 4. From these results we can have the following observations:

表 3 和表 4 提供了所有五个数据集的实验结果。从这些结果我们可以得到以下观察结果:

1) HGNN$^+$ achieves better or comparable performance compared with GCN, GAT and other graph-based methods. For example, HGNN$^+$ obtains gains of 6.6%, 8.49%, 8.17%, 9.81%, and 10.55% compared with GCN, GAT, GraphSAGE, GIN, and Graph-Conv, in terms of Acc when 5 samples are used for training, on the Facebook dataset.

1) HGNN$^+$ 与 GCN、GAT 和其他基于图的方法相比，取得了更好或相当的性能。例如，在 Facebook 数据集上，当使用 5 个样本进行训练时，HGNN$^+$ 在 Acc 方面与 GCN、GAT、GraphSAGE、GIN 和 Graph-Conv 相比分别获得了 6.6%、8.49%、8.17%、9.81% 和 10.55% 的提升。

2) Compared with other hypergraph-based methods, i.e., HyperGCN and Hyper-Atten, our proposed HGNN$^+$ can also yields consistent better performance. In particular, HGNN$^+$ outperforms HyperGCN and Hyper-Atten by 5.02% and 1.23% in terms of F1_ma when 5 samples are used for training, on the Github Web ML dataset.

2) 与其他基于超图的方法，即 HyperGCN 和 Hyper-Atten 相比，我们提出的 HGNN$^+$ 也能产生一致更好的性能。特别是，在 Github Web ML 数据集上，当使用 5 个样本进行训练时，HGNN$^+$ 在 F1_ma 方面比 HyperGCN 和 Hyper-Atten 分别高出 5.02% 和 1.23%。

3) With fewer training samples, the proposed method HGNN$^+$ can achieve more gains, which shows that the proposed methods can work well with limited training samples.

3) 使用更少的训练样本，提出的方法 HGNN$^+$ 可以获得更多的提升，这表明提出的方法在有限的训练样本下也能很好地工作。

4) The proposed HGNN$^+$ achieves a more remarkable performance improvement against graph-based methods on the social media network data than that on the publication network data.

4) 所提出的 HGNN + 在社交媒体网络数据上相对于基于图的方法实现了比在出版物网络数据上更显著的性能提升。

The better performance of the proposed framework can be attributed to the following factors. First, compared with the graph structure which can only represent pairwise correlation, the hypergraph structure is able to deeply exploit the high-order correlation among the data, even behind the simple pairwise correlation. As shown in the hypergraph generation procedure of our proposed framework, the hyperedge group using pairwise edge corresponds to the graph structure, while the hyperedge group using k-Hop neighbors can further represent the second order and even higher order reachable neighbors in the graph structure for each vertex. These higher order correlations are beyond the traditional pairwise relationship and yet lead to better representation of the latent data relationship. More importantly, such hypergraph structure can be very flexible to deal with multi-modal/multi-type representations, which is effective when handling heterogeneous data.

所提出框架的更好性能可归因于以下因素。首先，与仅能表示成对相关性的图结构相比，超图结构能够深入挖掘数据之间的高阶相关性，甚至是简单成对相关性背后的高阶相关性。如我们所提出框架的超图生成过程所示，使用成对边的超边组对应于图结构，而使用 k 跳邻居的超边组可以进一步表示图结构中每个顶点的二阶甚至更高阶可达邻居。这些高阶相关性超越了传统的成对关系，但却能更好地表示潜在的数据关系。更重要的是，这种超图结构在处理多模态/多类型表示时非常灵活，这在处理异构数据时很有效。

TABLE 3
Experimental Results When Using 5 Samples Per Category for Training

每类使用 5 个样本进行训练时的实验结果

Methods	Cora		Citeseer		Pubmed		Github Web ML		Facebook	
	Acc	F1_ma	Acc	F1_ma	Acc	F1_ma	Acc	F1_ma	Acc	F1_ma
GCN	0.6906	0.6765	0.5862	0.5398	0.6938	0.6899	0.7218	0.6679	0.5771	0.5462
GAT	0.7026	0.6911	0.6021	0.5510	0.7051	0.7038	0.7296	0.6641	0.5582	0.5362
GraphSAGE	0.6794	0.6648	0.5648	0.5247	0.6840	0.6806	0.7278	0.6718	0.5614	0.5405
GIN	0.6812	0.6675	0.5540	0.5195	0.6828	0.6797	0.7201	0.6428	0.5450	0.5194
GraphConv	0.6709	0.6571	0.5539	0.5219	0.6854	0.6800	0.6744	0.6150	0.5376	0.5140
HyperGCN	0.6951	0.6819	0.5890	0.5387	0.6976	0.6949	0.7256	0.6707	0.5775	0.5564
Hyper-Atten	0.7269	0.7118	0.5959	0.5484	0.7093	0.7050	0.7552	0.7086	0.6430	0.6179
HGNN	0.7143	0.6999	0.5471	0.5193	0.6973	0.6910	0.6872	0.6405	0.5520	0.5303
HGNN+	0.7319	0.7141	0.6064	0.5486	0.7138	0.7053	0.7637	0.7209	0.6431	0.6204

方法	科拉 (Cora)		科学引文索引 (Citeseer)		医学期刊数据库 (Pubmed)		GitHub 网络机器学习		脸书 (Facebook)	
	准确率 (Acc)	F1 值 (F1_ma)	准确率 (Acc)	F1 值 (F1_ma)	准确率 (Acc)	F1 值 (F1_ma)	准确率 (Acc)	F1 值 (F1_ma)	准确率 (Acc)	F1 值 (F1_ma)
图卷积网络 (GCN)	0.6906	0.6765	0.5862	0.5398	0.6938	0.6899	0.7218	0.6679	0.5771	0.5462
图注意力网络 (GAT)	0.7026	0.6911	0.6021	0.5510	0.7051	0.7038	0.7296	0.6641	0.5582	0.5362
图采样和聚合 (GraphSAGE)	0.6794	0.6648	0.5648	0.5247	0.6840	0.6806	0.7278	0.6718	0.5614	0.5405
图同构网络 (GIN)	0.6812	0.6675	0.5540	0.5195	0.6828	0.6797	0.7201	0.6428	0.5450	0.5194
图卷积 (GraphConv)	0.6709	0.6571	0.5539	0.5219	0.6854	0.6800	0.6744	0.6150	0.5376	0.5140
超图卷积网络 (HyperGCN)	0.6951	0.6819	0.5890	0.5387	0.6976	0.6949	0.7256	0.6707	0.5775	0.5564
超注意力 (Hyper-Atten)	0.7269	0.7118	0.5959	0.5484	0.7093	0.7050	0.7552	0.7086	0.6430	0.6179
超图神经网络 (HGNN)	0.7143	0.6999	0.5471	0.5193	0.6973	0.6910	0.6872	0.6405	0.5520	0.5303
超图神经网络升级版 (HGNN+)	0.7319	0.7141	0.6064	0.5486	0.7138	0.7053	0.7637	0.7209	0.6431	0.6204

The best results are marked in bold type, and the second-best results are marked with underline.

最佳结果用粗体标记，次佳结果用下划线标记。

From the aspect of correlation representation, the graph-based methods are described by the adjacency matrix. Although the adjacency matrix can concisely depict the connection structure of a graph, the complex higher-order information (connected component, k-order reachable neighbors, etc.) on the graph cannot be obtained directly. In most cases, both the information explicitly presented by the adjacency matrix (the connection structure of the graph) and the information implicitly expressed by the adjacency matrix (the complex higher-order information on the graph) is helpful for the representation learning of vertices on the graph. Existing methods based on the GNN only leverage the information that is explicitly presented by the adjacency matrix, hoping to sideways capture the high-order correlations on the graph for further representation learning by stacking multiple layers. However, stacking multiple layers of GCN may fail into the trap of rigid k-hop neighborhood smoothing. For example, each vertex's feature in the output layer of a three-layer GCN is generated by uniformly smoothing its 3-hop neighbor's features. In fact, the neighborhood information of different hops contributes differently to the learning task in different datasets, which is also verified in the ablation study on different hyperedge groups shown in Table 5. Thus, the GNNs with fixed number of layers may produce sub-optimal performance in different datasets. By contrast, our proposed framework can explicitly describe different "modality/ hop" information on the graph by defining multiple hyper-edge groups as well as introducing the weights of hyper-edge groups to balance the influence of different higher-order information on vertex representation learning.

从相关性表示的角度来看，基于图的方法由邻接矩阵描述。虽然邻接矩阵可以简洁地描绘图的连接结构，但图上复杂的高阶信息 (连通分量、k 阶可达邻居等) 无法直接获得。在大多数情况下，邻接矩阵明确呈现的信息 (图的连接结构) 和邻接矩阵隐含表达的信息 (图上复杂的高阶信息) 对图上顶点的表示学习都有帮助。现有的基于图神经网络 (Graph Neural Network，GNN) 的方法仅利用邻接矩阵明确呈现的信息，希望通过堆叠多层来间接地捕捉图上的高阶相关性以进行进一步的表示学习。然而，堆叠多层图卷积网络 (Graph Convolutional Network，GCN) 可能会陷入刚性 k 跳邻域平滑的陷阱。例如，三层 GCN 输出层中每个顶点的特征是通过均匀平滑其 3 跳邻居的特征生成的。实际上，不同跳的邻域信息在不同数据集中对学习任务的贡献不同，这也在表 5 所示的不同超边组的消融研究中得到了验证。因此，固定层数的 GNN 在不同数据集中可能会产生次优性能。相比之下，我们提出的框架可以通过定义多个超边组并引入超边组权重来明确描述图上不同的“模态/跳”信息，以平衡不同高阶信息对顶点表示学习的影响。

As for the hypergraph-based methods, the poor performance can be dedicated to their structural simplification or over-parametrization. HyperGCN bears unsatisfactory performance, probably due to the fact that it simplifies the initial hypergraph structure to perform graph convolution on hypergraphs. Such simplification is irreversible and thus will certainly lose crucial information. Hyper-Atten leverages the hyperedge-vertex attention module and therefore yields better performance compared with HyprGCN. Nonetheless, such a complex attention strategy introduces a large number of parameters and makes the model easily suffer from the overfitting problem. In contrast, HGNN$^+$ proposes the hyperedge group-level attention mechanism, which can consider the relationships among different hyperedge groups and vertices as well as cut down the volume of learnable parameters, thus effectively preventing overfitting and achieving more stable improvements.

至于基于超图的方法，其性能不佳可能归因于结构简化或参数过多。超图卷积网络 (HyperGCN) 性能不尽人意，可能是因为它简化了初始超图结构以在超图上执行图卷积。这种简化是不可逆的，因此肯定会丢失关键信息。超注意力网络 (Hyper - Atten) 利用超边 - 顶点注意力模块，因此与超图卷积网络 (HyprGCN) 相比性能更好。尽管如此，这种复杂的注意力策略引入了大量参数，使模型容易出现过拟合问题。相比之下，HGNN⁺ 提出了超边组级注意力机制，它可以考虑不同超边组和顶点之间的关系，并减少可学习参数的数量，从而有效防止过拟合并实现更稳定的改进。

The better performance gains from the cases with less labeled data indicates that the proposed framework can be more effective to deal with few labeled sample situation. When the labeled data is limited, which is the case in most applications, the data correlation plays more important role in the representation learning process. Therefore, a good and sufficient data correlation could help a lot in the task.

在标记数据较少的情况下获得更好的性能提升表明，所提出的框架在处理少量标记样本情况时可能更有效。当标记数据有限时 (大多数应用中都是这种情况)，数据相关性在表示学习过程中起着更重要的作用。因此，良好且充分的数据相关性对该任务有很大帮助。

TABLE 4

Experimental Results When Using Ten Samples Per Category for Training

每类使用十个样本进行训练时的实验结果

Methods	Cora		Citeseer		Pubmed		Github Web ML		Facebook	
	Acc	F1_ma	Acc	F1_ma	Acc	F1_ma	Acc	F1_ma	Acc	F1_ma
GCN	0.7632	0.7491	0.6383	0.5972	0.7305	0.7284	0.7737	0.7261	0.6577	0.6398
GAT	0.7670	0.7485	0.6472	0.6086	0.7378	0.7356	0.7739	0.7258	0.6382	0.6201
GraphSAGE	0.7325	0.7168	0.5932	0.5570	0.7230	0.7195	0.7598	0.7151	0.6413	0.6258
GIN	0.7319	0.7209	0.5964	0.5632	0.7259	0.7219	0.7459	0.6934	0.6135	0.5966
GraphConv	0.7314	0.7205	0.5931	0.5632	0.7164	0.7130	0.6862	0.6491	0.5988	0.5772
HyperGCN	0.7586	0.7451	0.6411	0.6015	0.7309	0.7282	0.7876	0.7375	0.6514	0.6377
Hyper-Atten	0.7684	0.7536	0.6398	0.5973	0.7336	0.7277	0.7865	0.7409	0.6961	0.6827
HGNN	0.7718	0.7579	0.6399	0.5945	0.7287	0.7235	0.7426	0.6957	0.6205	0.6055
HGNN+	0.7671	0.7496	0.6643	0.6196	0.7408	0.7327	0.7910	0.7500	0.6997	0.6853

方法	科拉 (Cora)		科学引文数据库 (Citeseer)		医学期刊数据库 (Pubmed)		GitHub 网络机器学习		脸书 (Facebook)	
	准确率 (Acc)	F1 值 (F1_ma)	准确率 (Acc)	F1 值 (F1_ma)	准确率 (Acc)	F1 值 (F1_ma)	准确率 (Acc)	F1 值 (F1_ma)	准确率 (Acc)	F1 值 (F1_ma)
图卷积网络 (GCN)	0.7632	0.7491	0.6383	0.5972	0.7305	0.7284	0.7737	0.7261	0.6577	0.6398
图注意力网络 (GAT)	0.7670	0.7485	0.6472	0.6086	0.7378	0.7356	0.7739	0.7258	0.6382	0.6201
图采样和聚合方法 (GraphSAGE)	0.7325	0.7168	0.5932	0.5570	0.7230	0.7195	0.7598	0.7151	0.6413	0.6258
图同构网络 (GIN)	0.7319	0.7209	0.5964	0.5632	0.7259	0.7219	0.7459	0.6934	0.6135	0.5966
图卷积 (GraphConv)	0.7314	0.7205	0.5931	0.5632	0.7164	0.7130	0.6862	0.6491	0.5988	0.5772
超图卷积网络 (HyperGCN)	0.7586	0.7451	0.6411	0.6015	0.7309	0.7282	0.7876	0.7375	0.6514	0.6377
超注意力 (Hyper-Atten)	0.7684	0.7536	0.6398	0.5973	0.7336	0.7277	0.7865	0.7409	0.6961	0.6827
超图神经网络 (HGNN)	0.7718	0.7579	0.6399	0.5945	0.7287	0.7235	0.7426	0.6957	0.6205	0.6055
超图神经网络升级版 (HGNN+)	0.7671	0.7496	0.6643	0.6196	0.7408	0.7327	0.7910	0.7500	0.6997	0.6853

The best results are marked in bold type, and the second-best results are marked with underline.

最佳结果用粗体标注，次佳结果用下划线标注。

TABLE 5

Ablation Study: Comparison on the Effectiveness of Different Hyperedge Groups With HGNN+

消融研究: 使用 HGNN+ 对不同超边组的有效性进行比较

3跳可能太大了，造成了干扰。2跳和1跳在不同的数据集上各有优劣，但是大体上还是都有比较好。大多数情况自适应权重好于同等权重

	Hyperedge Groups				Citeseer		Cora		Facebook		Github Web ML		Pubmed	
	pair	hop-1	hop-2	hop-3	Acc	F1_ma	Acc	F1_ma	Acc	F1_ma	Acc	F1_ma	Acc	F1_ma
Coequal	✓	✓	✓	✓	0.6009	0.5438	0.6515	0.6387	0.5956	0.5781	OOM	OOM	0.6481	0.6403
	✓	✓	✓		0.6141	0.5543	0.7216	0.7049	0.6332	0.5946	0.7009	0.6248	0.6974	0.6836
	✓	✓			0.5946	0.5523	0.7066	0.6864	0.6441	0.6128	0.7887	0.7367	0.7060	0.7033
	✓		✓		0.6142	0.5613	0.7182	0.6938	0.6275	0.5976	0.7040	0.6632	0.6968	0.6898
	✓				0.5876	0.5428	0.6903	0.6735	0.5767	0.5324	0.7219	0.6583	0.6928	0.6882
Adaptive	✓	✓	✓		0.6064	0.5486	0.7319	0.7141	0.6431	0.6204	0.7637	0.7209	0.7138	0.7053

	超边组				科学文献数据库 (Citeseer)		科拉数据集 (Cora)		脸书 (Facebook)		GitHub 网络机器学习		医学文献数据库 (Pubmed)	
	对；双；一对	一跳	两跳	三跳	准确率 (Acc)	F1 值 (F1_ma)	准确率 (Acc)	F1 值 (F1_ma)	准确率 (Acc)	F1 值 (F1_ma)	准确率 (Acc)	F1 值 (F1_ma)	准确率 (Acc)	F1 值 (F1_ma)
等化子	对勾	对勾	对勾	对勾	0.6009	0.5438	0.6515	0.6387	0.5956	0.5781	内存不足 (OOM)	内存不足 (OOM)	0.6481	0.6403
	对勾	对勾	对勾		0.6141	0.5543	0.7216	0.7049	0.6332	0.5946	0.7009	0.6248	0.6974	0.6836
	对勾	对勾			0.5946	0.5523	0.7066	0.6864	0.6441	0.6128	0.7887	0.7367	0.7060	0.7033
	对勾		对勾		0.6142	0.5613	0.7182	0.6938	0.6275	0.5976	0.7040	0.6632	0.6968	0.6898
	对勾				0.5876	0.5428	0.6903	0.6735	0.5767	0.5324	0.7219	0.6583	0.6928	0.6882
自适应的	对勾	对勾	对勾		0.6064	0.5486	0.7319	0.7141	0.6431	0.6204	0.7637	0.7209	0.7138	0.7053

The best results are marked in bold type, and the second-best results are marked with underlining. The OOM denotes the Out of Memory.

最佳结果用粗体标记，次佳结果用下划线标记。OOM 表示内存不足 (Out of Memory)。

We attribute the significant improvement that HGNN+ achieves on the social media network data to the rich high-order correlations behind the data. The social media network data encode diverse information such as address and hobby as vertex features, while the publication network data simply uses word one-hot encoding as vertex features. In addition to the explicit ”follow” associations, there are plenty of implicit complex relationships (e.g., communities of interest) in the social media network data, remains to be captured and learned by HGNN^{+} . These informative vertex features and complex vertex relationships enable the HGNN^{+} to achieve more remarkable improvements compared with graph-based methods. We must note that the current extension is just a simple implementation of using this graph structure data in our framework. Other hyper-edge generation methods can be also used in applications.

我们将 HGNN+ 在社交媒体网络数据上取得的显著改进归因于数据背后丰富的高阶相关性。社交媒体网络数据将诸如地址和爱好等多样信息编码为顶点特征，而出版网络数据仅使用单词独热编码作为顶点特征。除了明确的“关注”关联外，社交媒体网络数据中还存在大量隐含的复杂关系 (例如，兴趣社区)，有待 HGNN^{+} 捕获和学习。这些信息丰富的顶点特征和复杂的顶点关系使 HGNN^{+} 与基于图的方法相比能够实现更显著的改进。我们必须注意，当前的扩展只是在我们的框架中使用这种图结构数据的简单实现。其他超边生成方法也可用于应用中。

6.2.4 Ablation Experiments

6.2.4 消融实验

In this subsection, three ablation studies are conducted. First, we compare HGNN $^+$ with HGNN in Table 6. Then in Table 5 we demonstrate the effectiveness of the proposed adaptive fusion strategies. Finally, we conduct experiments to compare different convolutional strategies, i.e., GCNConv and HGNNConv+, and experimental results are shown in Table 7.

在本小节中，进行了三项消融研究。首先，我们在表 6 中将 HGNN $^+$ 与 HGNN 进行比较。然后在表 5 中展示了所提出的自适应融合策略的有效性。最后，我们进行实验比较不同的卷积策略，即 GCNConv 和 HGNNConv+，实验结果如表 7 所示。

Comparison with HGNN. For better comparison, we split hypergraph neural network into two parts: hypergraph structure and hypergraph convolution. In this case, HGNN

与 HGNN 的比较。为了更好地进行比较，我们将超图神经网络分为两部分: 超图结构和超图卷积。在这种情况下，HGNN

TABLE 6

Comparison of HGNN and HGNN+

HGNN 与 HGNN+ 的比较

		HGNNConv		HGNNConv+	
		hop-1	Adaptive	hop-1	Adaptive
Cora	Acc	0.7143	0.6990	0.7289	0.7319
	F1_ma	0.6999	0.6847	0.7151	0.7141
Citeseer	Acc	0.5741	0.6061	0.5828	0.6064
	F1_ma	0.5179	0.5449	0.5238	0.5486
Pubmed	Acc	0.6973	0.6938	0.7033	0.7038
	F1_ma	0.6910	0.6859	0.6983	0.7053

		超图神经网络卷积层		增强型超图神经网络卷积层	
		第 1 跳	自适应的	第 1 跳	自适应的
科拉数据集	准确率	0.7143	0.6990	0.7289	0.7319
	F1 宏平均	0.6999	0.6847	0.7151	0.7141
引文数据集	准确率	0.5741	0.6061	0.5828	0.6064
	F1 宏平均	0.5179	0.5449	0.5238	0.5486
PubMed 数据集	准确率	0.6973	0.6938	0.7033	0.7038
	F1 宏平均	0.6910	0.6859	0.6983	0.7053

The best results are marked in bold type.

最佳结果用粗体标记。

 is composed of hop-1 (structure) and HGNNConv (convolution), while HGNN $^+$ is composed of adaptive fusion from multiple hyperedge groups (structure) and HGNNConv+ (convolution). In Table 6, Adaptive means using default hyperedge group configuration and adaptive fusion. As shown in Table 6, the combination of adaptive and HGNNConv+ outperforms HGNNConv and hop-1 in all three datasets. When using the same hypergraph structure hop-1/adaptive, HGNConv+ yields better performance than HGNNConv. The reason lies in that when derived from spectral domain, HGNNConv uses chebyshev polynomials to reduce computation cost, which may lead to inaccurate structure representation. In contrast, HGNNConv+ directly adopts inherent hypergraph for message passing in representation learning without simplification and thus showing better performance.

由 hop-1(结构) 和 HGNNConv(卷积) 组成，而 HGNN $^+$ 由多个超边组的自适应融合 (结构) 和 HGNNConv+(卷积) 组成。在表 6 中，自适应意味着使用默认的超边组配置和自适应融合。如表 6 所示，自适应和 HGNNConv+ 的组合在所有三个数据集中都优于 HGNNConv 和 hop-1。当使用相同的超图结构 hop-1/自适应时，HGNNConv+ 比 HGNNConv 具有更好的性能。原因在于，从谱域推导时，HGNNConv 使用切比雪夫多项式来降低计算成本，这可能导致结构表示不准确。相比之下，HGNNConv+ 在表示学习中直接采用固有超图进行消息传递，无需简化，因此表现出更好的性能。

Overall, the HGNN framework only constructs hyperedges via linking vertex with its 1-hop neighborhoods for final hypergraph. The HGNN $^+$ framework further proposes hyper-edge group concept for hypergraph modeling, which not only uses 1-hop correlation but also includes other complex correlations. Each hyperedge group can be built to describe one type of correlation. In HGNN $^+$ framework, multiple hyperedge groups $\left(\mathcal{E}_{\text{pair}}, \mathcal{E}_{\text{hop}_k}, \mathcal{E}_{\text{attribute}}, \mathcal{E}^{\text{KNN}_k}_{\text{feature}}, \mathcal{E}^{\text{distance}\ d}_{\text{feature}}\right)$ can be built toward different correlation description. From the other aspect, the HGNN framework only use $\mathcal{E}_{\text{hop}_1}$ for hypergraph construction. Besides, the HGNN $^+$ framework designs an adaptive multiple hyperedge groups fusion strategy to generate a uniform hypergraph, which encodes multiple types of high-order correlation, simultaneously. In summary, the HGNN $^+$ framework takes advantage of hypergraph in multimodal data modeling, and explicit multiple correlations

总体而言，HGNN 框架仅通过将顶点与其 1 跳邻域链接来构建超边以形成最终超图。HGNN $^+$ 框架进一步提出了用于超图建模的超边组概念，它不仅使用 1 跳相关性，还包括其他复杂相关性。每个超边组可以构建来描述一种类型的相关性。在 HGNN $^+$ 框架中，可以针对不同的相关性描述构建多个超边组 $\left(\mathcal{E}_{\text{pair}}, \mathcal{E}_{\text{hop}_k}, \mathcal{E}_{\text{attribute}}, \mathcal{E}^{\text{KNN}_k}_{\text{feature}}, \mathcal{E}^{\text{distance}\ d}_{\text{feature}}\right)$。从另一方面来看，HGNN 框架仅使用 $\mathcal{E}_{\text{hop}_1}$ 进行超图构建。此外，HGNN $^+$ 框架设计了一种自适应多超边组融合策略来生成一个统一的超图，该超图同时编码多种类型的高阶相关性。总之，HGNN $^+$ 框架在多模态数据建模中利用了超图，并明确了多种相关性

TABLE 7

Ablation Study: Comparison on Different Convolutional Strategies When Five Samples are Used for Training

消融研究: 使用五个样本进行训练时不同卷积策略的比较

	GCN (w/o self-loop)		HGNN + (pair only)	
	Acc	F1_ma	Acc	F1_ma
Citeseer	0.5544	0.5013	0.5876	0.5428
Cora	0.6799	0.6687	0.6903	0.6735
Facebook	0.4793	0.4564	0.5767	0.5324
Github	0.6338	0.5851	0.7219	0.6583
Pubmed	0.6706	0.6675	0.6928	0.6882

	图卷积网络 (无自环)		超图神经网络 + (仅配对)	
	准确率	F1 宏平均	准确率	F1 宏平均
科学引文数据库	0.5544	0.5013	0.5876	0.5428
科拉数据集	0.6799	0.6687	0.6903	0.6735
脸书	0.4793	0.4564	0.5767	0.5324
GitHub	0.6338	0.5851	0.7219	0.6583
生物医学文献数据库	0.6706	0.6675	0.6928	0.6882

The best results are marked in bold type. modeling makes it easier for the later hypergraph convolutions to capture the hidden patterns among data.

最佳结果用粗体标注。建模使得后续的超图卷积更容易捕捉数据中的隐藏模式。

On Hyperedge Group. Compared with graph neural network, the proposed HGNN + framework utilizes hyper-graph to represent data correlations, in which the hyper-edge groups are the components to carry the high-order correlations. To investigate how such hyperedge groups work in the learning procedure, we conduct experiments with respect to different combinations of hyperedge groups, including $\mathcal{E}_{\text{pair}}$, $\mathcal{E}_{\text{hop-1}}$, $\mathcal{E}_{\text{hop-2}}$ and $\mathcal{E}_{\text{hop-3}}$. In the combination of hyperedge groups, all hyperedge groups share equal weights. The experimental results with respect to different hyperedge group combinations are shown in Table 5. From these results, we can have the following observations.

关于超边组。与图神经网络相比，所提出的 HGNN + 框架利用超图来表示数据相关性，其中超边组是承载高阶相关性的组件。为了研究这些超边组在学习过程中如何工作，我们针对超边组的不同组合进行了实验，包括 $\mathcal{E}_{\text{pair}}$, $\mathcal{E}_{\text{hop-1}}$, $\mathcal{E}_{\text{hop-2}}$ 和 $\mathcal{E}_{\text{hop-3}}$ 。在超边组的组合中，所有超边组共享相等的权重。关于不同超边组组合的实验结果如表 5 所示。从这些结果中，我们可以得到以下观察结果。

First, the method using just $\mathcal{E}_{\text{pair}}$, in which only the pairwise correlation is employed, performs worst in most cases. When high-order correlations, including $\mathcal{E}_{\text{hop-1}}$, $\mathcal{E}_{\text{hop-2}}$ and $\mathcal{E}_{\text{hop}-3}$, are employed, the performance could improve in most cases, which demonstrates the effectiveness of high-order correlation on representation learning.

首先,仅使用 $\mathcal{E}_{\text{pair}}$ 的方法,即仅采用成对相关性,在大多数情况下表现最差。当采用包括 $\mathcal{E}_{\text{hop-1}}$, $\mathcal{E}_{\text{hop-2}}$ 和 $\mathcal{E}_{\text{hop}-3}$ 在内的高阶相关性时，在大多数情况下性能会提高，这证明了高阶相关性在表示学习中的有效性。

Second, we can also notice that although the introducing of high-order correlation can improve the performance, there is no common pattern of hyperedge group combinations which can always perform best. It indicates that different high-order correlations may have varied impact on the representation learning. With the adaptive hyperedge weight optimization in the proposed framework, the performance can outperform or at least be close to that from the best hyperedge group combination, as shown in Table 5.

其次，我们还可以注意到，虽然引入高阶相关性可以提高性能，但不存在一种总能表现最佳的超边组组合的通用模式。这表明不同的高阶相关性可能对表示学习有不同的影响。在所提出的框架中，通过自适应超边权重优化，性能可以优于或至少接近最佳超边组组合的性能，如表 5 所示。

On Convolution Strategy. To evaluate the effectiveness of the proposed hypergraph convolution, we conduct experiments to compare GCN without self-loop and our HGNN$^+$ using just $\mathcal{E}_{\text{pair}}$, which only utilizes the pairwise correlation in the hypergraph structure, for fair comparison. The results on five datasets are provided in Table 7.

关于卷积策略。为了评估所提出的超图卷积的有效性，我们进行实验，将没有自环的 GCN 与仅使用 $\mathcal{E}_{\text{pair}}$ 的我们的 HGNN$^+$ 进行比较，后者仅利用超图结构中的成对相关性，以进行公平比较。五个数据集的结果如表 7 所示。

As shown in these results, the proposed HGNN$^+$ consistently outperforms GCN in all experiments on all evaluation metrics. Compared with the single layer graph convolution, a single layer hypergraph convolution is a hierarchical message passing (a vertex-hyperedge-vertex way referring to Section 5.2) that can handle information from multiple low-order/high-order correlation groups. Therefore, the proposed hypergraph convolution strategy is efficient on modeling the low-order structure with its hierarchical message passing strategy in each layer and thus leads to better performance.

如这些结果所示，在所提出的 HGNN$^+$ 在所有实验中的所有评估指标上都始终优于 GCN。与单层图卷积相比，单层超图卷积是一种分层消息传递 (一种指第 5.2 节的顶点 - 超边 - 顶点方式)，可以处理来自多个低阶/高阶相关组的信息。因此，所提出的超图卷积策略通过其每层的分层消息传递策略在对低阶结构进行建模方面是有效的，从而带来更好的性能。

6.3 Vertex Classification on the Data Without Graph Structure

6.3 无图结构数据上的顶点分类

In this part of the experiments, the classification task is conducted on the data which does not contain the explicit graph structure. These experiments aim to evaluate how the proposed hypergraph neural network framework can exploit data representation when there is no explicit graph structure, which is more common in real applications.

在这部分实验中，分类任务是在不包含显式图结构的数据上进行的。这些实验旨在评估所提出的超图神经网络框架在没有显式图结构时如何利用数据表示，这在实际应用中更为常见。

6.3.1 Datasets

6.3.1 数据集

Here, two public 3D object datasets are employed, including the ModelNet40 [40] dataset and the NTU [41] dataset. The ModelNet40 dataset consists of 12,311 3D objects from 40 popular categories, and the same training/testing split is

> 这里，使用了两个公共的 3D 对象数据集，包括 ModelNet40 [40] 数据集和 NTU [41] 数据集。ModelNet40 数据集由来自 40 个流行类别的 12,311 个 3D 对象组成，并且相同的训练/测试划分是

 applied as introduced in [40], where 9,843 objects are used for training and 2,468 objects are used for testing. The NTU dataset is composed of 2,012 3D shapes from 67 categories, including car, chair, chess, chip, clock, cup, door, frame, pen, plant leaf and so on. In the NTU dataset, 80% of data are used for training and the other 20% of data are used for testing. In this experiment, each 3D object is represented by the extracted features. Here, two 3D shape representation methods are employed, including Multi-view Convolutional Neural Network (MVCNN [42]) and Group-View Convolutional Neural Network (GVCNN [43]). These two methods are selected due to that they have shown satisfactory performance on 3D object representation. We follow the experimental settings of MVCNN and GVCNN to generate multiple views of each 3D object. Here, 12 virtual cameras are employed to capture views with an interval angle of 30 degrees, and then both the MVCNN and the GVCNN features are extracted accordingly.

> 如 [40] 中所述应用，其中 9843 个对象用于训练，2468 个对象用于测试。NTU 数据集由来自 67 个类别的 2012 个 3D 形状组成，包括汽车、椅子、国际象棋、芯片、时钟、杯子、门、框架、笔、植物叶子等。在 NTU 数据集中，80% 的数据用于训练，另外 20% 的数据用于测试。在本实验中，每个 3D 对象由提取的特征表示。这里，采用了两种 3D 形状表示方法，包括多视图卷积神经网络 (MVCNN [42]) 和组视图卷积神经网络 (GVCNN [43])。选择这两种方法是因为它们在 3D 对象表示上表现出了令人满意的性能。我们遵循 MVCNN 和 GVCNN 的实验设置来生成每个 3D 对象的多个视图。这里，使用 12 个虚拟相机以 30 度的间隔角度捕捉视图，然后相应地提取 MVCNN 和 GVCNN 特征。

6.3.2 Settings

> ### 6.3.2 设置

In this part of the experiments, we combine the two features as the vertex feature for all methods. The compared methods and the evaluation metrics are the same as that in Section 6.2.

> 在这部分实验中，我们将这两种特征组合作为所有方法的顶点特征。比较的方法和评估指标与 6.2 节中的相同。

Graph/Hypergraph Construction. In experiments without graph structure (on ModelNet40 and NTU datasets), K Nearest Neighbor (KNN) algorithm is adopted for hyper-graph construction. Specifically, we build two hyperedge groups $\mathcal{E}_{\text{mvcmn}}^{\text{KNN}_8}$ and $\mathcal{E}_{\text{gvcmn}}^{\text{KNN}_8}$ for MVCNN feature and GVCNN feature, respectively. The final hypergraph is constructed by fusing the two hyperedge groups with the coequal strategy. Different from the conference version, the graph structure is constructed by weighted hypergraph expansion (more details refer to Appendix B, available in the online supplemental material). This graph construction strategy is adopted to guarantee the same original connection structure for both graph-based methods and hyper-graph-based methods for a fair comparison.

图/超图构建。在没有图结构的实验中 (在 ModelNet40 和 NTU 数据集上)，采用 K 最近邻 (KNN) 算法进行超图构建。具体来说，我们分别为 MVCNN 特征和 GVCNN 特征构建两个超边组 $\mathcal{E}_{\text{mvcmn}}^{\text{KNN}_8}$ 和 $\mathcal{E}_{\text{gvcmn}}^{\text{KNN}_8}$ 。最终的超图通过将两个超边组以同等策略融合来构建。与会议版本不同，图结构通过加权超图扩展构建 (更多细节请参考附录 B，可在在线补充材料中获取)。采用这种图构建策略是为了确保基于图的方法和基于超图的方法具有相同的原始连接结构，以便进行公平比较。

6.3.3 Experimental Results and Discussions

6.3.3 实验结果与讨论

The experimental results on two datasets are provided in Table 8. As shown in these results, the proposed hypergraph neural network framework, i.e., HGNN $^+$ and HGNN, significantly outperforms all other compared methods. For example, HGNN$^+$ achieves gains of 3.75%, 4.02%, 3.48%, 4.02% and 3.22% compared with GCN, GAT, GraphSAGE, GIN and GraphConv in terms of Acc in the NTU dataset. Similar results can be observed in the ModelNet40 dataset.

两个数据集上的实验结果如表所示。如这些结果所示，所提出的超图神经网络框架，即 HGNN $^+$ 和 HGNN，明显优于所有其他比较方法。例如，HGNN$^+$ 在 NTU 数据集上的 Acc 方面与 GCN、GAT、GraphSAGE、GIN 和 GraphConv 相比，分别取得了 3.75%, 4.02%, 3.48%, 4.02% 和 3.22% 的增益。在 ModelNet40 数据集中也可以观察到类似的结果。

When there is no explicit graph structure, the proposed method performs much better than traditional graph neural network methods. These results indicate that the proposed framework is able to deeply exploit the underneath high-order correlation by generating a hypergraph structure. The superior performance of HGNN$^+$ and HGNN can sufficiently demonstrate the effectiveness of our proposed method on the classification task using data without graph structure.

当没有明确的图结构时，所提出的方法比传统的图神经网络方法表现得好得多。这些结果表明，所提出的框架能够通过生成超图结构深入挖掘底层的高阶相关性。HGNN$^+$ 和 HGNN 的优越性能充分证明了我们所提出的方法在使用无图结构数据的分类任务上的有效性。

6.4 Vertex Classification on the Data With Hypergraph Structure

6.4 超图结构数据上的顶点分类

In this part of the experiments, two datasets, i.e., Cooking- 200 and MovieLens2k-v2, where hypergraph structure naturally exists are selected. The objective of these experiments is to evaluate the effectiveness of the proposed hyper-graph convolution operator compared with the graph convolution operator on natural hypergraph data.

在这部分实验中，选择了两个自然存在超图结构的数据集，即 Cooking - 200 和 MovieLens2k - v2。这些实验的目的是评估所提出的超图卷积算子与图卷积算子在自然超图数据上相比时的有效性。

TABLE 8

Experimental Results on the ModelNet40 and NTU Dataset

ModelNet40 和 NTU 数据集上的实验结果

	ModelNet40		NTU	
	Acc	F1_ma	Acc	F1_ma
GCN	0.9485	0.9276	0.8043	0.7688
GAT	0.9575	0.9268	0.8016	0.7511
GraphSAGE	0.9473	0.9188	0.807	0.7699
GIN	0.9485	0.9275	0.8016	0.7590
GraphConv	0.9566	0.9370	0.8096	0.7664
HyperGCN	0.9546	0.9410	0.8177	0.7677
Hyper-Atten	0.9611	0.9419	0.8150	0.7616
HGNN	0.9680	0.9520	0.8311	0.7798
HGNN+	0.9692	0.9577	0.8418	0.7944

	模型网络 40(ModelNet40)		南洋理工大学 (NTU)	
	准确率 (Acc)	F1 宏平均 (F1_ma)	准确率 (Acc)	F1 宏平均 (F1_ma)
图卷积网络 (GCN)	0.9485	0.9276	0.8043	0.7688
图注意力网络 (GAT)	0.9575	0.9268	0.8016	0.7511
图采样和聚合方法 (GraphSAGE)	0.9473	0.9188	0.807	0.7699
图同构网络 (GIN)	0.9485	0.9275	0.8016	0.7590
图卷积 (GraphConv)	0.9566	0.9370	0.8096	0.7664
超图卷积网络 (HyperGCN)	0.9546	0.9410	0.8177	0.7677
超注意力 (Hyper-Atten)	0.9611	0.9419	0.8150	0.7616
超图神经网络 (HGNN)	0.9680	0.9520	0.8311	0.7798
超图神经网络升级版 (HGNN+)	0.9692	0.9577	0.8418	0.7944

The best results are marked in bold type.

最佳结果用粗体标记。

6.4.1 Datasets

6.4.1 数据集

The Cooking dataset is collected from Yummly.com [2] , in which vertex denotes the dish and hyperedge denotes the ingredient. Each dish is also associated with category information, which indicates the dish's cuisine like Chinese, Japanese, French, and Russian. To avoid vertex's feature over-smoothing, we drop the ingredients that contribute more than 200 dishes and contribute only one dish. After preprocessing, the Cooking-200 (including 7403 dishes, 2755 ingredients, and 20 cuisines) is generated. The Movie-Lens2k-v2 is an extension of the MovieLens10M dataset, published by the GroupLeans research group [3] . It links the movies of the MovieLens dataset with their corresponding web pages at Internet Movie Database [4] (IMDB) and Rotten Tomatoes movie review systems [5] . The MovieLens2k-v2 dataset includes 2113 users, 10197 movies, 13222 tags (47957 tag assignments, i.e., tuples [user, tag, movie]), 4060 directors, and 20 movie genres (like Adventure, Animation, Comedy, and Crime). Due to each movie may associate with more than one genre, experiments on the MovieLens dataset are indeed multi-label classification task. The vertices in the two datasets do not associate with vertex features.

烹饪数据集是从 Yummly.com 收集的 [2] , 其中顶点表示菜肴, 超边表示食材。每道菜肴还与类别信息相关联, 该信息表明菜肴的烹饪风格, 如中国菜、日本菜、法国菜和俄罗斯菜。为避免顶点特征过度平滑, 我们去除了贡献超过 200 道菜肴且仅贡献一道菜肴的食材。预处理后, 生成了 Cooking-200(包括 7403 道菜肴、2755 种食材和 20 种烹饪风格)。Movie-Lens2k-v2 是 GroupLeans 研究小组发布的 MovieLens10M 数据集的扩展版本 [3] 。它将 MovieLens 数据集中的电影与其在互联网电影数据库 [4] (IMDB) 和烂番茄电影评论系统 [5] 中的相应网页链接起来。MovieLens2k-v2 数据集包括 2113 个用户、10197 部电影、13222 个标签 (47957 个标签分配, 即元组 [用户, 标签, 电影])、4060 名导演和 20 种电影类型 (如冒险、动画、喜剧和犯罪)。由于每部电影可能与多种类型相关联, 因此在 MovieLens 数据集上的实验实际上是多标签分类任务。这两个数据集中的顶点不与顶点特征相关联。

6.4.2 Settings

6.4.2 设置

Considering that the identity matrix can identify each row (vertex feature) because of the orthogonality, the identity matrix is fed into the model as the initial vertex feature.

考虑到单位矩阵由于其正交性可以识别每一行 (顶点特征), 因此将单位矩阵作为初始顶点特征输入到模型中。

Train/validation/test Split. In both two datasets, we randomly sample 10 vertices for training and 10 vertices for validation for each category, and the rest vertices are used for testing.

训练/验证/测试划分。在这两个数据集中, 我们为每个类别随机抽取 10 个顶点用于训练, 10 个顶点用于验证, 其余顶点用于测试。

Hypergraph Construction. In the Cooking-200 dataset, each dish consists of several ingredients, and each ingredient can be shared with several dishes. Thus, the ingredient naturally acts as the hyperedge, which connects those related dishes (vertices). Finally, a hypergraph with 7403 vertices and 2755 hyperedges is constructed in the Cooking- 200 dataset. In the MovieLens2k-v2 dataset, the movie acts as the vertex, and the hyperedge can be built from the correlations of [movie, tag, weight] and [movie, director]. Consequently, two hyperedge groups - tag-based hyperedge group and director-based hyperedge group are constructed. To compare the learning ability of GCNConv, HGNNConv, and HGNNConv+, the adaptive fusion strategy is not adopted here. We directly concatenate the two hyperedge groups to generate the final hypergraph for a fair comparison in the MovieLens2k-v2 dataset.

超图构建。在 Cooking-200 数据集中，每道菜肴由几种食材组成，每种食材可以与多道菜肴共享。因此，食材自然地充当超边，连接那些相关的菜肴 (顶点)。最后，在 Cooking-200 数据集中构建了一个具有 7403 个顶点和 2755 条超边的超图。在 MovieLens2k-v2 数据集中，电影充当顶点，超边可以根据 [电影，标签，权重] 和 [电影，导演] 的相关性构建。因此，构建了两个超边组——基于标签的超边组和基于导演的超边组。为了比较 GCNConv、HGNNConv 和 HGNNConv+ 的学习能力，这里不采用自适应融合策略。我们直接将两个超边组连接起来，以在 MovieLens2k-v2 数据集中进行公平比较，生成最终的超图。

TABLE 9

Experimental Results on Cooking-200 and MovieLens2k-v2

Cooking-200 和 MovieLens2k-v2 上的实验结果

	Expansion	Cooking-200		MovieLens2k-v2		
		Acc	F1_ma	EMR	EB-Acc	EB-Pre
GCN	unweighted	0.3110	0.2608	0.0686	0.2081	0.3096
	weighted	0.3271	0.2849	0.0814	0.233	0.3363
HGNN	-	0.4564	0.3725	0.1043	0.2482	0.3652
HGNN $^+$	-	0.4785	0.3883	0.1214	0.2808	0.4175

	扩展	烹饪-200		MovieLens2k-v2		
		准确率	F1 值 (宏平均)	电子病历 (EMR)	EB 准确率	EB 预测
图卷积网络 (GCN)	无加权的	0.3110	0.2608	0.0686	0.2081	0.3096
	加权的	0.3271	0.2849	0.0814	0.233	0.3363
超图神经网络 (HGNN)	-	0.4564	0.3725	0.1043	0.2482	0.3652
超图神经网络 (HGNN) $^+$	-	0.4785	0.3883	0.1214	0.2808	0.4175

The best results are marked in bold type.

最佳结果用粗体标记。

Hypergraph Expansion. Considering that the hyper-graph incidence matrix cannot being directly handled by the graph neural network [2], two commonly used hyper-graph expansion methods [33], [45], i.e., unweighted clique expansion and weighted clique expansion, are employed to transfer the hypergraph structure into the simple graph structure. More details are provided in Appendix B, available in the online supplemental material.

超图扩展。考虑到超图关联矩阵无法直接由图神经网络处理 [2]，我们采用了两种常用的超图扩展方法 [33],[45]，即无加权团扩展和加权团扩展，将超图结构转换为简单图结构。更多细节见附录 B，可在在线补充材料中获取。

6.4.3 Experimental Results and Discussions

6.4.3 实验结果与讨论

Experimental results are shown in Table 9. The proposed hypergraph-based methods HGNN and HGNN $^+$ exhibit significant improvement compared with the graph-based method GCN in natural hypergraph real-world datasets. Specifically, as for the single-label classification task, HGNN$^+$ achieves gains of 16.75% and 15.14% on Acc compared with unweighted and weighted expansion GCN in the Cooking-200 dataset, respectively. As for the multi-label classification task, HGNN$^+$ achieves 10.79% and 8.12% on EB-Pre compared with the unweighted and weighted expansion GCNs in the MovieLens2k-v2 dataset respectively.

实验结果如表 9 所示。在自然超图真实世界数据集中，所提出的基于超图的方法 HGNN 和 HGNN $^+$ 与基于图的方法 GCN 相比有显著改进。具体而言，对于单标签分类任务，HGNN$^+$ 在 Cooking-200 数据集中，与无加权和加权扩展 GCN 相比，在准确率上分别提高了 16.75% 和 15.14%。对于多标签分类任务，HGNN$^+$ 在 MovieLens2k-v2 数据集中，与无加权和加权扩展 GCN 相比，在 EB-Pre 上分别提高了 10.79% 和 8.12%。

From the experimental results, we can have the following observations. First, the weighted hypergraph expansion GCN performs better than the unweighted-based way. The main reason is that the unweighted hypergraph expansion only inherits the connection relationships among vertices from the original hypergraph. In contrast, the weighted expansion links vertices with different intensities according to the original hyperedges and thus reserves more high-order information. Moreover, the hypergraph-based methods consistently exhibit much better performance than graph-based methods. The main reasons are two-fold. First, although hypergraph expansion methods like clique expansion can transfer the high-order hypergraph structure into the low-order graph structure so as to model the high-order correlations among data into a graph, it will still cause structure distortion and yield unsatisfactory performance, which also has been discussed in [46], [47], [48]. Besides, the HGNN and HGNN $^+$ are inherently proposed to learn in hypergraph structure. Specifically, the two-stage message passing strategy $\mathcal{V} \to \mathcal{E}, \mathcal{E} \to \mathcal{V}$ of HGNN and HGNN $^+$ can effectively capture the high-order information in hyper-graph compared with the the one-stage message passing strategy $\mathcal{V} \to \mathcal{V}$ adopted in graph-based methods, thus leading to the better performance.

从实验结果中，我们可以得到以下观察结果。首先，加权超图扩展 GCN 比基于无加权的方法表现更好。主要原因是无加权超图扩展仅从原始超图继承顶点之间的连接关系。相比之下，加权扩展根据原始超边以不同强度连接顶点，从而保留了更多高阶信息。此外，基于超图的方法始终比基于图的方法表现出更好的性能。主要原因有两个方面。首先，尽管像团扩展这样的超图扩展方法可以将高阶超图结构转换为低阶图结构，以便将数据之间的高阶相关性建模到图中，但它仍然会导致结构失真并产生不理想的性能，这在 [46],[47],[48] 中也有讨论。此外，HGNN 和 HGNN $^+$ 本质上是为在超图结构中学习而提出的。具体而言，与基于图的方法中采用的单阶段消息传递策略 <b2><b2> 相比，HGNN 和 HGNN $^+$ 的两阶段消息传递策略 <b1><b1> 可以有效地捕获超图中的高阶信息，从而带来更好的性能。

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2. https://www.yummly.com

2. https://www.yummly.com

3. https://grouplens.org/

3. https://grouplens.org/

4. https://www.imdb.com/

4. https://www.imdb.com/

5. https://www.rottentomatoes.com/

5. https://www.rottentomatoes.com/

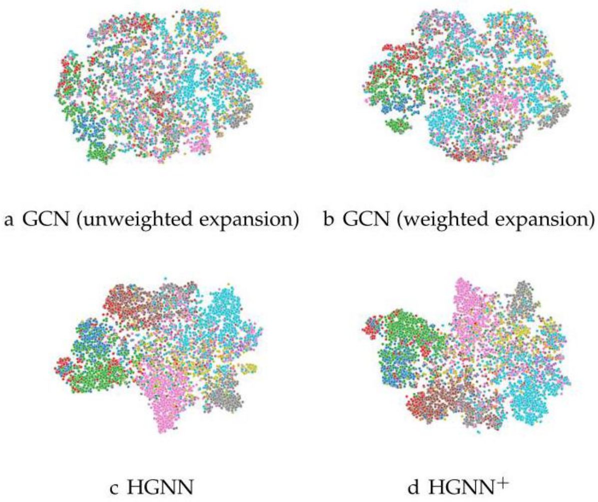

Fig. 7. A t-SNE visualization of graph-based methods and hypergraph-based methods on the Cooking-200 dataset.

图 7. 在 Cooking-200 数据集上基于图的方法和基于超图的方法的 t-SNE 可视化。

6.5 Visualization

6.5 可视化

Considering that there naturally exists hypergraph structure in the Cooking-200 dataset, indicating that it contains complex high-order correlations among data, the Cooking-200 dataset is selected for visualization to intuitively compare the learning ability of graph-based methods and hypergraph-based methods. The t-SNE method is utilized to visualize the output of the last-layer convolution and the results are shown in Fig. 7. It can be observed from the results that compared with graph-based methods, hypergraph-based methods like HGNN and HGNN$^+$ yield discernible clustering, which qualitatively verifies the effectiveness of the proposed method.

考虑到 Cooking-200 数据集中自然存在超图结构，这表明它包含数据之间复杂的高阶相关性，因此选择 Cooking-200 数据集进行可视化，以直观地比较基于图的方法和基于超图的方法的学习能力。使用 t-SNE 方法对最后一层卷积的输出进行可视化，结果如图 7 所示。从结果中可以观察到，与基于图的方法相比，像 HGNN 和 HGNN$^+$ 这样的基于超图的方法产生了明显的聚类，这从定性上验证了所提出方法的有效性。

7 THU-DEEPHYPERGRAPH: AN OPEN TOOLBOX OF THE HGNN+ FRAMEWORK

7 THU-DEEPHYPERGRAPH:HGNN+ 框架的开源工具箱

To facilitate the development of hypergraph-based representation learning, we develop THU-DeepHypergraph (THU-DH), an open-source python toolbox for the general hypergraph neural network framework, which is built upon PyTorch. As shown in Fig. 8, THU-DH can be decoupled into three parts: Graph Learning, Hypergraph Learning, and Structure Transform. The graph learning part includes the graph sampling, graph pooling, and a general graph-based message passing framework. The Structure Transform part implements some typical hypergraph expansion algorithms like clique expansion and star expansion, which can reduce the high-order data into the low-order data for graph learning on hypergraph dataset.

为了促进基于超图的表示学习的发展，我们开发了 THU-DeepHypergraph(THU-DH)，这是一个基于 PyTorch 的通用超图神经网络框架的开源 Python 工具箱。如图 8 所示，THU-DH 可以解耦为三个部分: 图学习、超图学习和结构转换。图学习部分包括图采样、图池化和一个通用的基于图的消息传递框架。结构转换部分实现了一些典型的超图扩展算法，如团扩展和星扩展，它可以将高阶数据降为低阶数据，以便在超图数据集上进行图学习。

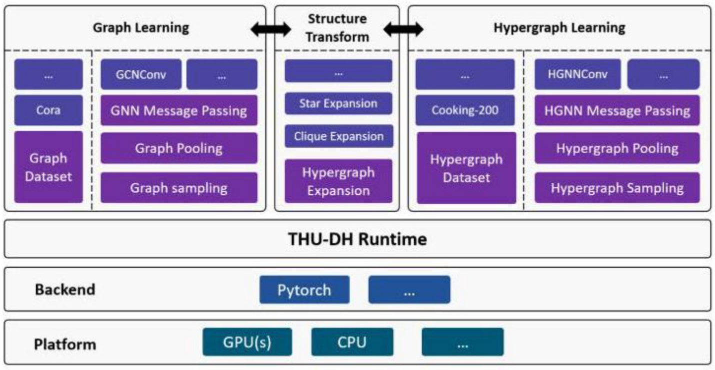

Fig. 8. A framework illustration of THU-DH toolbox.

图 8. THU-DH 工具箱的框架示意图。

As for the hypergraph learning, some hypergraph modeling algorithms have been integrated into the Hyper-graph Dataset module. Specifically, the hypergraph modeling can be further divided into two modules, i.e., hyperedge group generation and fusion, as stated in Section 4. To simplify the construction of hypergraph, THU-DH provides common APIs for hyperedge group generation, including pairwise edge-based, k -Hop neighbors-based, attributes-based and features-based methods. THU-DH also supports two strategies for hyperedge group fusion: coequal fusion and adaptive fusion. Here we recommend the adaptive fusion strategy since it can ensure more robust performance improvements. For hypergraph convolution, the convolution operators in the spectral domain (HGNNConv) and the spatial domain (HGNNConv+) have been implemented based on the HGNN Message Passing module in THU-DH. The Hypergraph Pooling module and Hypergraph Sampling module are designed for hypergraph learning on large scale hypergraph. Researchers can conveniently use this toolbox to handle various tasks, such as node classification, network classification, image segmentation, graph regression prediction, by assembling different modules according to the task characteristics. Data pre-processing algorithms included in the Hypergraph Dataset module are implemented for multiple tasks, such as pathological image sampling, magnetic resonance image enhancement, etc. We also provide some example codes and visualization tools to help researchers get started quickly and evaluate intuitively. We endeavor to make the toolbox more efficient. Specifically, sparse matrix techniques are used for the hypergraph representation and calculation, which greatly improves the running speed and decrease memory consumption.

至于超图学习，一些超图建模算法已集成到超图数据集模块中。具体而言，超图建模可进一步分为两个模块，即超边组生成和融合，如第 4 节所述。为简化超图的构建，清华深度超图 (THU-DH) 提供了用于超边组生成的通用应用程序编程接口 (API)，包括基于成对边、k -跳邻居、基于属性和基于特征的方法。THU-DH 还支持两种超边组融合策略: 平等融合和自适应融合。在此我们推荐自适应融合策略，因为它可以确保更强大的性能提升。对于超图卷积，已基于 THU-DH 中的超图神经网络消息传递模块实现了谱域 (HGNNConv) 和空域 (HGNNConv+) 中的卷积算子。超图池化模块和超图采样模块是为大规模超图上的超图学习而设计的。研究人员可以根据任务特点组装不同模块，方便地使用此工具箱来处理各种任务，如节点分类、网络分类、图像分割、图回归预测等。超图数据集模块中包含的数据预处理算法是针对多种任务实现的，如病理图像采样、磁共振图像增强等。我们还提供了一些示例代码和可视化工具，以帮助研究人员快速入门并直观地进行评估。我们努力使该工具箱更高效。具体而言，稀疏矩阵技术用于超图表示和计算，这大大提高了运行速度并减少了内存消耗。

8 CONCLUSION

8 结论

In this journal version, we extend our previous HGNN work and introduce a general hypergraph neural network framework HGNN$^+$ for representation learning. The proposed HGNN $^+$ framework has advantage on modeling high-order data correlations from multi-modal/multi-type data. Four types of data correlation generation methods are introduced in this paper and an adaptive hyperedge fusion strategy is provided to generate the overall hypergraph. A hypergraph convolution in the spatial domain is introduced to learn the representation. Experiments on 9 datasets and comparisons with state-of-the-art methods demonstrate the effectiveness of our proposed methods. The results and mathematical discussions reveal that the proposed framework is able to achieve the new state-of-the-art performance, especially when there is no explicit data correlations. The proposed HGNN $^+$ framework can be used in various of applications, such as data classification, retrieval and recommendation. A tool of the proposed framework, called THU-DeepHyper-graph, is released for public use.

在本期刊版本中，我们扩展了之前的超图神经网络 (HGNN) 工作，并引入了一个用于表示学习的通用超图神经网络框架 HGNN^{+} 。所提出的 HGNN $^{+}$ 框架在对多模态/多类型数据的高阶数据相关性进行建模方面具有优势。本文介绍了四种数据相关性生成方法，并提供了一种自适应超边融合策略来生成整体超图。引入了空域中的超图卷积来学习表示。在 9 个数据集上进行的实验以及与现有最先进方法的比较证明了我们所提出方法的有效性。结果和数学讨论表明，所提出的框架能够实现新的最先进性能，特别是在没有明确数据相关性的情况下。所提出的 HGNN $^{+}$ 框架可用于各种应用，如数据分类、检索和推荐。所提出框架的一个工具，称为清华深度超图 (THU-DeepHyper-graph)，已发布供公众使用。

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