

Graph Learning and Its Applications: A Holistic Survey

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Abstract—Graph learning is a prevalent domain that endeavors to learn the intricate relationships among nodes and the topological structure of graphs. Over the years, graph learning has transcended from graph theory to graph data mining. With the advent of representation learning, it has attained remarkable performance in diverse scenarios. Owing to its extensive application prospects, graph learning attracts copious attention. While some researchers have accomplished impressive surveys on graph learning, they failed to connect related objectives, methods, and applications in a more coherent way. As a result, they did not encompass current ample scenarios and challenging problems due to the rapid expansion of graph learning. Particularly, large language models have recently had a disruptive effect on human life, but they also show relative weakness in structured scenarios. The question of how to make these models more powerful with graph learning remains open. Different from previous surveys on graph learning, we provide a holistic review that analyzes current works from the perspective of graph structure, and discusses the latest applications, trends, and challenges in graph learning. Specifically, we commence by proposing a taxonomy and then summarize the methods employed in graph learning. We then provide a detailed elucidation of mainstream applications. Finally, we propose future directions.

Index Terms—Graph Learning, Deep Learning, Representation Learning

1 INTRODUCTION

GRAPH learning (GL) aims to model graphs, a type of non-Euclidean data that differs significantly from previous data structures in machine learning. Graphs are present in various real-world scenarios, such as social network [1], [2], academic network [3], [4], [5], e-commerce networks [6], [7], enterprise knowledge graphs [8], [9], [10]. It is crucial to extract rich information from the complex connections between nodes and the topological structure of graphs. Graph learning benefits various tasks and applications involving graphs.

Additionally, traditional applications can be transformed into graph data, such as computer vision [11], [12], language model [13], [14], physics [15], [16] and chemistry [17], [18]). The underline assumption is that there are many potential connections among different entities that are not observed directly. Thus, graph learning is not only a way to deal with natural graph structures but also a way of thinking about various kinds of problems.

Owing to the auspicious future of graph learning, it has attracted a lot of interest worldwide. However, despite previous theoretical works on graphs that help people understand various characters on graphs and provide basic analysis frameworks, these

works usually concentrate on small and simulated graphs. This constrains their applications in real scenarios, especially when intricate relationships and structures prevail on graphs.

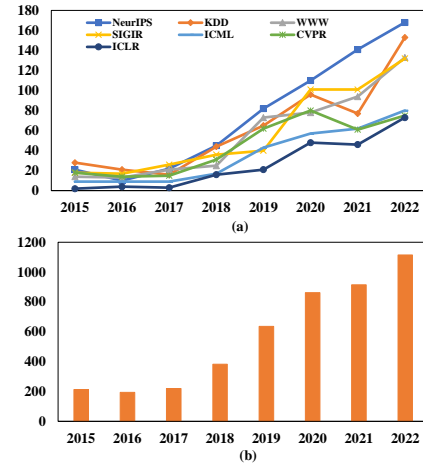


Fig. 1: Number of GL publications in recent years on top venues, including NeurIPS, KDD, WWW, SIGIR, ICML, CVPR and ICLR. Figures (a) and (b) depict the number of GL publications at top conferences and the total number, respectively.

Representation learning provides a successful way to deal with various kinds of complex problems in other traditional scenarios, which also sheds light on the progress of graph learning. As shown in Figure 1, the number of graph learning works has increased rapidly in recent years, reaching a new peak of 1115 papers in 2022 on top venues. There are thousands of works that focus on different objectives, methods, and applications of graph learning, making it imperative to survey these research and foster future progress on graph learning.

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Figure 2 exhibits a chronological overview of influential graph learning methods, which can be divided into three main types: graph mining methods, graph representation methods, and deep graph learning methods. In the early days of graph learning, most methods concentrated on characterizing graphs [1] or utilizing graph structure information to perform downstream tasks on small graphs [19], [20]. Nowadays, representation learning on graphs is predominant and can be broadly categorized into two types: graph embedding methods and graph neural network methods. Both methods aim to learn semantic representations of nodes, edges, or graphs. The former directly optimizes embeddings to preserve graph structure information, while the latter employs deep neural networks to model information passing processes on graphs, a technique that has been popular since early works [21], [22].

1.1 Discussion of the Novelty

While there have been some remarkable and thorough surveys in the field [47], [48], [49], [50], there is still a need for a holistic survey that connects related objectives, methods, and tasks in an organic and logical manner. Furthermore, there are hundreds of research papers on GL presented at top conferences every year, and their number continues to escalate rapidly. As a result of this rapid development, there is a lack of comprehensive surveys covering the latest applications, trends and challenges in the field, especially the combination of GL and large language models.

Therefore, we start with the graph structure, which makes it divergent from previous tabular data, by reviewing past and current works. Subsequently, we review the rapid development of GL, with the aim of promoting future research. Specifically, we summarize the technical trends of GL, including current pioneering works of large language models with graphs, mainstream applications, as well as benchmark datasets. Finally, based on the above, we discuss valuable future directions.

1.2 Contribution

As depicted in Figure 3, this survey provides an intuitive taxonomy that considers the objectives of graph learning. Specifically, we sort previous works based on the elements of graphs, such as nodes, edges, and graph structures. Based on this taxonomy, we survey related methods and tasks on graphs and demonstrate the great performance of graph learning on various real-world applications. Finally, we discuss current trends and challenges in graph learning that are expected to further stimulate research.

The main contributions of this survey are summarized below.

- We propose a holistic classification to review previous research with respect to two dimensions of objective and constituents. The former denotes data, models and tasks, and the latter pertains to node, edge and graph structure.
- we provide a detailed demonstration of representative works of different types of graph learning. We also conduct a thorough review of pioneering research on the combination of pre-trained language models, particularly large language models, and graph learning.
- We summarize the current applications and prevalent datasets of graph learning in the real world, which manifests the rapid advancement of this field. This underscores the significance of examining the latest works as well.
- We explore the current salient trends and challenges of graph learning and aspire to offer valuable directions for future research.

The remainder of this article is organized as follows. Section 2 proposes an intuitive taxonomy of previous works based on node, edge, and graph structure, from the viewpoint of data, model, and task. Section 3 demonstrates the main methods used for graph learning and current research trends. Section 4 concludes the applications of graph learning in the real world. Finally, section 5 discusses the challenges of graph learning today.

2 OBJECTIVES

Numerous methods have been proposed for mining complex information in graphs, focusing on various components. To categorize previous works, we divide them according to data, model, and task, and consider the basic components of graphs(i.e., nodes, edges, and graphs). This approach inherently links different methods that aim to achieve different objectives. We provide a brief definition of the notations to be used in the following parts, as shown in Table 1. Other notations that can be inferred from the context are not listed here.

TABLE 1: NOTATIONS AND EXPLANATIONS

Notations	Explanations
\mathcal{V}, \mathcal{E}	Node set and edge set
v_i, e_j	A node $v_i \in \mathcal{V}$ and edge $e_j \in \mathcal{E}$
$G = (\mathcal{V}, \mathcal{E})$	A graph G consists of \mathcal{V} and \mathcal{E}
A	The adjacent matrix of G
$\mathcal{T}^v, \mathcal{T}^e$	The node type set and edge type set
Ψ, ψ	Node type and edge type mapping function
$X \in \mathbb{R}^{ \mathcal{V} \times d}$	Node feature matrix with $ \mathcal{V} $ nodes and each node is with d dimension
$\mathcal{N}(v_i)$	The neighbours of node v_i
$w_{i,j}$	Edge weight between node v_i and node v_j
$\langle h, r, t \rangle$	Knowledge graph triplet, with head entity h , relation r and tail entity t
$\mathbf{T} = \{t_1, t_2, \dots, t_T\}$	Timestamp set of a dynamic graph
$q^n = (u_n, v_n, r_n, t_n)$	Event q^n consists of linked nodes v_i, v_j and relation r_n in time t_n
h_i	Representation of node v_i
σ	Activation function
LSTM	Long Short Term Memory networks

2.1 Data

In this subsection, we categorize current graphs based on their characteristics regarding node, edge, and graph structure. Note that all classifications are based on the data used in these works. In the preliminary stages, researchers may only be able to work with native graph structures, even if they encounter a complex problem, such as treating dynamic graphs as static graphs. However, in some scenarios, it may not be necessary to use advanced methods. For instance, methods that target complex graph structures may result in an unaffordable computing cost.

2.1.1 Node Perspective

A. Homophily Graph vs. Heterophily Graph

Homophily refers to the fact that connected nodes tend to belong to the same class or have similar characteristics. There are many types of network relationships that are found to be homophilous [1], for example, social network and academic network. Tang et al. [51] investigate the trust prediction problem with the homophily effect and gain a deep understanding of the role of homophily in trust prediction. Kossinets and Watts [52] investigate

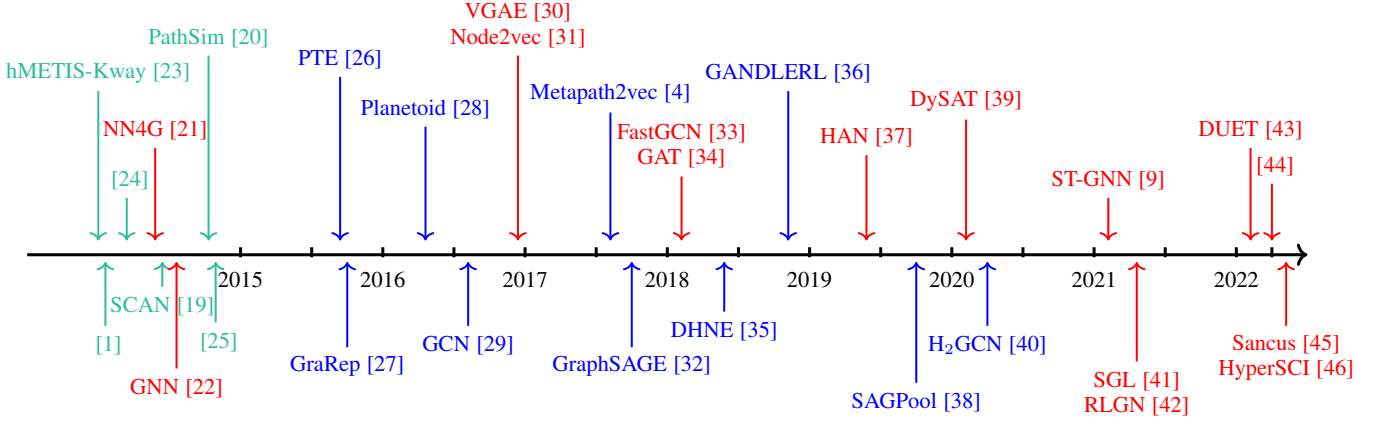


Fig. 2: Chronological overview of graph learning methods. Methods in green, blue and red are graph mining methods, graph embedding methods and graph neural network methods, respectively.

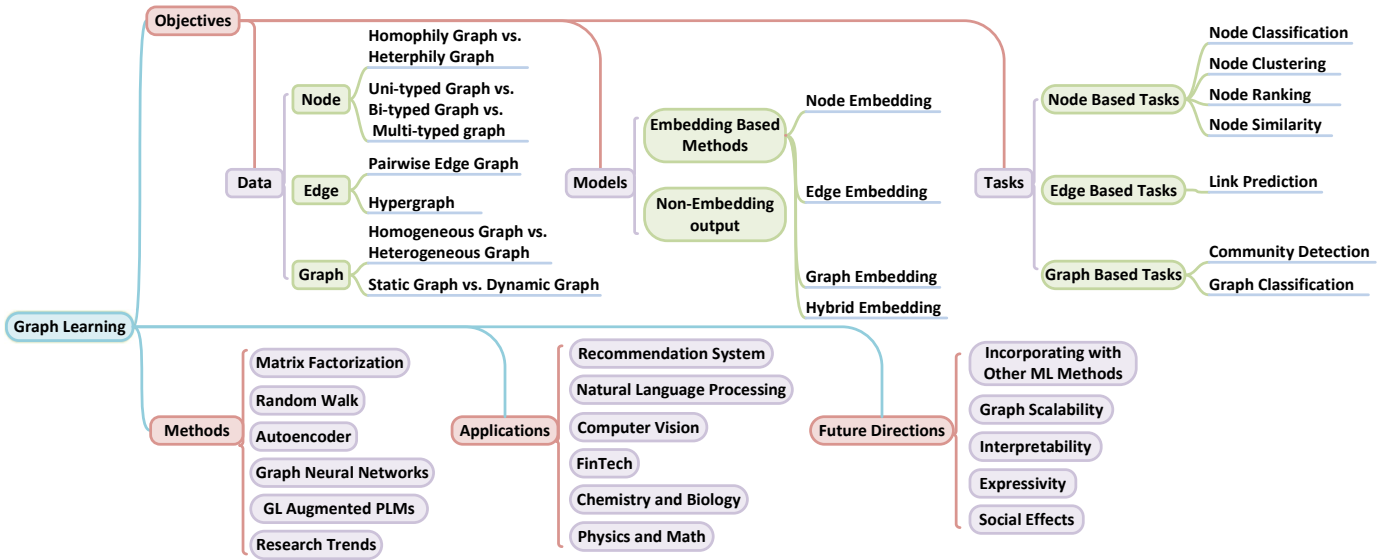


Fig. 3: A taxonomy of graph learning by Objectives, Methods, Applications and Future Directions.

the origins of homophily in a large university community. They conclude that the dynamic interplay of choice homophily can amplify even a modest preference for similar others, producing significant patterns of observed homophily.

In the real world, there are also settings where “opposites attract”, leading to heterophily networks. Heterophily means that the connected nodes may come from different categories or have different characteristics, for example, heterosexual dating networks and ecological food webs. Lazarsfeld and Merton [53] define heterophily as “the mirror opposite of homophily”. However, heterophily and homophily are not opposite, but complementary.

Most of the existing models are only applicable to homophily graphs. However, the graph structure in the real world usually shows a mixture of homophily and heterophily. There are two main types of approaches to solve the problem of heterophily. One is to design specified models to deal with heterophily graph. For instance, Chanpuriya and Musco [54] propose a new model that can adapt to both homophilous and heterophyllous graph structure. Zhu et al. [40] design H_2GCN , that can effectively accommodate heterophily and homophily. And the other way is to transfer heterophily graphs into homophily graphs. For instance,

Suresh et al. [55] transform the input graph into a computation graph, which has an enhanced level of assortativity. Moreover, they find it crucial to adaptively choose between structure and proximity when graphs have diverse mixing patterns.

B. Uni-typed Graph vs. Bi-typed Graph vs. Multi-typed Graph

Definition 1. Uni-typed graph & Bi-typed graph & Multi-typed graph A uni-typed graph can be defined as $\mathbf{G} = (\mathcal{V}, \mathcal{E})$. Here, \mathcal{V} denotes the set of nodes and \mathcal{E} denotes the set of edges. $\mathcal{V} = \{v_1, v_2, \dots, v_N\}$ and $\mathcal{E} = \{e_1, e_2, \dots, e_E\}$. Node type mapping function $\Psi(v_i) \in \mathcal{T}^v$. Edge type mapping function $\psi(e_j) \in \mathcal{T}^e$. $|\mathcal{T}^v| = 1$, $|\mathcal{T}^e| \in \mathbb{R}$. For a bi-typed graph, the difference is that $|\mathcal{T}^v| = 2$. For a multi-typed graph, the difference is that $|\mathcal{T}^v| > 2$.

According to the number of node types in graphs (see Definition 1), we can divide them into three types (i.e., uni-typed graph, bi-typed graph and multi-typed graph).

There exists only one type of node in uni-typed graphs. Page et al. [56] describe PageRank, a method rating web pages objectively and mechanically, which effectively measures people’s interest

and attention to web pages. Fortunato et al. [57] provide a comprehensive overview of community detection, from the definition of the main elements of the problem to the introduction of most development methods.

Bi-typed graphs denote graphs with two types of nodes, including bipartite graph and bi-typed multi-relational heterogeneous graph (BMHG), which are non-trivial in the real world. There are intra-type relations in BMHG, but not in a bipartite graph. Li et al. [58] study hierarchical representation learning of bipartite graphs. Previous methods fail to model BMHG efficiently as a result of ignoring the critical difference between the bi-typed nodes. Therefore, Zhao et al. [59] propose DHAN with intra-type and inter-type attention-based encoder under a hierarchical mechanism to model BMHG. Zhao et al. [60] construct a more comprehensive Market Knowledge Graph which contains bi-typed entities.

A multi-typed graph is a graph with three or more node types, which can be seen as subset of heterogeneous information networks (HINs). Hu et al. [5] present HGT for modeling web-scale heterogeneous graphs. Meta-paths are widely used in modeling multi-typed graphs due to their flexibility and interpretability to capture the complex semantic relation among objects. For instance, Dong et al. [4] develop two scalable representation learning models, named metapath2vec and metapath2vec++. Besides, automatically discovering meta-paths can mitigate the requirement of expertise [61].

2.1.2 Edge Perspective

A. Weighted Graph vs. Unweighted Graph

Graphs can be categorized into weighted and unweighted graphs based on whether the weights of their edges are equal.

Graphs with equal weights are called unweighted graphs, which are common in social networks. Previous methods have utilized graph distance measures [62] and network clustering [19] to model them. For instance, Xu et al. [19] propose Structural Clustering Algorithm for Networks, which could identify and isolate two types of vertices that play special roles - vertices that bridge clusters (hubs) and vertices that are marginally connected to clusters (outliers) based on graph structural similarity measure.

Edges are also assigned different weights, such as closeness extent in social networks and rating in e-commerce networks. To deal with the weighted graph, Umeyama [63] discusses an eigen decompositions of the adjacency matrices for weighted graph matching problem. In addition, some methods are proposed considering simplification [64] or compression [65].

B. Directed Graph vs. Undirected Graph

Undirected graphs refer to graphs that there always exist two symmetrical links for any types of edges, which are not unusual in community detection [66], natural language processing [67], etc.

Unlike undirected graphs, directed graphs describe asymmetric relationships between nodes, making them more versatile and applicable in various domains. For instance, Shi et al. [68] represent the skeleton data as a directed acyclic graph based on the kinematic dependency between the joints and bones in the natural human body, which can not be solved with an undirected graph.

Definition 2. Homogeneous Hypergraph. A homogeneous hypergraph can be defined as $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{T})$. Here, $v \in \mathcal{V}$ denotes the nodes. $e \in \mathcal{E}$ denotes the hyperedge. \mathcal{T} denotes hyperedge type set, and $|\mathcal{T}| = 1$ here. The relationship between nodes can be

represented by an incidence matrix $\mathbf{H} \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{E}|}$ with elements defined as:

$$\mathbf{H}(v, e) = \begin{cases} 1, & \text{if } v \in e \\ 0, & \text{otherwise.} \end{cases} \quad (1)$$

Definition 3. Heterogeneous Hypergraph. A heterogeneous hypergraph can be defined as $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{T})$. Here, \mathcal{V} denotes the set of nodes. $\mathcal{E} = \{e_1, e_2, \dots, e_E\}$ denotes hyperedge set. $\mathcal{T} = \{\Omega_1, \Omega_2, \dots, \Omega_M\}$ denotes hyperedge type set, and $|\mathcal{T}| > 1$ here. Hyperedge type map function $\psi: \psi(e_i) \in \mathcal{T}$.

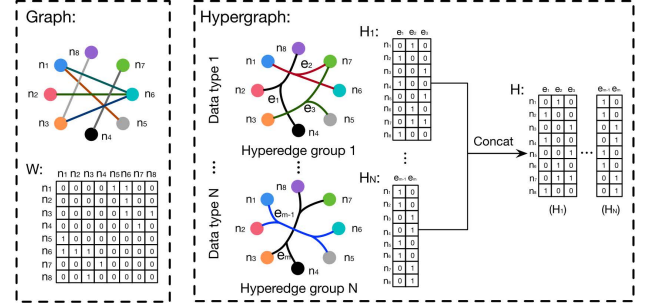


Fig. 4: The comparison between graph and hypergraph [69]

C. Homogeneous Hypergraph vs. Heterogeneous Hypergraph

Hypergraphs refer to the graph structure in which each edge can connect many nodes. Hypergraph theory was first proposed in [70], which mainly focused on hypergraph segmentation and the generalization of some traditional graph theories on hypergraphs. Afterwards, the research on hypergraphs has expanded to include a wider range of tasks and methods. For instance, Sun et al. [71] propose a hypergraph spectral learning formulation for multi-label classification, utilizing hypergraphs to leverage the correlation information among different labels. Nowadays, deep learning methods are being introduced for hypergraph representation [69].

Previous works mostly concentrate on homogeneous hypergraphs (see Definition 2), ignoring the heterogeneity in hypergraphs (i.e., different types of hyperedges). Recent works propose to model heterogeneous hypergraph (see Definition 3). For instance, Sun et al. [72] first project the heterogeneous hypergraph into a series of snapshots. They then utilize a wavelet basis with an efficient polynomial approximation to conduct localized hypergraph convolution. Heterogeneous hypergraphs also have various applications, such as studying contagions [73].

2.1.3 Graph Perspective

A. Homogeneous Graph vs. Heterogeneous Graph

Definition 4. Homogeneous graph & Heterogeneous graph A homogeneous graph can be defined as $\mathcal{G} = (\mathcal{V}, \mathcal{E})$. Here, \mathcal{V} denotes the set of nodes and \mathcal{E} denotes the set of edges. $\mathcal{V} = \{v_1, v_2, \dots, v_N\}$ and $\mathcal{E} = \{e_1, e_2, \dots, e_E\}$. Node type mapping function $\Psi(v_i) \in \mathcal{T}^v$. Edge type mapping function $\psi(e_j) \in \mathcal{T}^e$. $|\mathcal{T}^v| = 1$, $|\mathcal{T}^e| = 1$. For a heterogeneous graph, the difference is that $|\mathcal{T}^v| + |\mathcal{T}^e| > 1$.

We formally define the homogeneous graph in Definition 4, in which there are only one node type and one relationship type. Homogeneous graphs are most basic and widely studied graph type. Inspired by Graph Convolutional Networks (GCN) [29], Hamilton et al. [32] present GraphSAGE, a scalable approach for semi-supervised learning on graph-structured data. Velivckovic et

al. [34] propose Graph Attention Networks (GAT), which assigns different weights to neighbors' information.

But most of the real-world graphs can be naturally modeled as heterogeneous graphs, as Definition 4 shows, with more than one node type or relationship type in a graph. Multiple types of nodes, edges and rich attribute information bring great challenges to model heterogeneous graphs. Based on the way to utilize heterogeneous edges, we divide current methods into two categories: 1. *Link-based heterogeneous graph embedding*: Chen et al. [74] treat each link type as a relation and use a relational-specific matrix to transform nodes into different metric spaces. 2. *Path-based heterogeneous network representation*: Meta-path is a path that contains a sequence of relations, which are defined on different types of objects. Wang et al. [37] propose to utilize hierarchical attention mechanism to model path-based heterogeneous information, which becomes popular nowadays.

B. Static Graph vs. Dynamic Graph

Definition 5. Discrete-time dynamic graph. A discrete-time dynamic graph (DTDG) can be defined as a set: $\{\mathcal{G}^1, \mathcal{G}^2, \dots, \mathcal{G}^T\}$ in which $\mathcal{G}^t = \{\mathcal{V}^t, \mathcal{E}^t\}$, \mathcal{G}^t is a snapshot in time t , \mathcal{V}^t is the node set in \mathcal{G}^t and the \mathcal{E}^t is the edge set in \mathcal{G}^t .

Definition 6. Continuous-time dynamic graph. A continuous-time dynamic graph (CTDG) can be defined as a set of event quadruples $\{q^1, q^2, \dots, q^N\}$, where $q^n = (u_n, v_n, r_n, t_n)$ means that node u_n links to node v_n with relation r_n in time t_n . Each time t_n is only assigned with corresponding event quadruple q_n .

Definition 7. Dynamic hypergraph. A Dynamic hypergraph can be defined as $\mathcal{G} = (\mathcal{V}, \mathcal{E}^t, \mathcal{T})$. Here, \mathcal{V} denotes the set of nodes. $\mathcal{E}^t = \{e_1, e_2, \dots, e_E\}$ denotes hyperedge set. $\mathcal{T} = \{\Omega_1, \Omega_2, \dots, \Omega_M\}$ denotes hyperedge type set. Hyperedge type map function $\psi: \psi(e) \in \mathcal{T}$, Hyperedge time map function $\psi: \psi(e_i) \in \mathbf{T} = \{t_1, t_2, \dots, t_T\}$.

Static graphs do not show any state changes over time. Research related to static graphs can be divided into two categories based on the convolution method used: 1. *Spectral-based Graph Convolutional Networks*: The core idea of spectral convolution is to replace the convolution kernel in the spectral domain with the diagonal matrix. Essentially, GCN is a localized first-order approximation of spectral graph convolution [29]. 2. *Spatial-based Graph Convolutional Networks*: The space-based approach defines graph convolution based on the spatial relationships of nodes. Spatial-based Graph Convolutional Networks essentially propagates node information along the edges. For example, Niepert et al. [75] propose a framework for learning convolutional neural networks for arbitrary graphs and a general approach to extract locally connected regions from graphs.

Dynamic graphs are more complex as they contain critical time information (i.e., links and nodes may appear and disappear over time). According to the time granularity, dynamic graphs can be divided into discrete (DTDG, see Definition 5) and continuous dynamic graphs (CTDG, see Definition 6).

Discrete dynamic graphs are often represented by multiple network snapshots taken at different time intervals. In this context, we can identify two types of discrete dynamic graph neural networks (DGNN) for DTDG. 1. *Stacked DGNNs* model each snapshot with a GNN, and then stack the outputs of previous GNNs into a time series model. For example, Sankar et al. [39] propose DySAT, which computes node representations through joint self-attention along the two dimensions (i.e., structural neighborhood and tem-

poral dynamics). Structural Self-Attention adopt similar operation as GAT [34] to aggregate neighbors' information. Temporal Self-Attention is designed to capture the patterns of time changes in the motion graph as follows:

$$Z_v = \beta_v (X_v W_v), \beta_v^{ij} = \frac{\exp(e_v^{ij})}{\sum_{k=1}^T \exp(e_v^{ik})},$$

$$e_v^{ij} = \frac{((X_v W_q)(X_v W_k)^T)_{ij}}{\sqrt{F^z}} + M_{ij}, \quad (2)$$

where $\beta_v \in \mathbb{R}^{T \times T}$ is the attention weight matrix obtained by the multiplicative attention function and $M \in \mathbb{R}^{T \times T}$ is a mask matrix with each entry $M_{ij} \in \{-\infty, 0\}$ to enforce the autoregressive property. In the latest study [76], researchers investigate how to model the evolutionary and multi-scale interactions of time series. 2. *Integrated DGNNs* splice the GNN and the time series model into one layer to form the encoder. To solve the problem of frequent change of the node set, Pareja et al. [77] propose EvolveGCN, which adapts the GCN model along the temporal dimension without resorting to node embeddings.

In fact, DTDG can be considered as a simplified case of CTDG, because we can always transform a CTDG with fine grain into graph snapshots with coarse-grain. Currently, there are three main CTDG methods available for continuous modeling. (1) *RNN-based methods* maintain node embeddings by RNN-based architectures. For example, DyGNN [78] updates node information by capturing the sequential information of edges (interactions), the time intervals between edges and information propagation coherently. DyGNN consists of two components: the update component and the propagation component. Both components include an interact unit, an update unit, and a merge unit, but with slight differences. The update component updates the interaction information of the involved nodes, aiming to capture the direct influence of an interaction. Afterwards, the propagation component propagates interaction information to more related nodes, thus capturing indirect influence. The update unit is a LSTM-style operation, considering weight decay of time. (2) *Random process methods* can also be parameterized by neural networks. For example, Trivedi et al. [79] propose a framework for dynamic graphs that posits representation learning as a latent mediation process bridging two observed processes (i.e., dynamics of the network (realized as topological evolution) and dynamics on the network (realized as activities between nodes)). (3) *Time encoding methods* represent time information as a vector. This is similar to position embedding in language models [80]. Earlier works learned positional embedding to capture the absolute position of nodes or edges. Current research mostly uses sinusoidal position encoding to encode relative time distance of nodes [5].

Moreover, dynamic hypergraphs (see Definition 7) have also garnered significant attention. For instance, Zhang et al. [81] propose the first dynamic hypergraph structure learning method, aiming to simultaneously optimize the label projection matrix (a common task in hypergraph learning) and the hypergraph structure itself. The objective function for dynamic hypergraph structure learning is a dual optimization problem as following:

$$\begin{aligned}
\arg \min_{\mathbf{F}, 0 \preceq \mathbf{H} \preceq \mathbf{I}} \mathcal{Q}(\mathbf{F}, \mathbf{H}) &= \Psi(\mathbf{F}, \mathbf{H}) + \beta \Omega(\mathbf{H}) + \lambda \mathcal{R}_{\text{emp}}(\mathbf{F}) \\
&= \text{tr} \left(\left(\mathbf{I} - \mathbf{D}_v^{-\frac{1}{2}} \mathbf{H} \mathbf{W} \mathbf{D}_e^{-1} \mathbf{H}^T \mathbf{D}_v^{-\frac{1}{2}} \right) \right. \\
&\quad \left. \left(\mathbf{F} \mathbf{F}^T + \beta \mathbf{X} \mathbf{X}^T \right) \right) + \lambda \|\mathbf{F} - \mathbf{Y}\|_F^2, \quad (3)
\end{aligned}$$

where β and λ are parameters to balance different components in the objective function. $\Psi(\mathbf{F}, \mathbf{H})$ is a commonly used hypergraph regularizer for the label projection matrix \mathbf{F} , which should be smooth on the hypergraph structure \mathbf{H} . $\Omega(\mathbf{H})$ is the constraint of \mathbf{H} on the input features \mathbf{X} . $\mathcal{R}_{\text{emp}}(\mathbf{F})$ is the empirical loss.

One of the drawback of existing method is that the hypergraph structure is fixed during the training, which is not flexible. Therefore, Jiang et al. [82] propose DHGNN, which is composed of the stacked layers of two modules: dynamic hypergraph construction and hypergraph convolution. Zhu et al. [83] propose a new feature selection method by dynamically constructing a hypergraph Laplacian matrix in the framework of sparse feature selection.

2.2 Models

In this subsection, we generally divide the output into two typical categories: none-embedding outputs and embedding outputs. The former refers to task-specific output, such as node similarity [84], node correspondences [85], and local and global consistency [2], while the latter includes representations of nodes, edges, graphs, and the hybrid of these.

2.2.1 Non-Embedding Output

Before the emergence of graph representation learning, many excellent data mining methods were proposed to model various networks. Jeh and Widom [84] adopt a naive method to output the similarity of the structural context. Koutra et al. [85] manage to find the node correspondences between two given graphs for aligning bipartite graphs. Sun et al. [20] propose PathSim for similarity search in heterogeneous networks. Intuitively, two similar peer objects should share comparable visibility and the relation between them should be symmetric. Therefore, the meta-path-based similarity measure, called PathSim, is confined to only symmetric meta-paths. Given a symmetric meta-path P , PathSim between two objects of the same type, x and y , is achieved by the following equation:

$$s(x, y) = \frac{2 \times |\{p_{x \rightsquigarrow y} : p_{x \rightsquigarrow y} \in \mathcal{P}\}|}{|\{p_{x \rightsquigarrow x} : p_{x \rightsquigarrow x} \in \mathcal{P}\}| + |\{p_{y \rightsquigarrow y} : p_{y \rightsquigarrow y} \in \mathcal{P}\}|}, \quad (4)$$

where $p_{x \rightsquigarrow y}$ denotes a path instance between x and y , and $p_{x \rightsquigarrow x}$.

2.2.2 Embedding-based Methods

In light of the popularity of representation learning, researchers are increasingly focused on learning semantic embeddings in graphs and applying them to various downstream tasks. In the following subsections, we will introduce four types of outputs of graph representation learning: node embedding, edge embedding, graph embedding, and hybrid embedding.

A. Node Embedding

Node embedding is one of the most fundamental outputs in graph representation learning, with the goal of capturing nodes' semantic and graph structure information. Node embedding can be applied to most structural scenarios, such as social networks [86] and academic networks [87], and even traditional non-structure scenarios like document networks [26], chemistry [18], and computer vision [88]. Anchor links refer to links between the same users across different social networks. To offer a robust method for anchor links prediction, Man et al. [89] employ node embedding with awareness of observed

anchor links as information to capture major and specific structural regularities, and then learn a stable cross-network.

Despite previous works that focused on structural scenarios, node embeddings can also be applied to non-structural scenarios. For example, in a document network, a node could be a word, sentence, paragraph, or document, each carrying different semantic information. To address the gap where most text embedding methods cannot handle labeled information, Tang et al. [26] represent both the labeled information and word information into a heterogeneous text network. They construct three bipartite networks: word-word, word-document, and word-label networks to learn the embeddings, and then minimize the sum of their objective functions. For example, to embed the word-word network, they use the following objective function:

$$O_{ww} = - \sum_{(i,j) \in E_{ww}} w_{ij} \log p(v_i | v_j), \quad (5)$$

where $p(v_i | v_j)$ denotes the conditional probability of vertex v_i in set \mathcal{V}_A given vertex v_j in set \mathcal{V}_B . The objective functions for the other two networks are similar.

Different from the previously mentioned works, many studies focus on attributed networks, where nodes or edges contain attribute information. Park et al. [90] propose to jointly integrate node embeddings from multiplex networks by minimizing the disagreements among the specific node embeddings and discriminating true samples, regardless of their relation types.

B. Edge Embedding

In certain tasks, we may be interested in the features of edges, such as link classification [91], which requires obtaining edge embedding. We can categorize the research on edge embedding into two aspects based on the data types: HINs and Knowledge Bases (KB).

Research on edge embeddings related to HINs typically focuses on capturing path-based information. For example, Shi et al. [92] employ weighted meta-path concepts to predict weights that represent user preferences on paths for personalized recommendations. Zhou et al. [36] propose a novel edge representation learning framework that combines generative adversarial network-based multi-label classification with density-adaptive local edge representation learning to produce high-quality, low-dimensional edge embeddings. They propose to learn edge homophily by making edges with common vertices have similar representations and vice versa, as following:

$$\begin{aligned}
\mathcal{L}_{\text{Prox}} &= \omega_2 \sum_{x_s, x_t \in E, x_s \wedge x_t \neq \emptyset} \|\mathbf{y}_s - \mathbf{y}_t\|_2^2 + \\
&\quad (1 - \omega_2) \sum_{x_s, x_t \in E, x_s \wedge x_t = \emptyset} \max \{0, m - \|\mathbf{y}_s - \mathbf{y}_t\|_2^2\}, \quad (6)
\end{aligned}$$

where \mathbf{x}_s and \mathbf{x}_t denote edges.

Research on KBs is also an important aspect of edge embedding research. Toutanova et al. [93] propose the first exact dynamic programming algorithm to efficiently incorporate all relation paths of bounded length for KB completion.

C. Graph Embedding

Graph embedding, rather than substructure embedding, represents the structural properties of an entire graph in a latent vector space. Graph pooling is a widely used technique for learning graph embeddings, and there are two main methods: graph coarsening and node selection. Graph coarsening involves clustering nodes first and then synthesizing a super node to achieve the pooling effect. Ying et al. [94] propose a graph pooling module that can generate hierarchical representations of graphs. Node selection involves selecting some important nodes to replace the original graph. Based on self-attention, Lee et al. [38] utilize the node selection pooling method to learn hierarchical representations using relatively few parameters. They first obtain self-attention scores using graph convolution as follow: $\text{idx} = \text{top} - \text{rank}(Z, \lceil kN \rceil)$, where $k \in (0, 1]$ denotes the pooling ratio. idx is an indexing operation and Z_{mask} is the feature attention mask. The top $\lceil kN \rceil$ nodes are selected based on the value of Z that represents the self-attention score, and Z_{mask} is equal to Z_{idx} . An input graph is processed by the following operation:

$X' = X_{\text{idx},:}$, $X_{\text{out}} = X' \odot Z_{\text{mask}}$, where $X_{\text{idx},:}$ is the row-wise indexed feature matrix.

In addition to graph pooling, other research focuses on direct graph representation learning methods. For example, Pan et al. [95] propose an adversarial graph embedding framework that encodes a graph into a compact representation.

D. Hybrid Embedding

Hybrid embedding involves combining different types of embeddings, which can often lead to better model performance compared to using a single type of embedding.

The KB typically stores information as $\langle h, r, t \rangle$, making the hybrid of substructure embedding very common in KB. Unlike traditional methods that rely on random paths between fixed entity pairs, Das et al. [96] learn to navigate the graph conditioned on the input query, in order to find predictive paths for addressing tasks where only one entity is known but the relation is not.

The combination of node embedding and graph embedding can bring mutual benefits to machine learning tasks. Hassani and Khasahmadi [97] learn node and graph-level representations by contrasting structural views of graphs.

An increasing number of studies have started to incorporate all three types of embedding, consisting of node embedding, edge embedding, and graph embedding. For instance, Cao et al. [98] propose a bipartite graph embedding approach to address the challenge of preserving the global properties of a bipartite graph. They use a noise-contrastive loss to optimize embeddings as following:

$$\mathcal{L}_m = -\frac{1}{|E| + |\tilde{E}|} \left(\sum_{i=1}^{|\tilde{E}|} \mathbb{E}_G \left[\log \mathcal{D} \left(\mathbf{g}_{(u,v)_i}^h, \mathbf{g} \right) \right] + \sum_{i=1}^{|\tilde{E}|} \mathbb{E}_{\tilde{G}} \left[\log \left(1 - \mathcal{D} \left(\tilde{\mathbf{g}}_{(u,v)_i}^h, \mathbf{g} \right) \right) \right] \right), \quad (7)$$

where \mathcal{D} aims to score local-global representation: $\mathcal{D}(\mathbf{g}_{(u,v)_i}^h, \mathbf{g}) = \sigma \left((\mathbf{g}_{(u,v)_i}^h)^T W_b \mathbf{g} \right)$. \mathbf{g} and $\mathbf{g}_{(u,v)_i}^h$ denote the global representation and local input, respectively.

2.3 Tasks

In this subsection, we summarize previous works based on their target tasks. Different tasks have different requirements for these methods, which results in significant differences between models.

2.3.1 Node-based Tasks

A. Node Classification and Clustering

Node classification and clustering are basic tasks in graph learning and occur in specific scenarios. From the perspective of graph representation learning, they are often seen as downstream tasks in experiments to verify the effect of the model [29], [90]. Some research enhances representation learning with the help of graph structure [27]. Huang et al. [99] utilize label information to help the representation learning of attributed network embedding. In addition, Sun et al. [72] learn node embedding by transforming heterogeneous hypergraphs into a series of snapshots and applying localized hypergraph convolution on them.

B. Node Ranking

Node ranking is a vital part of graph analysis, with great significance for some areas such as virus marketing. A lot of efficient methods were proposed for node ranking methods in the past. The famous PageRank algorithm [56] is based on web page citation ranking and has a promising effect on the Google search engine. To study the fine-grained GNN fairness problem, Dong et al. [100] propose a novel node ranking framework to calculate the individual fairness by ranking with the similarity between node instances. Besides, node ranking is widely used to assist other tasks. For example, Gilbert and Levchenko [101] take vertex ranking as an essential strategy for graph compression.

C. Node Similarity Measurement

Node similarity refers to measuring the similarity between different nodes on the graph. It has always been essential research in node tasks and has widely occurred in fields like information retrieval. Jeh and Widom [84] measure the similarity of the structural context according to the relationships between nodes, which represent the items in the text. Zhang et al. [102] propose a distributed framework to capture the graph structure correlation and node attribute similarity on the graph, integrating node attribute similarity into the original graph to form a hybrid graph, and then utilizing a method of random walk with restart for node similarity search. Saxena et al. [103] perform link prediction by capturing node similarity and network structure for efficient embedding.

2.3.2 Edge-based Tasks

Link Prediction. Link prediction aims to discover hidden connections that may exist between nodes, which is important and exists widely in real scenarios, such as medicine and biology [94]. Over the years, researchers have proposed many improved methods for link prediction. For example, Clauset et al. [104] propose a method for leveraging network data to infer network hierarchies, reproducing the topological properties of networks and predicting the missing links based on the properties of network hierarchies. Zhu et al. [105] incorporate the Bellman-Ford algorithm into the GNNs framework to assist the link prediction task. Among various scenarios, social networks is one of the best known one for link prediction's application. Xu et al. [106] define two different types of links and learn two representations for each node, assisting link prediction by mining different semantic information of links in social networks.

2.3.3 Graph-based Tasks

A. Community Detection Community detection is a research area that focuses on identifying locally densely connected subgraphs by clustering nodes based on one or more features. This field has been extensively studied since Newman proposed the concept of modularity [66]. One approach to modeling dynamic community structure is the classical stochastic block model-based optimization approach proposed by Anagnostopoulos et al. [107]. Another approach, proposed by Chen et al. [108], involves modifying GNNs by adding non-traceback operators, which allow them to exploit edge adjacency information for community detection. GNNs are also useful for detecting overlapping communities due to their ability to handle complex networks [109]. This is particularly important because communities in real-world graphs are often not disjointed.

B. Graph Classification Graph classification is a technique that aggregates all node data into a vector representing the entire graph structure for classification, similar to node classification. To preserve the structural information of the graph, pooling is a common approach. Hamilton et al. [32] apply an elementwise max-pooling operation to aggregate information across neighbors. Ying et al. [94] introduce a differentiable pooling method for GNNs to extract complex, hierarchical structures of real-world graphs. For multitask graph classification tasks, Pan et al. [110] propose an algorithm that classifies each subgraph feature into one of three categories shared by specific tasks.

3 METHODS

In this section, we divide methods into two major types: traditional models and graph neural networks. Traditional models can be further divided into three types: matrix factorization, random walk-based, and autoencoder-based models. We first survey traditional models, some of which are still active or combined with GNNs nowadays, and provide many inspirations for current models. GNNs usually exhibit higher expressivity and better performance compared to traditional models. We conclude by discussing two aspects of GNNs.

3.1 Matrix Factorization

Factorization-based algorithms [27], [111], [112] obtain node embeddings by decomposing a matrix which measures the probabilities that nodes tend to connect. The matrix can take various forms, such as the node adjacency matrix, Laplace matrix, node transfer probability matrix, Katz similarity matrix, and others. For instance, Cao et al. propose GraRep [27] to learn node representations in weighted graphs. They propose to integrate global structural information, which contains long distance relationship and distinct connections between nodes. Inspired by skip-gram model [113], they construct probability transition matrix, which finally measures the relationship between vertices. Besides, implementing factorization effectively and efficiently on those matrices is crucial. Ahmed et al. [111] propose GF, the first method to obtain a graph embedding in $O(|E|)$ time. GF factorizes the adjacency matrix by minimizing the following loss function:

$$\phi(Y, \lambda) = \frac{1}{2} \sum_{(i,j) \in E} (W_{ij} - \langle Y_i, Y_j \rangle)^2 + \frac{\lambda}{2} \sum_i \|Y_i\|^2, \quad (8)$$

where W_{ij} is the edge weight between nodes (i, j) , which can be replaced as the inner product of the two nodes. Y_i, Y_j are the representation of node i and node j respectively, λ is the regular coefficient. Ou et al. [112] propose HOPE, which can be seen as an improvement on GF. The key idea of HOPE is to preserve asymmetric transitivity, which captures structure information of graphs. The approach first propose a class of high-order proximity measurements and then utilizes a time-efficient generalized SVD to solve them.

3.2 Random Walks

The random walk-based approach involves sampling a graph with a large number of paths. These paths indicate the context of the connected vertices and are obtained by starting the walk from randomly selected initial nodes. Once the paths are built, a series of probabilistic models can be executed on these randomly sampled paths to learn the node representation. We can divide the methods based on the random walk approach into two categories: structure-based random walks and auxiliary information-based random walks.

3.2.1 Structure-Based Random Walks

In practical applications, many networks only have structural information and lack vertex attribute information. Identifying graph structure information, such as important nodes and invisible links, can be challenging without vertex information. One efficient way to solve this problem is through structure-based random walks.

Inspired by Word2vec [114], Perozzi et al. [115] propose DeepWalk as a means of capturing the connection relationships between nodes in a graph data structure. DeepWalk consists of two modules: random sampling on graphs to generate node sequences and training a skip-gram model to obtain node embeddings. To capture the diversity of connection patterns in the network, Grover et al. [31] propose node2vec, which generates neighbor sequences by sampling nodes with different probabilities. Specifically, it allows the sample strategy to be biased towards depth first search or breadth first search. Modern random walk algorithms are typically equipped with a restart strategy. For example, Zhang et al. [116] utilize random walk with restart strategy to sample heterogeneous neighbors.

3.2.2 Auxiliary Information-based Random Walks

Auxiliary information-based random walks is proposed to take advantage of the attribute information of nodes. Yang et al. [28] propose a semi-supervised graph learning framework for nodes with attribute information. They first sample pairs of instances and context using random walk, and then formulate a loss function based on them. The context aims to jointly model graph structure information and label information. Since the predicted label depends on the nodes' input attribute, the sampled distribution contains both graph structure information and node attribute information.

3.3 Autoencoder-based methods

Graph Autoencoders (GAEs) use an encoder to project the original graph into low-dimensional representations. These representations are then fed into a decoder to reconstruct the graph. By minimizing the reconstruction loss, the learned representations contain topology information and can be used for downstream tasks. For example, Cao et al. [117] use stacked denoising autoencoders to encode and decode positive point-wise mutual information (PPMI) matrices through multilayer perceptrons. In contrast to previous works, Hamilton et al. [32] encode node features with two graph convolutional layers. Velickovic et al. [118] drive local network embeddings to capture global structural information by maximizing local mutual information. Instead of simply reconstructing the graph adjacency matrix, which may lead to overfitting due to the capacity of the autoencoder, Kipf et al. [30] propose VGAE, a variational version of VAE, to learn the data distribution. VGAE assumes that the empirical distribution $q(Z|X, A)$ should be as close as possible to the prior distribution $p(Z)$.

Using multiple graphs, GAE is able to learn the distribution of graph generations by encoding the graph as a hidden representation and decoding the graph structure from a given hidden representation. Simonovsky and Komodakis [119] propose GraphVAE, which models the existence of nodes and edges as independent random variables. By assuming the posterior distribution $q_\phi(z|G)$ defined by an encoder and the generative distribution $p_\theta(G|z)$ defined by a decoder, GraphVAE optimizes the variational lower bound.

$$L(\phi, \theta; G) = E_{q_\phi(z|G)} [-\log p_\theta(G | \mathbf{z})] + KL[q_\phi(\mathbf{z} | G) \| p(\mathbf{z})], \quad (9)$$

where $p(\mathbf{z})$ follows a Gaussian prior, ϕ and θ are learnable parameters. With a ConvGNN as the encoder and a simple multi-layer perception as the decoder, GraphVAE outputs a generated graph with its adjacency matrix, node attributes, and edge attributes.

3.4 Graph Neural Networks

Graph Neural Networks (GNNs) utilize deep neural networks to model message-passing processes on graphs, achieving excellent performance in various tasks and scenarios. Current methods can be divided into two categories: learning and inference. The former covers research related to the extent that GNNs use supervising signals. The latter demonstrates previous works considering whether GNNs can be used to infer unseen graphs.

3.4.1 Learning Perspective

A. Supervised Methods Most GNNs are trained using supervised signals, including the labels of nodes [5], [120], edges [36], [121], and graphs [110], [122], which denote the properties of graphs. Similar to traditional supervised learning, supervised graph learning also utilizes cross-entropy and mean squared error (MSE) for classification and regression tasks. For example, Peng et al. [122] propose a motif-based attentional graph convolution neural network to classify chemical compounds. Zhao et al. [120] construct an enterprise knowledge graph where nodes represent companies and persons, and optimize the proposed model with cross-entropy loss: $\mathcal{L} = -\sum_{i \in \mathcal{Y}_L} y_i \log(\tilde{y}_i)$. The labels indicate the state of the companies, whether they are in bankruptcy or still surviving.

B. Semi-supervised Methods Semi-supervised learning utilizes both labeled and unlabeled data simultaneously, making it suitable for scenarios where only a few labeled samples are available and the rest of the data samples are unlabeled. Hu et al. [123] propose HGAT, a method for semi-supervised short text classification. HGAT leverages limited labeled data and large unlabeled data through information propagation along a graph. The method presents a flexible HINs framework for modeling short texts, which can integrate any type of additional information and capture their relations to address semantic sparsity. Graph-based Semi-Supervised Learning (SSL) aims to transfer the labels of a handful of labeled data to the remaining massive unlabeled data via a graph. Wan et al. [124] propose a novel GCN-based SSL algorithm to enrich the supervision signals by utilizing both data similarities and graph structure. Jiang et al. [125] propose

GLCN, which combines semi-supervised learning method with GCN model to classify tags.

C. Self-supervised Methods

Self-supervised learning methods primarily use auxiliary tasks to extract supervised information from large-scale unsupervised data and train the network using this constructed supervised information. There are four main types of self-supervised methods suitable for graphs. The first type uses node feature similarity clustering to obtain pseudo tags and achieve self-supervised training. For example, M3S [126] leverages the DeepCluster technique, a popular form of self-supervised learning, and designs a corresponding alignment mechanism in the embedding space to refine the Multi-Stage Training Framework. The alignment mechanism aims to transform the categories in clustering to the classes in classification. Specifically, the aligned class is calculated as follow:

$$c^{(l)} = \arg \min_m \|v_l - \mu_m\|^2, \quad (10)$$

where μ_m refers to center of class m in labeled data and v_l is center of cluster l in unlabeled data. The second type constructs a supervision signal based on the correlation within the input data or context connections to achieve self-supervised training. Wu et al. [41] propose SGL, which enhances node representation learning by exploring internal relationships between nodes and building supervisory signals based on internal correlations of input data. Another method involves masking the node features of the center and reconstructing the node features of the center by using the features of its neighbors. The reconstruction error serves as the self-supervised loss function for optimization [127]. Wang et al. [128] propose HeCo, which leverages network schema and meta-path structure as two different views for cross-view contrast learning. HeCo uses a view mask mechanism to extract positive and negative embeddings from both views, enabling cooperative and mutually supervised learning between the two views.

D. Unsupervised Methods

Unsupervised learning involves learning statistical rules or the intrinsic structure of data from unlabeled data, commonly using techniques such as clustering, dimension reduction, and probability estimation. Unsupervised learning on graphs is similar to self-supervised learning on graphs, where models are optimized using cross-entropy loss or contrast loss. Additionally, some models employ alternative methods to improve performance. Kipf et al. [129] propose NRI, which optimizes reconstruction error and Kullback-Leibler divergence during training process. Some models use combinatorial loss functions to optimize unsupervised graph learning. Tang et al. [130] introduce LUFs, which leverages the concept of pseudo-class labels to guide unsupervised learning, and it optimizes the model by:

$$\begin{aligned} \min_{\mathbf{W}} \text{Tr}(\mathbf{W}^\top \mathbf{X} \mathbf{L} \mathbf{X}^\top \mathbf{W}) + \beta \|\mathbf{W}\|_{2,1} \\ + \alpha \text{Tr}(\mathbf{W}^\top \mathbf{X} (\mathbf{I}_n - \mathbf{F} \mathbf{F}^\top) \mathbf{X}^\top \mathbf{W}), \end{aligned} \quad (11)$$

where \mathbf{F} is the weighted social dimension indicator matrix. $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n) \in \mathbb{R}^{m \times n}$ is the conventional representation of node set $\mathbf{u} = \{u_1, u_2, \dots, u_n\}$. The mapping matrix $\mathbf{W} \in \mathbb{R}^{m \times c}$ assigns each data point with a pseudo-class label where c is the number of pseudo-class labels. The pseudo-class label indicator matrix is $\mathbf{Y} = \mathbf{W}^\top \text{diag}(\mathbf{s}) \mathbf{X} \in \mathbb{R}^{c \times n}$.

3.4.2 Inference Perspective

A. Transductive Methods

Definition 8. Transductive GNNs Given a graph $G = (\mathcal{V}, \mathcal{E})$, label information \mathcal{Y} and Transductive Graph Neural Networks (TGNNs). TGNNs' training and testing processes are all performed on \mathcal{G} with $\mathcal{Y}_{\text{train}}, \mathcal{Y}_{\text{test}} \subseteq \mathcal{Y}$ and $\mathcal{Y}_{\text{train}} \cap \mathcal{Y}_{\text{test}} = \emptyset$.

Transductive learning (see Definition 8) involves applying existing knowledge to a given dataset. In the context of TGNNs, this means training the model with both training and test set data, and then evaluating the model's performance on the test set. In other words, transductive learning is the process of using known information to

make predictions on new data [1], [41].

B. Inductive Methods

Definition 9. Inductive GNNs Given Transductive Graph Neural Networks (IGNNs), IGNNs' training and testing are performed on different graphs (i.e., $G_{\text{train}} \cap G_{\text{test}} = \emptyset$).

Inductive learning (see Definition 9) refers to learning when the test set or validation set samples are not used during training (or when the test set and validation sets are not visible during training). The advantage of IGNNs is that they use the information of known nodes to generate embeddings for unknown nodes. GraphSAGE [32] is a representative example of inductive learning on graphs. It is a general inductive framework that computes node representations by sampling neighborhoods of each node and then performing a specific aggregator for information fusion. In this way, the node feature information (e.g., text attributes) efficiently generates node embeddings for previously unseen data [108]. Unlike GraphSAGE [32], Chen et al. [33] propose FastGCN, the model that interprets graph convolutions as integral transforms of embedding functions and samples the nodes in each layer independently. Teru et al. [131] propose GraIL, which reasons over local subgraph structures. This allows it to generalize to unseen entities and graphs after training. Traditional inductive learning approaches such as node2vec [31] can also be used.

There are also works considering **both transductive and inductive learning**. Some of them use different datasets with different learning settings, while others use the same datasets. For example, Velickovic et al. [34] employ a two-layer GAT model on three standard citation network benchmark datasets (Cora, Citeseer, and Pubmed) for transductive learning tasks. However, for inductive learning tasks on graphs, they utilized a three-layer GAT model for the PPI dataset. Yang et al. [28] adopt a different approach to dealing with the problem. Specifically, for each dataset, they divide all instances into three parts: labeled data, unlabeled data, and test data. Inductive methods are trained on the labeled and unlabeled data and tested on the test data. Transductive methods are trained on labeled and unlabeled data, and test data without labels. Although the same datasets are used, in the transductive variant of the method, the class labels are determined by both the learned embeddings and input feature vectors, while in the inductive setting, the embeddings are defined as a parametric function of the feature vectors, so predictions can be made on instances not seen during training.

3.5 GL Augmented Pre-trained Language Models

Pre-trained Language Models (PLMs) are trained on encyclopedic and commonsense corpora, endowing them with great capabilities for various natural language processing (NLP) tasks, such as question answering and sentiment analysis. However, most PLMs lack the ability to perform specific domain tasks [154]. One effective way to solve this problem is to combine PLMs with structured knowledge [155]. Moreover, structured knowledge has shown superiority in enhancing the explainability of PLMs' outputs [156]. In this section, we first demonstrate how graph structure knowledge helps improve vanilla PLMs. Then we show the combination of graph learning and Large Language Models (LLMs).

3.5.1 Vallina Pre-trained Language Models

Vallina Pre-trained Language Models (PLMs) are models based on transformer architecture and trained on a general corpus, which can be used for various downstream tasks with fine-tuning. We introduce the latest representative methods in different tasks where structural knowledge assists in improving the Vallina PLMs, including methods aiming at specific tasks and task-free methods. Vallina PLMs are widely used for the Question Answer (QA) task, but most of them lack the ability to represent latent relationships between concepts. To solve this problem, Zhang et al. [155] propose GREASELM, which fuses the representations from Vallina PLMs and GNNs. Passage re-ranking helps Vallina PLMs retrieve better messages. Previous Vallina PLMs-based methods cannot deal with the vocabulary mismatch problem and

TABLE 2: REPRESENTATIVE WORKS IN TERMS OF CITATIONS

Title	Venue	Year	Citation
Emergence of scaling in random networks [132]	Science	1999	43381
Semi-supervised classification with graph convolutional networks [29]	ICLR	2016	21665
Birds of a feather: Homophily in social networks [1]	Annual Review of Sociology	2001	21563
Community structure in social and biological networks [133]	PNAS	2002	17978
The pagerank citation ranking: Bringing order to the web [56]	WWW	1999	17609
Finding and evaluating community structure in networks [134]	Physical Review E	2004	16206
Community detection in graphs [57]	Physics Reports	2010	11486
Maximizing the spread of influence through a social network [24]	KDD	2003	9642
The link prediction problem for social networks [135]	CIKM	2003	6665
Convolutional neural networks on graphs with fast localized spectral filtering [136]	NeurIPS	2016	6631
Translating Embeddings for Modeling Multi-relational data [137]	NeurIPS	2013	6216
Graph attention networks [34]	ICLR	2017	5627
The graph neural network model [22]	IEEE Transactions on Neural Networks	2008	5368
Finding community structure in networks using the eigenvectors of matrices [138]	Physical review E	2006	5284
Line: Largescale information network embedding [139]	WWW	2015	5135
Neural message passing for quantum chemistry [140]	ICML	2017	5119
Spectral networks and locally connected networks on graphs [141]	ICLR	2013	4501
How powerful are graph neural networks? [142]	ICLR	2018	4239
The emerging field of signal processing on graphs: Extending high-dimensional data analysis to networks and other irregular domains [143]	IEEE Signal Processing Magazine	2013	3632
Graph embedding and extensions: A general framework for dimensionality reduction [144]	TPAMI	2006	3471
Friends and neighbors on the web [145]	Social Networks	2003	3461
Convolutional networks on graphs for learning molecular fingerprints [146]	NeurIPS	2015	3251
Graphs over time: densification laws, shrinking diameters and possible explanations [147]	KDD	2005	3056
Knowledge graph embedding by translating on hyperplanes [148]	AAAI	2014	3030
The dynamics of viral marketing [149]	ACM Transactions on the Web	2007	2981
Graph evolution: Densification and shrinking diameters [150]	TKDD	2007	2979
Social structure from multiple networks. i. blockmodels of roles and positions [151]	American Journal of Sociology	1976	2921
A measure of betweenness centrality based on random walks [152]	Social Networks	2005	2749
Detecting community structure in networks [153]	The European Physical Journal B	2004	2709
Simrank: a measure of structural-context similarity [84]	KDD	2002	2558

lack domain knowledge. Thus, Dong et al. [157] introduce explicit knowledge to Vallina PLMs. They first obtain a reliable knowledge meta-graph from noisy and incomplete knowledge graphs and then utilize the meta-graph and Vallina GLMs as two encoders to get final outputs. Saha et al. [158] find that with limited supervision, Vallina PLMs cannot generate structured outputs that meet graph constraints and are semantically correct. They propose a simple yet effective graph perturbation method and utilize it with Max-Margin and InfoNCE losses, which lead to significant improvements. There are also task-free methods. For instance, Yu et al. [159] propose JAKET, a joint pre-training framework, to leverage both Vallina PLMs and GNNs. The design achieves good performance on several knowledge-aware NLP tasks.

3.5.2 Large Language Models

Unlike vanilla PLMs, Large Language Models (LLMs) are trained on massive datasets and have billions of parameters, such as OPT (175 billion parameters) [160], PaLM 2 [161], and GPT-4 [162]. The huge number of parameters makes LLMs capable of dealing with complex problems and achieving amazing performance on various tasks, including multi-modal tasks. However, using flattened texts as inputs limits LLMs' performance in some scenarios, especially for knowledge-intensive tasks. To overcome this drawback, there are two main ways to improve LLMs, as shown in Figure 5. Additionally, we introduce works on LLMs' abilities in graph reasoning.

A. LLMs as Knowledge Extractor. The first way to use LLMs is as a knowledge extractor for GNNs. For instance, GraphCare [163] focuses on healthcare prediction, a specific scenario that requires medical knowledge. To address this challenge, GraphCare extracts knowledge from both LLMs and external biomedical KGs to generate patient-specific KGs, which are then used for healthcare prediction with GNNs. Shi et al. [156] utilize ChatGPT to extract refined and structured knowledge from raw data, and then feed this knowledge to GCN for text classification. The proposed method also improves the interpretability of the results.

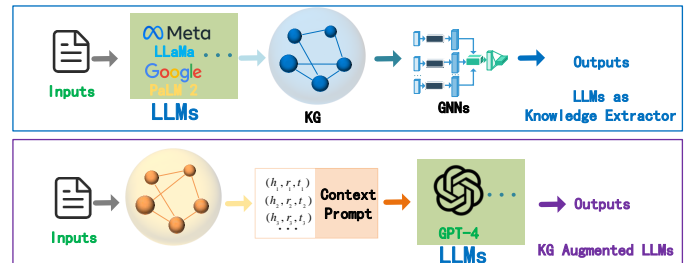


Fig. 5: Current ways to improve LLMs with graphs.

B. KG Augmented LLMs. Another way is to feed LLMs with structured prompts. Due to the limited context window, LLMs suffer from difficulty in understanding thousands of tokens. To address this, Andrus et al. [164] propose extracting an external dynamic KG from the original story text and using it as a prompt to enhance LLMs. Similarly, Bi et al. [165] transform natural language inputs into code-format inputs and use them as schema-aware prompts to improve LLMs' performance. Choudhary and Reddy [166] claim that LLMs lack the ability to deal with complex queries. To address this, they decompose input queries using KGs and convert them into LLM prompts, resulting in a final set of answers. Additionally, Chen et al. [167] propose LMExplainer, which aims to learn the explanation of language models. They use KG and GAT to extract the key decision signals of language models. LMExplainer then uses the input context, model predicted output, trigger sentence, and extracted key components as prompts for LLMs to provide explanations of language models.

C. Graph Reasoning LLMs have performed well on some tasks with structured inputs, such as code generation. However, they exhibit flaws when it comes to graph learning tasks. To address this problem, Jiawei Zhang proposes Graph-ToolFormer, a framework that teaches LLMs to utilize external graph reasoning API tools [168]. Wang et al.

propose NLGraph, a comprehensive benchmark for LLMs’ abilities in solving graph-based problems [169]. They found that LLMs can demonstrate preliminary graph reasoning, but they are vulnerable to graphs with spurious correlations. Zhu et al. [170] test LLMs’ abilities on KG construction and reasoning and concluded that LLMs can address complex problems but lag behind SOTA models. Guo et al. [171] also evaluate the proficiency of LLMs in comprehending graph data.

3.6 Research Trends

We present representative methods, considering their citations in Table 2. From the table, we can draw the conclusion that early works focused on characteristics of graphs, such as homophily [1] and dynamics [39], and proposed various tasks on graphs, such as community detection [133], link prediction [135], and influence maximization [24]. Nowadays, influential works are concerned with how to model and solve those problems effectively [29], [34]. Furthermore, a huge number of works focusing on LLMs have emerged in recent months. Consequently, more attention is being paid to enhancing LLMs with graph learning to improve their reasoning abilities.

We also show active authors in graph learning in Figure 6 and high-frequency words in graph learning in Figure 7. From Figure 6, it is easy to recognize influential individuals with regard to the amount of publications in top conferences. It is even more interesting to find that GNNs have become mainstream in graph learning, with the most important applications being in recommendation systems and language models. On the one hand, this means that those two scenarios are natural to be modeled as graphs, resulting in great performance. On the other hand, other scenarios have not been explored sufficiently, such as Fintech and interpretability, which should receive more attention.



Fig. 6: Active authors of graph learning at top conferences.

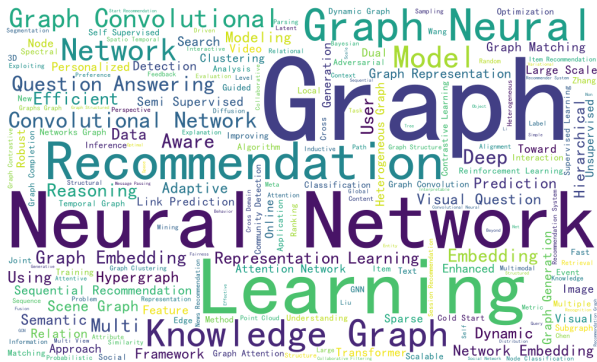


Fig. 7: High-frequency words in graph learning.

4 APPLICATIONS

This section introduces the current major applications of graph learning in the real world. These include traditional machine learning

scenarios such as recommendation systems, natural language processing, computer vision, and FinTech. There are also burgeoning applications in scientific scenarios such as chemistry, biology, physics, and mathematics. Finally, we summarize popular datasets used in graph learning.

4.1 Recommendation System

Recommendation systems are information filters that recommend items that users need or are interested in. Previous related research has mainly been based on collaborative filtering and then deep neural networks. In recent years, due to the advantage of graph neural network modeling linked data, they have been widely used in recommendation systems to model the relation between users and products [172], [41].

4.1.1 Heterogeneous Graph

The heterogeneous graph is often used to model users and items with two different properties in recommendation systems. Dong et al. [173] perform link prediction and recommendation across heterogeneous social networks. Shi et al. [92] propose the concept of semantic paths by setting weights on heterogeneous information graphs and meta-paths to assist the model in better integrating heterogeneous information. Then, Shi et al. [174] utilize a novel network embedding method on HINs to explore high-level structural information of users and items.

4.1.2 Hypergraph

The hypergraph describes high-order relationships between multiple users and items for recommendation. Yu et al. [175] propose a multi-channel hypergraph convolutional network to exploit high-order user relations such as social relations between users and their same purchase behavior. Yang et al. [176] use hypergraph neural networks to model global multi-behavior dependencies based on the dynamic heterogeneous relations of users and items. Xia et al. [177] propose a hypergraph transformer framework based on a self-supervised approach to enhance user representation with user-item interactions.

4.1.3 Dynamic Graph

The dynamic graph incorporates time dimension into recommendation system. For the dynamism of users in online communities, Song et al. [178] propose a recommendation method based on a dynamic graph attention network, which models user’s dynamic interest changes and the influence of interaction between users to infer users’ interests. Zhang et al. [179] model different users’ history sequences instead of individual user’s sequences with a dynamic graph framework for user sequence recommendation. In addition, there are some other research directions using graph learning to assist recommender systems [180].

4.2 Natural Language Processing

Natural Language Processing (NLP) is a crucial area of artificial intelligence. It takes language as the research object and aims to realize the understanding and application of human language by machine. Following are some typical research directions.

4.2.1 Text Classification

Text classification is a classic problem in NLP research. For the weakly supervised text classification, Peng et al. [67] model keywords graph structure and calculate the correlation between keywords with the help of GNN. While unlike many applications of CNN, Yao et al. [14] propose the TextGCN model to learn representations of words and documents. Similarly, Lin et al. [181] adopt a graph-based CNN to capture long-distance semantic information for text classification.

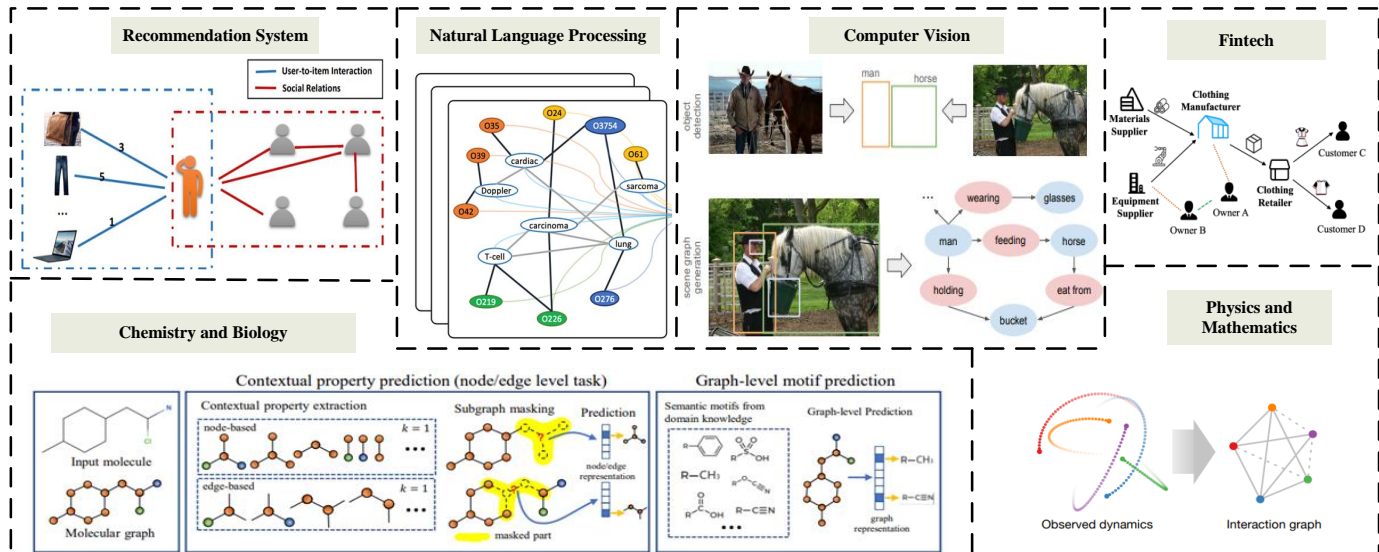


Fig. 8: Examples of applications. These applications include Recommendation System [172], Natural Language Processing [14], Computer Vision [88], Fintech [9], Chemistry and Biology [18], Physics and Mathematics [129].

4.2.2 Information Extraction

Relation extraction aims to identify target relations in text entities and is one of the primary tasks of information extraction [182]. Rocktaschel et al. [183] incorporate the matrix factorization method to learn the embedding representation of entity pairs and relations to improve the generalization ability of relation extraction. Song et al. [184] propose a graph-state LSTM model that models document graphs while preserving the graph structure, thereby reducing the information loss caused by graph splitting. Zhang et al. [185] utilize the GCN model to extract entity dependencies in text based on the dependency tree and design a new pruning strategy to ensure the accuracy of the information.

4.2.3 Knowledge Graph

The knowledge graph is essentially a heterogeneous information network with rich information [186], [187], [188]. It focuses on the representations of nodes and the relationship between nodes. Zhao et al. [121] propose MRGAT to model the constructed heterogeneous relational graph, which includes three semantic subgraphs, for knowledge graph entity typing. Based on TransE [137], Wang et al. [189] model node relationship as a hyperplane for translation to better keep the mapping properties of the original relationship. Schlichtkrull et al. [17] adopt the R-GCN model to model relational data on the knowledge base for link prediction and entity classification. Liu et al. [190] improve the encoding method and apply the GNN model to inductive knowledge graph completion. In order to perform the joint reasoning between the question answering and the knowledge graph, Yasunaga et al. [13] learn the representation on the graph of the joint composition of the two aspects with the GNN method.

4.2.4 Question Answering

Question answering is a crucial task in natural language generation. Zhang et al. [155] integrate PLMs and GNN for encoding to capture language contextual relations. In addition, visual question answering is also a hot research topic in recent years. Teney et al. [191] utilize graph structure to model scene objects and given problems instead of CNN or LSTM to take full advantages of the structural information. In the ‘fact-based’ research direction, Narasimhan et al. [192] model entity graphs with GCN to reason about answers.

4.3 Computer Vision

Graph structure data is widely used in many computer vision tasks, including images, videos, and icons. Researchers have explored the

use of graph structures in various aspects, such as scene graph generation and object recognition.

Scene Graph is a directed graph that represents the semantic information of the scene, where nodes represent objects and edges represent the relationships between objects. Xu et al. [88] propose an end-to-end model that generates structured scene representation from an input image using scene graphs. Yang et al. [193] propose Graph R-CNN, that is both effective and efficient at detecting objects and their relations in images. They also propose an attentional Graph Convolutional Network (aGCN) that effectively captures contextual information between objects and relations.

Additionally, Jain et al. [194] propose to combine the power of high-level spatio-temporal graphs and the success of Recurrent Neural Networks (RNNs) in sequence learning. Wang et al. [195] propose EdgeConv, which operates on dynamically computed graphs in each layer of the network. It is suitable for CNN-based high-level tasks on point clouds, including classification and segmentation. Sarlin et al. [12] introduce SuperGlue, a neural network that matches two sets of local features by jointly finding correspondences and rejecting non-matchable points. This allows for joint reasoning about the underlying 3D scene and feature assignments.

4.4 FinTech

Fintech refers to the application of AI and other computer technologies to the traditional financial industry to improve the effect and efficiency of its operation. Financial market, including enterprises, persons and regulators, naturally forms a giant complex network which is worth to mine. Thus, graph learning is widely applied in Fintech, mainly divided into two aspects: company and individual.

4.4.1 Company Aspect

A. Supply Chain Network

Supply chain is an important part of business operations. To solve the visibility problem on the supply chain, Kosasih and Brintrup [196] detect potential buyers on the car network through a GNN method. Yang et al. [9] propose a novel GNN model to mine the supply chain relationships of small and medium-sized enterprises for financial risk prediction. In stock movement prediction, Cheng and Li [197] utilize supply chains and other relations to build company relations and then use GAT to model the company’s momentum spillover effect for prediction.

B. Guarantee Network

Guarantee network is mainly the product of small- and medium-sized enterprises (SMEs) guaranteeing each other to improve credit rating. To monitor the potential default risk on the guarantee network, Cheng et al. [198] calculate the risk score of the contagion chain based on the graph-structured loan data. Cheng et al. [8] also leverage GAT to learn network node representations and predict the default probability of a company according to its temporal behavior and structural position in the guarantee network.

C. Investment-shareholding Relation Network

It is natural to treat investment-shareholding relation network as heterogeneous graphs to model spillover effects for stock predictions [197], [199], asset pricing [200] and risk propagation [201]. Based on the investment relation in the capital market, Cheng et al. [202] utilize GCN to model the relationship between the target company and its related companies on graph for stock movement prediction. Li et al. [203] also propose LSTM-RGCN, a model to simulate the linkages between stocks to enhance the effect of prediction. Zheng et al. [204] put forward a heterogeneous-attention-network-based model to explore the bankruptcy prediction problem of SMEs by leveraging the relational information in accessible financial networks. Besides, hypergraph can also promote prediction of enterprise risk [120]. Zhang et al. [10] model bank data as a heterogeneous information network and thoroughly mine the relations existing in the financial activities of small and micro-enterprise users under the commercial banking service scenario to assist in default analysis [201].

4.4.2 Individual Aspect

Credit Risk Assessment. Credit risk assessment aims to detect and identify users' potential fraud or default. Cheng et al. [205] propose a spatial-temporal graph attention network method for credit card fraud detection depending on time and location transaction information, which jointly learns attention weights with 3D convolutional network. Liu et al. [206] focus on the problem of fraud detection with the imbalanced class on the graph, adopting a supervised GNN method combined with a specific sampling strategy. They leverage a label-balanced sampler to establish sub-graphs and aggregate information from choosed neighborhood to form the representation of the target nodes. Chen and Tsourakakis [207] design an AntiBenford subgraph framework and corresponding algorithm based on Benford's law, detecting abnormal subgraphs on the cryptocurrency transaction network and identifying abnormal transaction data.

4.5 Chemistry and Biology

GNNs have been used in Chemistry and Biology. When applied to molecules, for example, their natural graph structure can be leveraged. In this structure, atoms and chemical bonds can be regarded as nodes and edges, respectively.

Molecular representation learning has been studied by many scholars. Coley et al. [208] treat molecules as undirected graphs with attributed nodes and edges. Rong et al. [18] propose a framework, GROVER, which learns rich structural and semantic information of molecules from enormous unlabelled molecular data.

Besides, many works aim to model protein structures. Jumper et al. [209] propose the AlphaFold2 to predict the three-dimensional structure of proteins, which transforms pair representations into directed edges. GraphBind [210] uses GNNs to embed the latent local patterns of structural and bio-physicochemical characteristics for identifying nucleic-acid-binding residues on proteins.

Additionally, graph learning has many healthcare applications in chemistry and biology. For instance, Gaudelot et al. [211] present a multidisciplinary academic-industrial review of graph machine learning within the context of drug discovery and development.

4.6 Physics and Mathematics

Graph learning in physics mainly focuses on physical scenes understanding, dynamic systems, etc. Sanchez-Gonzalez et al. [15] introduce a new class of learnable models based on graph networks

which implement an inductive bias for object- and relation-centric representations of complex, dynamical systems to understand and interact with everyday physical scenes. To tackle a limitation of the sparsely discretized data which cause value error, Seo et al. [212] propose SDL and combine it with recurrent graph networks to build PA-DGN, which automatically learns the underlying spatiotemporal dynamics in graph signals. Chen et al. [16] use graph-based meta learning approach to separately predict water quantity and quality variables for river segments in stream networks, considering physical characteristics of stream segments. GNNs are also used in math problems. For example, Prates et al. [213] use GNNs to solve the decision variant of the Traveling Salesperson Problem, a highly relevant NP-Complete problem.

4.7 Datasets

We provide a summary of the most popular datasets in Table 3. In recommendation systems, users, items, and their interactions are represented as heterogeneous nodes and edges, resulting in various graph types such as bi-typed graphs, hypergraphs, and dynamic graphs. Social networks often exhibit homogeneity, while networks in fintech and academic settings tend to be heterogeneous on both nodes and edges. For NLP and CV scenarios, graphs are constructed indirectly, so the number of nodes and edges depends on the experiment settings. In contrast, knowledge graphs, a specific type in NLP, consist of knowledge triples. Finally, in chemistry and biology, both nodes and edges in those graphs usually have attributes, which distinguish them from other datasets.

5 FUTURE DIRECTIONS

Despite the achievements of GL, many challenges remain unsolved. This section, we summarize major trends and challenges, which are also future directions of GL. In particular, we identify five directions that are worth considering: incorporating other ML methods, graph scalability, interpretability, expressivity and social effects.

5.1 Incorporating with Other ML Methods

Graph neural network often encounters various limitations in practical application. Reinforcement learning, meta-learning, few shot and other mainstream models in machine learning have great advantages in different aspects, and are gradually applied to GNN field to solve various problems. Here we mainly introduce three types.

5.1.1 Reinforcement Learning

Reinforcement Learning (RL) consists of an agent, environment, state, action, and reward. Through reinforcement learning, the agent adjusts what actions it should take in various states to obtain the maximum reward according to the new state and the reward feedback from the environment. When combined with graph neural networks, RL models are used for decision-making, rewards, or both. Wan et al. [61] propose MPDRL, which provides a multi-hop reasoning strategy in the reinforcement learning framework for inferring the next promising connection between the source and the target entities. Das et al. [96] introduce MINERVA, a neural reinforcement learning algorithm that learns to navigate a graph and find a predicted path for the target entities. Meiroum et al. [42] propose RLGN, which formulates the setup as a sequential decision problem over a temporal graph process. In face of an exponential state space, combinatorial action space, and partial observability, they design a novel tractable scheme to control dynamical processes on temporal graphs.

5.1.2 Meta-Learning

Meta-Learning means learning to learn. It aims to enable models to acquire the ability to "learn" so that they can quickly learn new tasks based on acquiring existing "knowledge" and it can significantly improve tasks with insufficient training data. The applications of meta-learning in graph problems include node embedding, node classification, link prediction, node/edge level shared representation,

TABLE 3: A TABLE OF DATA SUMMARY

Scenarios	Dataset	Nodes	Edges	Description
Recommendation System	Amazon [179]	2.098×10^7	8.283×10^7	This is a large crawl of product reviews from Amazon.
	IMDB [26]	1,199,919	3,782,463	A binary sentiment analysis dataset.
	Flickr [2]	499,610	8,545,307	A popular photo sharing network on Flickr.
	LastFM [2]	136,420	1,685,524	Social network of LastFM users from Asia.
NLP	WordNet18 [17]	146,005	656,999	This dataset includes 18 relations scraped from WordNet.
	DBpedia [214]	3,966,924	13,820,853	Structured information from Wikipedia.
	FB15k [17]	14,951	1,345	KB relation triples and textual mentions of Freebase entity pairs.
	NELL [61]	1.7×10^6	2.4×10^6	This dataset offers the common sense knowledge rules.
	YAGO [61]	1×10^6	1.2×10^8	A KG that augments WordNet.
CV ¹	Visual Genome [88]	38	22	This dataset connects language and vision using crowdsourced dense image.
	COCO [11]	-	-	An object detection, segmentation, key-point detection, and captioning dataset.
	CAD [194]	40	-	A dataset comprised of video sequences of humans performing activities.
	INRIA Person [215]	-	-	A dataset of images of persons used for pedestrian detection.
	Cityscapes [216]	-	-	A database focusing on semantic understanding of urban street scenes.
Fintech	SMEsD [120]	3,976	21,818	A multiplex enterprise KG consisting of SMEs and related persons in China.
	DGraph [217]	3,700,550	4,300,999	This graph represents a realistic user-to-user social network in financial industry.
	eBay-small [218]	2.89×10^5	6.13×10^5	A real transaction network on eBay for fraud detection.
Chemistry and Biology	MUTAG [17]	1.793×10^4	1.979×10^4	A collection of nitroaromatic compounds.
	NCI1 [110]	2.987×10^4	3.23×10^4	A dataset related to anti-cancer screening.
	PTC [110]	1.456×10^4	1.5×10^4	A collection of chemical compounds reporting the carcinogenicity for rats.
	Tox21 [18]	2.235×10^4	2.332×10^4	A dataset represents chemical compounds.
	ENZYMES [94]	3.263×10^4	6.214×10^4	A dataset of protein tertiary structures.
	PROTEINS [94]	3.906×10^4	7.282×10^4	A dataset of proteins classified as enzymes or non-enzymes.
Academic	Pubmed [29]	8,341,043	737,869,083	This dataset consists of publications pertaining to diabetes.
	DBLP [26]	317,080	1,049,866	DBLP collaboration network.
	MAG240M [3]	244,160,499	1,728,364,232	An academic graph extracted from Open Graph Benchmark.
	OAG [5]	1,858,395	3,965,744	A large Knowledge Graph unifying Microsoft Academic Graph and Aminer.
	AMiner [4]	1,369,055	8,650,089	A large academic network.
Social Network	Google+ [86]	28,943,739	462,994,069	A network contains a snapshot of the Google+ social structure.
	YouTube [108]	3,223,589	9,375,374	A network of YouTube users and their friendship connections.
	Twitter [106]	465,017	834,797	A dataset containing information about who follows whom on Twitter.
	Livejournal [2]	4,847,571	68,993,773	LiveJournal online social network.

¹ The numbers of nodes and links in the CV part are counted per image on average.

graph level shared representation, etc. Huang et al. [219] propose G-META, which uses local subgraphs to convey subgraph-specific information and learns transferable knowledge more quickly through metagrapms. Chen et al. [220] propose MetaR, which solves few-shot link prediction by passing relation-specific meta-information, which enables the model to learn the most important knowledge and learn faster, corresponding to the related element and the gradient element in the MetaR respectively.

5.1.3 Few-shot Learning

Few-shot learning is a type of Meta-Learning applied to supervised learning. In little-shot learning, the N-way K-shot problem challenges models to learn how to distinguish N categories from $N \times K$ data. To tackle this problem, Kim et al. [221] propose the EGNN. Instead of learning to predict node labels, EGNN predicts edge labels on graphs and iteratively updates them by leveraging intra-cluster similarity and inter-cluster dissimilarity. This explicit clustering approach enables few-shot learning. Common approaches to implement few-shot learning include data augmentation [222] and regularization [223].

5.2 Graph Scalability

Graph neural networks have proven highly effective in learning from graph-structured data and are now widely used across various domains. However, graphs in some domains can be both large and heterogeneous, often containing millions or even billions of vertices

and edges of different types. To address this challenge, various training models have been proposed for large-scale graphs. In this article, we introduce common approaches for implementing few-shot learning, focusing on two key aspects.

5.2.1 Mini-batch Training

Mini-batch training is a widely used technique for training large-scale graph data, where only a part of the graph nodes are selected for training each time. Several neighborhood sampling methods have been proposed for mini-batch training, including the most basic method of node sampling [32], as well as layer sampling [33] and subgraph sampling [5], which are commonly used.

5.2.2 Embedding Compression

Node embeddings can enhance performance in certain tasks, but the associated number of parameters increases linearly with the number of nodes, which can lead to computational challenges. To address this issue, embedding compression methods have been proposed. Yeh et al. [224] developed a node embedding compression method that uses a bit vector to compactly represent each node, rather than a floating-point vector. The compression method parameters can be trained simultaneously with graph neural networks [225]. Meanwhile, Cui et al. [226] used a reinforcement learning agent with an imbalance-aware reward function to sample from both majority and minority classes, and then applied a graph coarsening strategy to reduce the search space of the agent.

5.3 Interpretability

The problem of machine learning interpretability is divided from the perspective of interpretable objects. The first is post-hoc interpretable models for existing models [227]. The second is a pre-event interpretability model with both excellent performance and interpretability of downstream tasks [228]. Graph structure data contains not only the node features, but also the network topology, which makes it different from the general interpretability of machine learning methods. Current post-hoc interpretability mainly includes two levels: instance level and model level. Amara et al. [229] propose a framework to evaluate explanations of current methods.

5.3.1 Instance-level interpretability

Instance-level interpretability focuses on the interpretability of the classification results for a given node. Ying et al. [227] propose to determine important nodes, node characteristics, and key pathways that ultimately have much influence on the classification of a particular node as interpretability. Different from existing explainers for GNNs, DIR-GNNs [230] explain GNNs on graph-structured data from a causal perspective.

5.3.2 Model-level interpretability

Model-level interpretability focuses on global, generic patterns and treats them as intrinsic logic for graph neural network classification. Luo et al. [231] use reinforcement learning to iteratively generate subgraphs as the global interpretability result. There are also some researchers implement the transparency interpretability of graph neural network models, for example, Dai et al. [232] propose a new framework which can find K-nearest labeled nodes for each unlabeled node to give explainable node classification. Other scholars have applied the interpretability of graph neural networks to different domains, Schnake et al. [233] use the GNN-LRP model to test under different scenarios of the graph neural networks, including text emotion classification, quantum chemistry, and image classification.

5.4 Expressivity

5.4.1 Over-smoothing

Over-smoothing is a crucial problem in GNNs. As most GNNs are based on the assumption that similar nodes tend to connect, the representations of nodes tend to become similar after several layers of convolution, which we know as over-smoothing. So far, there are mainly two methods to alleviate over-smoothing.

A. Model-specific Methods

This type of methods mainly focuses on designing a special anti-over-smoothing module for a specific GCN model, therefore they varies from model to model. For instance, Klicpera et al. [234] combine the PageRank algorithm with GCN to improve the traditional propagation method, reducing the number of parameters and making the neighborhood larger and adjustable to alleviate over-smoothing. Chen et al. [235] propose GCNII with two mechanisms of initial residual and identity mapping to ensure that the model still obtain promising results while depth added.

B. General Methods

General methods are a more flexible methods with better portability and scalability, which are not specific to the model. They usually through the idea such as regularization to mitigate over-smoothing. Do et al. [236] propose a new regularization method DropNode, which randomly discards parts of the graph to reduce the connectivity of the entire graph. Zeng et al. [237] utilize a subgraph extractor to exclude noisy nodes. The extracted subgraph is composed of a small number of key neighbor nodes, which will finally be transformed into informative representation to prevent the entire graph from being over-smoothing.

5.4.2 Expressive Power

The theoretical research of GNNs' expressive power is a hot issue in graph learning. In recent years, researchers have attempted to study the higher-order Weisfeiler-Lehman (WL) tests, such as 1-2-3 GNN [238]. Similarly, Xu et al. [142] put forward a theoretical framework for analyzing the expressive power of GNN, and design the GIN with strong expressive power based on the neighborhood aggregation framework. Meantime, some researchers put efforts into enhancing the rooted subtree of 1-WL with additional features. Wijesinghe et al. [239] leverage a novel locally isomorphic structure hierarchy to incorporate the structural information so that the proposed model GraphSNN has stronger expressive power than WL tests.

5.4.3 Equivariant GNNs

Graph Neural Networks come in many varieties, but they should always be either invariant (meaning the permutation of the nodes in the input graph does not affect the output) or equivariant (meaning the permutation of the input permutes the output). Invariant and equivariant networks have been successfully used for learning images, sets, point clouds, and graphs. Keriven et al. [240] construct networks with a single hidden layer, and applied either an invariant or equivariant linear output layer with an equivariant linear operator and a pointwise non-linearity. Satorras et al. [241] introduce a new model for learning graph neural networks equivariant to rotations, translations, reflections and permutations called Equivariant Graph Neural Networks (EGNNs). Batzner et al. [242] present an E(3)-equivariant neural network approach for molecular dynamics simulations.

5.5 Social Effects

5.5.1 Fairness

GNNs have demonstrated significant potential in modeling graph-structured data. However, like other machine learning models, GNNs may make predictions based on protected sensitive attributes, e.g., skin color and gender. Two kinds of biases may exist in graph-structured data: one is the bias that exists widely in various types of data such as tables, texts, graphs; The other is the bias characteristic of graph-structured data. These biases may compromise the fairness of GNNs, leading to flaws in their predictions.

For GNNs fairness algorithms, we classify them into adversarial debiasing [243], fairness constraints [244], and other methods [245]. Dong et al. [243] propose novel definitions and metrics to measure the bias in an attributed network, which leads to the optimization objective to mitigate bias, feeding GNNs with less biased data. Song et al. [244] propose a novel GNN framework, GUIDE, which operates on the similarity matrix of individuals to learn personalized attention to achieve individual fairness without group level disparity. Zhang et al. [245] explore a more general case where quantities of unlabeled data are provided, leading to a new form of learning paradigm, namely fair semi-supervised learning.

5.5.2 Privacy

The private information in the model training set may be leaked in the published model or the provided service. The defense against different privacy attacks is the research direction of many scholars. Hsieh et al. [246] present a graph perturbation-based approach, NetFense, to against GNN-based privacy attacks. NetFense can simultaneously keep graph data unnoticeability, maintain the prediction confidence of targeted label classification, and reduce the prediction confidence of private label classification. Wu et al. [247] propose FedPerGNN, a federated GNN framework for privacy preserving recommendation, which utilize decentralized graph mining.

6 CONCLUSION

Graphs are ubiquitous in the real world, highlighting the importance of mining complex relationships and structural information. With the advent of deep learning, graph learning has become an efficient method for modeling various kinds of graphs, including traditional

social networks, such as academic networks and enterprise knowledge graphs, etc., and graphs transformed based on text, image and tabular data. The prosperous development of graph learning has led to thousands of related works that address problems on graphs from different perspectives. While there have been some influential surveys that sort through previous large amounts of literature, there is still a lack of a comprehensive survey that concludes previous works in a more logical and organic way. Moreover, the high-speed development of this area makes it difficult to cover current applications, trends, and future challenges that are vital to further research on graph learning. To remedy this, we collect and analyze the latest works to provide meaningful suggestions. In this survey, we first sort previous and current works based on the elements of graphs (i.e., node, edge, and graph structure), considering data model and tasks. Then, we sort representative methods of graph learning, covering latest works on the combination of PLMs and graph learning. We particularly focus on LLMs augmented with graph learning. Afterward, we conclude current applications in different scenarios. Finally, we propose future directions of graph learning to promote further research.

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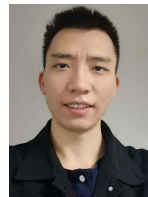
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