Graph-level Neural Networks: Current Progress and Future Directions

Ge Zhang†, Jia Wu†, Jian Yang†, Shan Xue‡, Wenbin Hu§, Chuan Zhou‡
Hao Peng‡, Quan Z. Sheng†, Charu Aggarwal‡

† School of Computing, Macquarie University, Sydney, Australia
‡ School of Computing and Information Technology, University of Wollongong, Australia
§ School of Computer Science, Wuhan University, Wuhan, China

Abstract

Graph-structured data consisting of objects (i.e., nodes) and relationships among objects (i.e., edges) are ubiquitous. Graph-level learning is a matter of studying a collection of graphs instead of a single graph. Traditional graph-level learning methods used to be the mainstream. However, with the increasing scale and complexity of graphs, Graph-level Neural Networks (GLNNs), deep learning-based graph-level learning methods have been attractive due to their superiority in modeling high-dimensional data. Thus, a survey on GLNNs is necessary. To frame this survey, we propose a systematic taxonomy covering GLNNs upon deep neural networks, graph neural networks, and graph pooling. The representative and state-of-the-art models in each category are focused on this survey. We also investigate the reproducibility, benchmarks, and new graph datasets of GLNNs. Finally, we conclude future directions to further push forward GLNNs. The repository of this survey is available at https://github.com/GeZhangMQ/Awesome-Graph-level-Neural-Networks.

1 Introduction

The research on graph-structured data can be traced back to the 18th century [Biggs et al., 1986]. Since then, graph-level learning that takes a number of graphs (i.e., a graph dataset) as the study object has attracted great attention. Graph Isomorphism (GI) that determines whether two graphs are isomorphic has been the pioneer topic of graph-level learning as far back as the 1940s [Bondy and Hemminger, 1977]. In the 1970s, GI was defined as the “disease” of graph theory, and a lot of algorithms researching it have emerged [Weisfeiler and Leman, 1968; McKay and Piperno, 2014]. Moving into the 21st century, due to the thriving of machine learning and deep learning, graph classification [Shervashidze et al., 2011; Xu et al., 2018], embedding [Narayanan et al., 2017], regression [Gilmer et al., 2017], and generation [You et al., 2018] have been the main tasks of graph-level learning.

Graph structures give the unified modeling manner for many real-world entities. For example, the chemical compound, interactions between proteins, and a human brain can be described as the molecular graph, protein-to-protein graph, and brain network, respectively. Graph-level learning has been of great practical significance. For instance, since the 1960s, scientists have utilized graphs to model molecules [Morgan, 1965] and designed molecular fingerprints to assist chemical dataset substructure searching [Ralaivola et al., 2005; Duvenaud et al., 2015]. Graph regression has been becoming an effective manner for molecular property prediction [Gilmer et al., 2017] and drug discovery [Chen et al., 2018]. Graph classification can discriminate the brains affected by neurological disorders from healthy individuals [Wang et al., 2017]. Most recently, graph-level learning has been applied to the open catalyst project that aims to find new catalyst molecules [Chanussot et al., 2021].

Traditional graph-level learning methods have demonstrated good performance on small-sized graphs but output highly-sparse results for large-scaled graph datasets. In addition, the GI issue that only has quasipolynomial-time so-
lutions [Babai, 2016] is involved in some traditional methods. The computational complexity of these methods has quadratic or even exponential growth with the increase of data size. Beyond traditional methods, GLNNs have achieved state-of-the-art performance on graph-level learning, particularly when it comes to high-dimensional graph data. GLNNs cater to graph-level learning by: (1) automatically learning nonlinear features from graphs; 2) explicitly encoding graphs into compact numerical representations; 3) learning task-specific graph representations and addressing graph-level learning tasks in an end-to-end fashion (see Figure 1).

Existing survey papers mainly concentrating on node-level learning tasks that analyze node/edge/structure of a single graph, such as network embedding [Cui et al., 2018], community detection [Su et al., 2021], and anomaly detection [Ma et al., 2021]. There are also two up-to-date surveys [Wu et al., 2020; Zhang et al., 2020] that focus on node-level neural networks. [Kriege et al., 2020] and [Nikolentzos et al., 2021] review graph kernels (one type of traditional graph classification methods), but they only introduce GLNNs roughly and even do not provide taxonomy.

To the best of our knowledge, this is the first survey devoted to GLNNs. This paper is intended to help new practitioners understand graph-level learning and enable researchers to have a grasp of the current progress of GLNNs. The contributions of this survey are summarized as:

- **Systematic Taxonomy:** We propose a systematic taxonomy for GLNNs (see Figure 2). In each category, representative algorithms and the latest progress are introduced. We also summarized papers about the reproducibility, benchmarks, new datasets of GLNNs.

- **High-impact References:** Our references mainly come from the well-established conferences in machine learning (e.g., NeurIPS, ICLR, ICML, KDD, AAAI, IJCAI, CIKM, ICDM, and WWW).

- **Future Directions:** We discuss the future directions of GLNNs and hope this part can inspire researchers and further promote the development of GLNNs-GNNs.

## 2 Definitions

**Definition 1.** (Graph) A graph can be represented as $G = \{V, E\}$, where $V$ and $E$ denote the set of $n$ nodes and $m$ edges, respectively. The graph structure can be represented by an adjacency matrix $A \in \{0, 1\}^{n \times n}$, where $A_{u,v} = 1$ denoted there is an edge between nodes $u$ and $v$, otherwise 0. The node $v$ and edge $E_{u,v}$ can be annotated with vector $x_u \in \mathbb{X}$ and $s_{u,v} \in \mathbb{S}$, respectively, where $\mathbb{X} \in \mathbb{R}^{n \times b}$ and $\mathbb{S} \in \mathbb{R}^{m \times d}$.

**Definition 2.** (Graph-level Learning) It takes a graph dataset $G = \{G_1, ..., G_N\}$ as inputs, and it outputs results of a graph-level learning task. The prominent property of a graph is permutation-invariant — enumerating the ordering of nodes does not change its structure. Hence, the graph-level learning algorithm is supposed to be permutation-invariant, i.e., the prediction result about a graph does not affect by permutations on its node ordering.

**Definition 3.** (Graph-level Neural Networks) GLNNs perform graph-level learning tasks on the graph dataset $G$ in an end-to-end fashion. Generally, GLNNs encode the graph $G_i \in G$ into a vectorized representation (a.k.a., embedding) $h_{G_i}$, followed that the task-specific results will be output.

## 3 A Development of Graph-level Learning

In this section, we briefly review three types of traditional graph-level learning methods first. Then, we explain why the deep learning-based method GLNNs is more desirable. The taxonomy of graph-level learning from traditional methods to GLNNs is shown in Figure 2.

**Graph Kernels (GKs).** GKs calculate pairwise kernel values (i.e., similarity) of graphs through well-defined kernel functions to obtain the Gram matrix where each entry denotes the kernel value of pairwise graphs. Afterward, employing off-the-shelf machine learning techniques to perform graph-level learning tasks on the Gram matrix, such as Support Vector Machines for classification, $K$-Means for clustering, and Gaussian Processes for regression. The representative method include Weisfeiler-Lehman GKs [Shervashidze et al., 2011][Togninalli et al., 2019], graphlet GKs [Shervashidze et al., 2009], and random walk GKs [Kang et al., 2012].

**Subgraph Mining-based Approaches.** Frequent subgraph-based methods [Thoma et al., 2010] generally represent each graph by a series of frequent subgraphs (i.e., the subgraphs with the occurrence in the graph dataset beyond a threshold) beforehand. Then, machine learning techniques can be applied to handcrafted graph representations. There are also informative subgraph-based [Kudo et al., 2004] and dense subgraph-based methods [Lanciano et al., 2020].

**Graph Embedding.** Based on handcrafted features, GKs and subgraph mining-based approaches output deterministic instead of learnable results. Moreover, pairwise similarity calculation in GKs and the GI issue associated with subgraph mining-based approaches make these algorithms suffer from computation bottlenecks. Practitioners have turned to data-driven graph embedding, such as graph2vec [Narayanan et al., 2017] and AWE [Ivanov and Burnaev, 2018], which can learn knowledge from graphs automatically and output learned task-agnostic graph representations explicitly.

**Why GLNNs are Needed?** GLNNs bring significant benefits to the graph-level learning community. They provide a general framework to encode graphs into task-specific representations and predict graphs in an end-to-end system. Benefiting from deep learning, GLNNs can learn the highly non-linear features from the large-scale sparse graph data effectively. Moreover, non-structural features (e.g., node and edge attributes) can be naturally integrated into GLNNs as the supplements for graph structures. Next, we will discuss GLNNs based on deep neural networks, graph neural networks, and graph pooling in detail.

## 4 GLNNs - Deep Neural Networks (DNNs)

In this section, we survey GLNNs based on three types of DNNs, i.e., Convolution Neural Networks (CNNs), Capsule Neural Networks (CapsNets), and Recurrent Neural Networks (RNNs). These DNNs were originally proposed for learning grid-structured data (e.g., image) and sequence-
structured (e.g., text and speech) data, instead of the non-Euclidean structure data—graphs.

### 4.1 CNN-based Approaches

Generalizing CNNs to graph-structured data in the high-dimensional and irregular domain is non-trivial, due to the unordered nodes and the unbounded node neighborhood. One of the straightforward ways is to transform each graph to be the girded data. For example, through selecting nodes sequence and assembling regular node neighborhoods, PATCHY-SAN [Niepert et al., 2016] successfully applied CNNs to the graph classification task. On the contrary, some algorithms apply the idea of spatial CNNs to graph-level learning. For example, in DCNN [Atwood and Towsley, 2016], the node feature transformation is based on a three-dimensional tensor that contains the multi-hop node neighborhood information. Through averaging the learned node representations of each graph, DCNN obtains the graph representation. Another method ECC [Simonovsky and Komodakis, 2017] learns the node representation by applying weighted summation to its neighbors’ representations coming from the former neural layer. The weights are edge-specific and learned by the feature transformation on edge attributes. ECC coarsens a graph into a node to obtain the graph representation.

### 4.2 CapsNet-based Approaches

CapsNets [Hinton et al., 2011] were proposed to address the issue that CNNs cannot effectively capture spatial relationships among features. CapsNets extend the scalar neuron to a vector-structured capsule, in which each vector element is responsible for capturing different features such as position, pose, and texture of the input. Analogically, GCAPS-CNN [Verma and Zhang, 2018] and GapsGNN [Zhang and Chen, 2018] leverage the idea of CapsNets to preserve high-level properties of graphs into graph representations. Moreover, GCAPS-CNN achieves permutation-invariance by calculating the covariance of layer outputs.

### 4.3 RNN-based Approaches

As a type of neural networks in which all nodes are connected directly or indirectly, RNNs are specialized in capturing sequential patterns in data [Medsker and Jain, 2001]. [You et al., 2018] proposed an RNN-based graph generation model in which nodes and edges are formed in a sequence. [Lee et al., 2018] emphasized that significant structures are confined to a small part of a graph. Hence, they used substructures sampled by RNNs to do the graph classification task.

### 5 GLNNs - Graph Neural Networks (GNNs)

Currently, GNNs are the standard toolkit for learning node representations [Wu et al., 2020]. As the key component of GNNs, graph convolution can be defined either in the spatial domain or spectral domain. To achieve permutation-invariant GLNNs-GNNs for graph-level learning, a trivial idea is to employ a GNN followed by a readout function, such as summation-based, averaging-based, and jumping knowledge-based functions. The former two types of readout obtain the graph representation \( h_G \) by summing/averaging node representations \( h_v, \forall v \in V(G) \). The latter one aggregates node representation across all convolution layers, that is \( h_G = \sum_{v \in V(G)} h_v^{(0)} \) \ldots \( h_v^{(L)} \) where \( h_v^{(l)} \) is the representation of node \( v \) output by the \( l \)-th graph convolution layer, and “;” denotes the concatenation operation. The most widely used GLNNs-GNNs are Messaging Passing Neural Networks (MPNNs) [Gilmer et al., 2017]. MPNNs belong to spatial graph convolution where each node updates its representation by aggregating vectorized representations of its neighbors.

We investigate the expressivity of GLNNs-GNNs first. Then, spectral GLNNs-GNNs will be discussed. In addition, we introduce models focusing on improving the generalization of GLNNs-GNNs and explaining GLNNs-GNNs’ predictions. This section ends with a discussion of employing other techniques to improve GLNNs-GNNs.

#### 5.1 The Expressivity of GLNNs-GNNs

Since GLNNs-GNNs are proposed for graph-level learning, it is critical to investigate the power of the expressivity of GLNNs-GNNs in distinguishing graph structures. Generally, researchers call such a power “expressivity”. Employing the Weisfeiler-Leman graph isomorphism testing (WL-test, [Weisfeiler and Leman, 1968]) to describe GLNNs-GNNs’ expressivity is attractive at present. The WL-test contains the neighborhood aggregation-based message passing similar to MPNNs. [Xu et al., 2018] firstly proved that the upper bound of MPNNs in distinguishing graph structures is the 1-dimensional WL test (1-WL). They emphasized that it is the injective message passing making 1-WL so powerful. By adding multi-layer perceptrons
behind each graph convolution layer to guarantee the injective message passing. Gin is that equivalent to the 1-WL is proposed. However, 1-WL equivalence MPNNs cannot distinguish graphs that are indistinguishable by 1-WL, such as regular graphs. Also, 1-WL cannot count substructures in a graph other than the star-shaped pattern [Arvind et al., 2020; Chen et al., 2020b], but substructures (e.g., triangles, cycles) are critical for learning social networks and molecular graphs.

By introducing more inductive biases, scientists have presented MPNNs beyond the expressivity of 1-WL. For example, in analogy to k-WL (the extension of 1-WL), [Morris et al., 2019] proposed k-GNNs which perform message passing on pre-defined subgraphs consisting of k-nodes and achieves the same expressivity as k-WL. However, when k ≥ 3, achieving k-GNNs is at the cost of exponential increase in computing complexity, since k-GNNs perform calculations on k-ranked tensors. [Maron et al., 2019] proposed PPGLN, which achieves the 3-WL equivalent expressivity by designing a 2-GNN augmented with a quadratic projection. In addition, [Bouritsas et al., 2020] and [Bevilacqua et al., 2021] enriched MPNNs through employing pre-processing substructures as additional features and automatically selecting discriminative substructures, respectively.

Practically, theoretically more powerful MPNNs fail to beat their 1-WL equivalent counterparts on most graph datasets [Dwivedi et al., 2020]. This is because when graph attributes can perform as supplements of structural information, almost all graphs can be distinguished by 1-WL. Hence, it is not worth achieving more powerful MPNNs at the cost of high complexity. Adding unique node identities [Murphy et al., 2019] or random features [Sato, 2020] into graphs can achieve more powerful MPNNs within linear complexity. In addition, breaking the key property of graph convolution - local updates [Battaglia et al., 2018] is the other reason why theoretically more powerful GLNNs-GNNs do not achieve superior performance in experiments. To tackle this problem, [Balcilar et al., 2021] proposed GNML3 based on the eigendecomposition of graph Laplacian in the spectral domain. Through encoding graph signals from various frequencies, and casting critical computation operations in Matrix Query Languages (MATLANG, that is originally proposed to measure the expressivity of linear algebra) into graph convolution, GNML3 is equivalent to 3-WL experimentally. [Bodnar et al., 2021] introduced the simplicial complexes into graph convolution to achieve GLNNs-GNNs with expressivity no less than 3-WL while ensuring local updates. Notably, inspired by MATLANG, [Geerts and Reutter, 2022] presented that describing GLNNs-GNNs’ expressivity can be released from the intricacies of the WL-test by employing tensor languages to model GLNNs-GNNs.

5.2 Spectral GLNNs-GNNs

Existing MPNNs work as a low-pass filter that can only preserve graph signals in low frequencies [Balcilar et al., 2020]. However, multi-scale graph signals are critical for graph-level learning, say, graph signals in high frequencies can highlight the differences among graphs. Spectral GLNNs-GNNs that define graph convolution in the spectral domain can capture multi-scale graph signals under robust theoretical guarantees. In addition to GNML3, other spectral GLNNs-GNNs also achieve good performance on graph-level learning. For example, [Zheng et al., 2021] defined framelet-based graph convolution that can filter high- and low-frequency signals by tensorized framelet transforms. Based on the spectral density computation, [Sawlani et al., 2021] proposed a method to capture graph signals in multi-scale beyond the extremum. After performing the spectral analysis about mainstream GNNs, [Balcilar et al., 2020] presented a spectral graph convolution with a custom frequency profile that achieves good performance on graph classification.

5.3 The Generalization of GLNNs-GNNs

Investigating the generalization ability of GLNNs-GNNs from small to large graphs is necessary since real-world graphs have various sizes and labeling big graphs is difficult. [Xu et al., 2021] theoretically analyzed the size-generalization capability of GLNNs-GNNs that have a single graph convolution layer. [Yehudai et al., 2021] suggested detecting local structures that are both significant in small-sized and large-sized graphs to improve GLNN-GNNs in size generalization. On the other hand, [Ma et al., 2020] and [Chauhan et al., 2020] explored how to improve the generalization of GLNNs-GNNs under the few-shot setting where only a few (even zero) graphs have the same graph label with unseen graphs. In addition, [Alon and Yahav, 2021] emphasized that most of GLNNs-GNNs have the over-squashing issue that each node’s receptive field grows exponentially, but long-range interactions among nodes cannot be captured. However, long-range interactions are critical, say, the property of methylnonane compound depends on the atoms located on the molecule’s opposite sides. Empirically, appending a fully-adjacent layer in which nodes are fully-connected can help GLNNs-GNNs capture long-range interactions.

5.4 Explaining GLNNs-GNNs’ Predictions

The black-box nature of GLNNs prevents academia and industries from trusting their predictions. The mainstream to explain GLNNs-GNNs is to detect nodes and substructures in a graph that can dominate GLNNs-GNNs’ predictions on it. These explanation models work in a post-hoc fashion and can be roughly divided into perturbation-based [Yuan et al., 2020a; Luo et al., 2020; Ying et al., 2019], surrogate model-based [Huang et al., 2020], and gradient-based [Pope et al., 2019]. One drawback of these models [Ying et al., 2019; Yuan et al., 2020b] is that they can only perform on instance-level —a complete training of the explanation model can only explain the prediction of GLNNs-GNNs on a single graph. [Yuan et al., 2020a] proposed the reinforcement learning-based XGNN that can explain GLNNs-GNNs’ prediction on a specific graph class after a complete training. Furthermore, [Luo et al., 2020] presented PGExplainer to explain GLNNs-GNNs collectively and inductively.

5.5 GLNNs-GNNs Combined with Other Methods

In this subsection, we discuss algorithms improving GLNNs-GNNs by combining them with contrastive learning and GKS: Combining GLNNs-GNNs with Contrastive Learning: Most GLNNs-GNNs work in a supervised fashion. How-
ever, annotating graphs is costly. For example, labeling chemical compounds need Density Functional Theory calculation. It leads to the demand for self-supervised techniques. Contrastive learning [Hjelm et al., 2019] has attracted a surge of interest. Generally, contrastive learning-based models train an encoder by contrasting representations having statistical dependencies and those that do not. Analogically, [Sun et al., 2019] proposed InfoGraph that learns task-agnostic graph representations by maximizing statistical dependencies between the graph and its nodes and minimizing statistical dependencies between the graph and nodes from other graphs. [You et al., 2020] investigated the impact of data augmentation in graph contrastive learning. [Qu et al., 2020] proposed contrastive learning-based graph presentation pre-training model that is optimized by maximizing the agreement between graphs’ original and augmented views.

Combining GLNNs-GNNs with GKs: Leveraging the benefits of GKs to improve GLNN-GNNs is feasible [Lei et al., 2017] [Chen et al., 2020a]. For example, GLNNs-GNNs are hard to train due to non-convex objective functions and over-parameterized properties. [Du et al., 2019] proposed a computationally efficient graph classification model in which the graph convolution is replaced by the calculation of pairwise graph kernel values. [Long et al., 2021] noticed that GKs naturally involve the substructure comparison. Hence, they introduced random walk-based GKs into graph convolution to improve GLNNs-GNNs in terms of distinguishing graphs.

6 GLNNs: Graph Pooling

Graph pooling performs graph-level learning by downsizing the graph. However, it is non-trivial due to the irregular structure of graphs. Recently, differentiable graph pooling has been the mainstream. It can be roughly divided into two types of approaches, i.e., the global and the hierarchical pooling.

6.1 Global Pooling

Global pooling, acting as a bridge between the graph representation and output layers, is generally utilized only once in a GLNN. The simplest global pooling is the readout function. A number of GLNNs [Xu et al., 2018] [Atwood and Towsley, 2016] [Simonovsky and Komodakis, 2017] apply the readout function on nodes to obtain graph representations. DGCNN [Zhang et al., 2018] is a graph classification model leveraging the sorting-based global pooling. After encoding nodes by graph convolution similar to GCN [Kipf and Welling, 2017], nodes in each graph will be sorted based on their structural roles and graphs can be pooled into the same size. Afterward, CNNs can be employed to classify graphs. Compared with PATHY-SAN [Niepert et al., 2016] that also transforms graphs to be grided data, DGCNN can be optimized by backpropagation since it can record the sorting order of nodes. [Lee et al., 2021] mapped nodes to the latent space composed of k structural prototypes and pooled nodes in the same prototype together. The graph representation can be obtained by concatenating embeddings coming from different prototypes.

6.2 Hierarchical Pooling

Hierarchical pooling learns coarsen-grained graph structures by gradually applying the pooling layer to downsize the graph. One type of hierarchical pooling is the cluster assignment-based method that clusters nodes in a graph and regards clusters as new nodes to form the pool graph. After several pooling operations, the graph can be coarsened into a node and represented by a vector. The cluster assignment can be obtained via deterministic [Bruna et al., 2014] and learnable clustering. DiffPool [Ying et al., 2018] is one of the representatives based on learnable clustering. Compared with inherently flat GLNNs-GNNs, DiffPool can learn hierarchical representations for graphs. Analogly to DiffPool, other cluster-assignment-based graph pooling methods, such as MinCutPool [Bianchi et al., 2020], MemGNN [Khasahmadi et al., 2020] and SAGPool [Lee et al., 2019] are proposed. In addition, Top-K Pooling [Gao and Ji, 2019] is the node selection-based hierarchical pooling that selects the nodes with top-k scores into the pooled graph in each pooling layer. In DiffPool, storing dense cluster assignment matrices needs quadratic storage complexity. [Cangea et al., 2018] proposed to use the top-k node selection to achieve hierarchical pooling without sacrificing sparsity.

Some practitioners proposed that the rich structural information is overlooked by existing graph pooling. They tackled the problem by encoding high-order structures explicitly. For example, [Ma et al., 2019] and [Yuan and Ji, 2020] introduced the graph Fourier transform and conditional random fields into graph pooling to capture more structural information, respectively. [Ranjan et al., 2020] scored substructures instead of nodes for top-k selection.

6.3 Emerging Graph Pooling Techniques

Pooling layers are usually put into GLNNs-GNNs as the component to downsize graphs. [Mesquita et al., 2020] conducted a sanity check for investigating the impact of hierarchical pooling on GLNNs-GNNs. Experiment results demonstrate that the cluster assignment-based hierarchical pooling does not witness a performance decrease when adopting random clustering or performing clustering on the complement graph. A possible reason is that graph convolution preceded by pooling can smooth graphs sufficiently. Hence, conducting more ablation experiments to validate newly proposed hierarchical pooling methods is necessary. In addition, existing graph pooling fails to keep stable performance on different datasets. [Wei et al., 2021] proposed to address this problem by the data-specific graph pooling that can adaptively sample off-the-shelf pooling methods for the input graph dataset.

7 Reproducibility, Benchmarks, and Datasets

Lacking standard experiment procedures has been a major threat to the reproducibility of GLNNs. [Errica et al., 2020] re-evaluated GLNNs-GNNs on the graph classification task under rigorous experiments concerning unified train-validation-test split, model selection and assessment processes. Furthermore, they also provided two graph structure-agnostic baselines to help practitioners characterize the contribution of newly proposed GLNNs-GNNs. [Dwivedi et al., 2020] are also concerned by the reproducibility issue. Based on PyTorch and DGL [Wang et al., 2019], they presented a benchmarking framework that fairly evaluates GLNNs-GNNs on graph classification and regression tasks.
Existing graph datasets (e.g., TU collection [Morris et al., 2020]) are criticized for their small size, isomorphism bias [Ivanov et al., 2019], and random data splits. Recently, practitioners have presented new graph datasets to improve the graph-level learning community. For example, [Freitas et al., 2021] introduced a graph dataset named MalNet for graph-level learning. [Hu et al., 2020] proposed the Open Graph Benchmark (OGB), in which graph datasets are large-scaled, have multiple task categories, and are from diverse domains. Notably, these new datasets propose challenges for GLNNs in scalability, imbalanced learning, explainability, and out-of-distribution generalization.

8 Future Directions

In this section, we highlight seven future directions for GLNNs based on the latest progress.

8.1 Equivariant GLNNs-GNNs

It is the permutation-invariant property of message passing that limits GLNNs-GNNs’ expressivity [Kondor et al., 2018] [Wijesinghe and Wang, 2022]. [Haan et al., 2020] proposed permutation-equivariant message passing —the local output is changed corresponding to the permutation. In addition, practitioners proposed message-passing mechanisms that are equivariant to more graph transformation. For example, [Klicpera et al., 2021] presented GemNet in which the message passing is graph permutation- and rotation-equivariant. [Satorras et al., 2021] introduced graph translation and reflection-equivariant message passing into GLNNs-GNNs. The above two methods achieve state-of-the-art performance on molecular property prediction. Designing graph transformation-equivariant message passing to improve GLNNs-GNNs’ expressivity is a new trend.

8.2 Graph Pooling with Difference Awareness

Existing graph pooling especially the top-k node selection-based has argued that nodes with great importance should be placed into pooled graphs. However, there is no rigorous definition of “importance”. In practice, graph convolution acts as a low-pass filter, and nodes with high similarities are put into pooled graphs [Mesquita et al., 2020]. However, a pooled graph consisting of dissimilar nodes is critical for graph-level learning. For example, a pair of different atoms can empower completely different properties to two molecules. How to construct a node difference-aware graph pooling method has not been explored yet.

8.3 Imbalanced Graph-level Learning

Learning imbalanced data in which a significant gap among the number of instances in different classes is a longstanding issue faced by machine learning. When learning the data with imbalanced class distributions, algorithms usually demonstrate poor generalization in the class with minority instances. However, almost all GLNNs overlook this issue. [Freitas et al., 2021] offered a new graph dataset that has imbalanced class distribution. The graph-level learning community urgently needs the baselines targeting imbalanced learning.

8.4 Out-of-Distribution Generalization of GLNNs

GLNNs assume that train and test data from the same distribution. However, the assumption is usually invalid in the open-world environment. Testing data could be out-of-distributed (OOD) regarding graph sizes and other characteristics of training data. [Bevilacqua et al., 2021] proposed to learn environment-robust graph representation by describing the mechanism of distribution shift. In addition, GLNNs aiming at the OOD scenario are almost unexplored. We refer readers who are interested in this issue to this paper [Hu et al., 2020] for graph data splitting that satisfies OOD.

8.5 Performant Parameters

As the non-convex model, GLNNs-GNNs need careful initialization and training to obtain performant parameters. However, with the ever-complex architecture of GLNNs-GNNs and the increasing size of the data scale, searching performant parameters becomes GPU-consuming. [Knyazev et al., 2021] proposed a model that learns knowledge about predicting performant parameters at the training stage and predicts performant parameters for unseen deep learning architectures through a single forward pass at the test stage. Such an optimization architecture exposes determining performant parameters of GLNNs-GNNs to a new direction.

8.6 Applying GLNNs to Classify Brain Networks

Brain network data are scarce since obtaining a network needs to scan an individual’s brain. A brain network contains a small number of nodes that denote the brain’s region of interest (ROI). Different brain networks are composed of the same ROIs. Neuroscientists desire to understand which regions play a decisive role when distinguishing brains having neurological disorders from healthy individuals. Hence, brain network classification needs to simplify GLNNs that have a small number of parameters, identity awareness, and high explanation. However, existing GLNNs do not meet the requirements mentioned above [Lanciano et al., 2020].

8.7 Encoding Relations among Graphs

GLNNs treat each graph as an independent individual. However, graphs can be regarded as interrelating entities. For example, relations among graphs could be established based on common substructures. Building relations among graphs and encoding them into graph representations have the potential to tackle the issue that GLNNs only embed limited structure information into graph representations [Wang et al., 2020].

9 Conclusions

GLNNs have brought a new paradigm and a large number of state-of-the-art models for the graph-level learning community. A considerable number of high-impact publications about GLNNs are badly in need of a survey with systematic taxonomy. In this survey, we briefly reviewed traditional graph-level learning methods. Then we summarized GLNNs into three categories and deeply investigated the development and contributions of each category. The reproducibility and benchmarks of GLNNs and new graph datasets were also discussed. Finally, we identified seven potential future directions to further promote the research area with fast-growing.
References

[Alon and Yahav, 2021] U. Alon and E. Yahav. On the bottleneck of graph neural networks and its practical implications. In ICLR, 2021.

[Arvind et al., 2020] V. Arvind, F. Fuhlbrück, J. Köbler, et al. On weisfeiler-leman invariance: subgraph counts and related graph properties. J Comput Syst Sci, 113:42–59, 2020.

[Atwood and Towsley, 2016] J. Atwood and D. Towsley. Diffusion-convolutional neural networks. In NeurIPS, 2016.

[Babai, 2016] L. Babai. Graph isomorphism in quasipolynomial time. In STOC, pages 684–697, 2016.

[Balcilar et al., 2020] M. Balcilar, G. Renton, P. Héroux, et al. Analyzing the expressive power of graph neural networks in a spectral perspective. In ICLR, 2020.

[Balcilar et al., 2021] M. Balcilar, P. Héroux, B. Gaižuė, et al. Breaking the limits of message passing graph neural networks. In ICML, 2021.

[Battaglia et al., 2018] P. W. Battaglia, J. B. Hamrick, V. Bapst, et al. Relational inductive biases, deep learning, and graph networks. arXiv, 2018.

[Bevilacqua et al., 2021] B. Bevilacqua, Y. Zhou, and B. Ribeiro. Size-invariant graph representations for graph classification extrapolations. In ICML, 2021.

[Bevilacqua et al., 2022] B. Bevilacqua, F. Frasca, D. Lim, et al. Equivariant subgraph aggregation networks. In ICLR, 2022.

[Bianchi et al., 2020] F. M. Bianchi, D. Grattirola, and C. Alippi. Spectral clustering with graph neural networks for graph pooling. In ICML, pages 874–885, 2020.

[Biggs et al., 1986] N. Biggs, E. K. Lloyd, and R. J. Wilson. Graph Theory, 1736–1936. OUP, 1986.

[Bodnar et al., 2021] C. Bodnar, F. Frasca, Y. G. Wang, et al. Weisfeiler and lehman go topological: Message passing simplicial networks. In ICML, 2021.

[Bondy and Hemminger, 1977] J. A. Bondy and R. L. Hemminger. Graph reconstruction—a survey. J Graph Theory, 1(3), 1977.

[Bouritsas et al., 2020] G. Bouritsas, F. Frasca, S. Zafeiriou, et al. Improving graph neural network expressivity via subgraph isomorphism counting. arXiv, 2020.

[Bruna et al., 2014] J. Bruna, W. Zaremba, A. Szlam, et al. Spectral networks and locally connected networks on graphs. In ICLR, 2014.

[Cangea et al., 2018] C. Cangea, P. Veličković, N. Jovanović, et al. Towards sparse hierarchical graph classifiers. In NeurIPS, 2018.

[Chanussot et al., 2021] L. Chanussot, A. Das, S. Goyal, et al. Open catalyst 2020 (oc20) dataset and community challenges. ACS Catal., 11(10):6059–6072, 2021.

[Chauhan et al., 2020] J. Chauhan, D. Nathani, and M. Kaul. Few-shot learning on graphs via super-classes based on graph spectral measures. In ICLR, 2020.

[Chen et al., 2018] H. Chen, O. Engkvist, Y. Wang, et al. The rise of deep learning in drug discovery. Drug Discov, 23(6), 2018.

[Chen et al., 2020a] D. Chen, L. Jacob, and J. Mairal. Convolutional kernel networks for graph-structured data. In ICLR, 2020.

[Chen et al., 2020b] Z. Chen, L. Chen, S. Villar, et al. Can graph neural networks count substructures? In NeurIPS, 2020.

[Cui et al., 2018] P. Cui, X. Wang, J. Pei, et al. A survey on network embedding. IEEE Trans. Knowl. Data Eng., 2018.

[Du et al., 2019] S. S. Du, K. Hou, R. R. Salakhutdinov, et al. Graph neural tangent kernel: Fusing graph neural networks with graph kernels. In NeurIPS, volume 32, pages 5723–5733, 2019.

[Duvenaud et al., 2015] D. Duvenaud, D. Maclaurin, J. Aguilera-Iparraguirre, et al. Convolutional networks on graphs for learning molecular fingerprints. In NeurIPS, 2015.

[Dwivedi et al., 2020] V. P. Dwivedi, C. K. Joshi, T. Laurent, et al. Benchmarking graph neural networks. arXiv, 2020.

[Errica et al., 2020] F. Errica, M. Podda, D. Bacciu, et al. A fair comparison of graph neural networks for graph classification. In ICLR, 2020.

[Freitas et al., 2021] S. Freitas, Y. Dong, J. Neil, et al. A large-scale database for graph representation learning. In NeurIPS, 2021.

[Gao and Ji, 2019] H. Gao and S. Ji. Graph u-nets. In ICML, 2019.

[Geerts and Reutter, 2022] F. Geerts and J. L. Reutter. Expressiveness and approximation properties of graph neural networks. In ICLR, 2022.

[Gilmer et al., 2017] J. Gilmer, S. Schoenholz, P. F. Riley, et al. Neural message passing for quantum chemistry. In ICML, 2017.

[Haan et al., 2020] P. Haan, de, T. Cohen, and M. Welling. Natural graph networks. In NeurIPS, 2020.

[Hinton et al., 2011] G. E. Hinton, A. Krizhevsky, and S. D. Wang. Transforming auto-encoders. In ICANN, pages 44–51, 2011.

[Hjelm et al., 2019] R. D. Hjelm, A. Fedorov, S. Lavoie-Marchildon, et al. Learning deep representations by mutual information estimation and maximization. In ICLR, 2019.

[Hu et al., 2020a] W. Hu, M. Fey, M. Zitinik, et al. Open graph benchmark: Datasets for machine learning on graphs. In NeurIPS, 2020.

[Huang et al., 2020] Q. Huang, M. Yamada, Y. Tian, and other. Graphlime: Local interpretable model explanations for graph neural networks. arXiv, 2020.

[Ivanov and Burnaev, 2018] S. Ivanov and E. Burnaev. Anonymous walk embeddings. In ICML, pages 2186–2195, 2018.

[Ivanov et al., 2019] S. Ivanov, S. Sviridov, and E. Burnaev. Understanding isomorphism bias in graph data sets. arXiv, 2019.

[Kang et al., 2012] U. Kang, H. Tong, and J. Sun. Fast random walk graph kernel. In SDM, pages 828–838. SIAM, 2012.

[Khasahmadi et al., 2020] A. H. Khasahmadi, K. Hassani, P. Moradi, et al. Memory-based graph networks. In ICLR, 2020.

[Kipf and Welling, 2017] T. N. Kipf and M. Welling. Semi-supervised classification with graph convolutional networks. In ICLR, 2017.

[Klicpera et al., 2021] J. Klicpera, F. Becker, and S. Günnemann. Gemnet: Universal directional graph neural networks for molecules. In NeurIPS, 2021.

[Knyazev et al., 2021] B. Knyazev, M. Drozdžal, G. W. Taylor, et al. Parameter prediction for unseen deep architectures. In NeurIPS, 2021.

[Kondor et al., 2018] R. Kondor, H. T. Son, H. Pan, et al. Covariant compositional networks for learning graphs. In ICLR, 2018.

[Kriege et al., 2020] N. M. Kriege, F. D. Johansson, and C. Morris. A survey on graph kernels. Appl. Netw. Sci., 5(1):1–42, 2020.

[Kudo et al., 2004] T. Kudo, E. Maeda, and Y. Matsumoto. An application of boosting to graph classification. In NeurIPS, 2004.

[Lanciano et al., 2020] T. Lanciano, F. Bonchi, and A. Gionis. Explainable classification of brain networks via contrast subgraphs. In KDD, pages 3308–3318, 2020.

[Lee et al., 2018] J. B. Lee, R. Rossi, and X. Kong. Graph classification using structural attention. In KDD, 2018.

[Lee et al., 2019] J. Lee, I. Lee, and J. Kang. Self-attention graph pooling. In ICLR, pages 3734–3743, 2019.

[Lee et al., 2021] D. Lee, S. Kim, S. Lee, et al. Learnable structural semantic readout for graph classification. In ICDM, 2021.

[Lei et al., 2017] T. Lei, W. Jin, R. Barzilay, et al. Deriving neural architectures from sequence and graph kernels. In ICDM, 2017.

[Long et al., 2021] Q. Long, Y. Jin, Y. Wu, et al. Theoretically improving graph neural networks via anonymous walk graph kernels. In WWW, pages 1204–1214, 2021.

[Luo et al., 2020] D. Luo, W. Cheng, D. Xu, et al. Parameterized explainer for graph neural network. In NeurIPS, 2020.

[Ma et al., 2019] Y. Ma, S. Wang, C. C. Aggarwal, et al. Graph
convolutional networks with eigenpooling. In KDD, 2019.

[Ma et al., 2020] N. Ma, J. Bu, J. Yang, et al. Adaptive-step graph meta-learner for few-shot graph classification. In CIKM, 2020.

[Ma et al., 2021] X. Ma, J. Wu, S. Xue, et al. A comprehensive survey on graph anomaly detection with deep learning. IEEE Trans. Knowl. Data Eng., 2021.

[Maron et al., 2019] H. Maron, H. Ben-Hamu, H. Serviansky, et al. Provably powerful graph networks. In NeurIPS, 2019.

[Mckay and Piperno, 2014] B. D. McKay and A. Piperno. Practical graph isomorphism, ii. J. Symbolic Comput., 60:94–112, 2014.

[Medsker and Jain, 2001] L. R. Medsker and L. Jain. Recurrent neural networks. Design and Applications, 5:64–67, 2001.

[Mesquita et al., 2020] D. Mesquita, A. H. Souza, and S. Kaski. Rethinking pooling in graph neural networks. In NeurIPS, 2020.

[Morgan, 1965] H. L. Morgan. The generation of a unique machine description for chemical structures-a technique developed at chemical abstracts service. J. chem. doc., 5(2):107–113, 1965.

[Morris et al., 2019] C. Morris, M. Ritzert, M. Fey, et al. Weisfeiler and leman go neural: Higher-order graph neural networks. In AAAI, pages 4602–4609, 2019.

[Morris et al., 2020] C. Morris, N. M. Kriege, F. Bause, et al. Benchmark data sets for graph kernels. https://chrsmrrs.github.io/datasets/, 2020.

[Murphy et al., 2019] R. Murphy, B. Srinivasan, V. Rao, et al. Relational pooling for graph representations. In ICML, 2019.

[Narayanan et al., 2017] A. Narayanan, M. Chandramohan, R. Venkatesan, et al. graph2vec: Learning distributed representations of graphs. CoRR, abs/1707.05005, 2017.

[Niepert et al., 2016] M. Niepert, M. Ahmed, and K. Kutzkov. Learning convolutional neural networks for graphs. In ICML, pages 2014–2023, 2016.

[Nikolentzos et al., 2021] G. Nikolentzos, G. Siglidis, and M. Vazirgiannis. Graph kernels: A survey. J. Artif. Intell., 2021.

[Pope et al., 2019] P. E. Pope, S. Kolouri, M. Rostami, et al. Explainability methods for graph convolutional neural networks. In CVPR, pages 10772–10781, 2019.

[Qiu et al., 2020] J. Qiu, Q. Chen, Y. Dong, et al. Gcc: Graph contrastive coding for graph neural network pre-training. In KDD, pages 1510–1520, 2020.

[Ralaivola et al., 2005] L. Ralaivola, S. J. Swamidass, H. Saigo, et al. Graph kernels for chemical informatics. Neural Netw., 18(8):1093–1110, 2005.

[Ranjan et al., 2020] E. Ranjan, S. Sanyal, and P. Talukdar. Asap: Adaptive structure aware pooling for learning hierarchical graph representations. In AAAI, pages 5470–5477, 2020.

[Sato, 2020] R. Sato. A survey on the expressive power of graph neural networks. arXiv, 2020.

[Satorras et al., 2021] G. Satorras, E. Hoogeboom, and M. Welling. Provably powerful graph networks. In IJCAI, 2021.

[Sawlani et al., 2021] S. Sawlani, L. Zhao, and L. Akoglu. Fast attributed graph embedding via density of states. In ICDM, 2021.

[Shervashidze et al., 2009] N. Shervashidze, S. Vishwanathan, T. Petri, et al. Efficient graphlet kernels for large graph comparison. In AISTATS, pages 488–495, 2009.

[Shervashidze et al., 2011] N. Shervashidze, P. Schweitzer, E. J. Van Leeuwen, et al. Weisfeiler-lehman graph kernels. J Mach Learn Res, 12(9), 2011.

[Simonovsky and Komodakis, 2017] M. Simonovsky and N. Komodakis. Dynamic edge-conditioned filters in convolutional neural networks on graphs. In CVPR, pages 3693–3702, 2017.

[Su et al., 2021] X. Su, S. Xue, F. Liu, et al. A comprehensive survey on community detection with deep learning. IEEE Trans. Neural Netw. Learn. Syst., 2021.

[Sun et al., 2019] F. Sun, J. Hoffmann, V. Verma, et al. Infograph: Unsupervised and semi-supervised graph-level representation learning via mutual information maximization. In ICLR, 2019.

[Thoma et al., 2010] M. Thoma, H. Cheng, A. Gretton, et al. Discriminative frequent subgraph mining with optimality guarantees. Stat Anal Data Min, 3(5):302–318, 2010.

[Togninalli et al., 2019] M. Togninalli, E. Ghisu, F. Llinares-López, et al. Wasserstein weisfeiler-lehman graph kernels. In NeurIPS, 2019.

[Verma and Zhang, 2018] S. Verma and Z. Zhang. Graph capsule convolutional neural networks. In ICML&IJCAI workshop, 2018.

[Wang et al., 2017] S. Wang, L. He, B. Cao, et al. Structural deep brain network mining. In KDD, pages 475–484, 2017.

[Wang et al., 2019] M. Wang, D. Zheng, Z. Ye, et al. Deep graph library: A graph-centric, highly-performant package for graph neural networks. In ICLR Workshop, 2019.

[Wang et al., 2020] H. Wang, D. Lian, Y. Zhang, L. Qin, and X. Lin. Gognn: Graph of graphs neural network for predicting structured entity interactions. In IJCAI, 2020.

[Wei et al., 2021] L. Wei, H. Zhao, Q. Yao, et al. Pooling architecture search for graph classification. In CIKM, 2021.

[Weisfeiler and Leman, 1968] B. Weisfeiler and A. Leman. The reduction of a graph to a canonical form and the algebra which appears therein. NTI, Series, 2(9):12–16, 1968.

[Wijesinghe and Wang, 2022] A. Wijesinghe and Q. Wang. A new perspective on “how graph neural networks go beyond weisfeiler-lehman”. In ICLR, 2022.

[Wu et al., 2020] Z. Wu, S. Pan, F. Chen, et al. A comprehensive survey on graph neural networks. IEEE Trans Neural Netw Learn Syst, 32(1):4–24, 2020.

[Xu et al., 2018] K. Xu, W. Hu, J. Leskovec, et al. How powerful are graph neural networks? In NeurIPS, 2018.

[Xu et al., 2021] K. Xu, M. Zhang, J. Li, et al. How neural networks extrapolate: From feedforward to graph neural networks. In ICLR, 2021.

[Yehudai et al., 2021] G. Yehudai, E. Fetaya, E. Meirom, et al. From local structures to size generalization in graph neural networks. In ICML, pages 11975–11986, 2021.

[Ying et al., 2018] R. Ying, J. You, C. Morris, et al. Hierarchical graph representation learning with differentiable pooling. In NeurIPS, 2018.

[Ying et al., 2019] R. Ying, D. Bourgeois, J. You, et al. Gnnexplainer: Generating explanations for graph neural networks. In NeurIPS, 2019.

[You et al., 2018] J. You, R. Ying, X. Ren, et al. Graphrnn: Generating realistic graphs with deep auto-regressive models. In ICML, pages 5708–5717, 2018.

[You et al., 2020] Y. You, T. Chen, Y. Sui, et al. Graph contrastive learning with augmentations. In NeurIPS, 2020.

[Yuan and Ji, 2020] H. Yuan and S. Ji. Structpool: Structured graph pooling via conditional random fields. In ICLR, 2020.

[Yuan et al., 2020a] H. Yuan, J. Tang, X. Hu, et al. Xgnn: Towards model-level explanations of graph neural networks. In ICLR, 2020.

[Yuan et al., 2020b] H. Yuan, H. Yu, S. Gui, et al. Explainability in graph neural networks: A taxonomic survey. arXiv, 2020.

[Zhang and Chen, 2018] X. Zhang and L. Chen. Capsule graph neural network. In ICLR, 2018.

[Zhang et al., 2018] M. Zhang, Z. Cui, M. Neumann, et al. An end-to-end deep learning architecture for graph classification. In AAAI, 2018.

[Zhang et al., 2020] Z. Zhang, P. Cui, and W. Zhu. Deep learning on graphs: A survey. IEEE Trans. Knowl. Data Eng., 34(1), 2020.

[Zheng et al., 2021] X. Zheng, B. Zhou, J. Gao, et al. How framelets enhance graph neural networks. ICML, 2021.