Graph Learning under Distribution Shifts: A Comprehensive Survey on Domain Adaptation, Out-of-distribution, and Continual Learning

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Abstract—Graph learning plays a pivotal role and has gained significant attention in various application scenarios, from social network analysis to recommendation systems, for its effectiveness in modeling complex data relations represented by graph structural data. In reality, the real-world graph data typically show dynamics over time, with changing node attributes and edge structure, leading to the severe graph data distribution shift issue. This issue is compounded by the diverse and complex nature of distribution shifts, which can significantly impact the performance of graph learning methods in degraded generalization and adaptation capabilities, posing a substantial challenge to their effectiveness. In this survey, we provide a comprehensive review and summary of the latest approaches, strategies, and insights that address distribution shifts within the context of graph learning. Concretely, according to the *observability* of distributions in the inference stage and the *availability* of sufficient supervision information in the training stage, we categorize existing graph learning methods into several essential scenarios, including graph domain adaptation learning, graph out-of-distribution learning, and graph continual learning. For each scenario, a detailed taxonomy is proposed, with specific descriptions and discussions of existing progress made in distribution-shifted graph learning. Additionally, we discuss the potential applications and future directions for graph learning under distribution shifts with a systematic analysis of the current state in this field. The survey is positioned to provide general guidance for the development of effective graph learning algorithms in handling graph distribution shifts, and to stimulate future research and advancements in this area.

Index Terms—Graph learning, graph neural network, domain adaptation, out-of-distribution learning, continual learning

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1 INTRODUCTION

G RAPH structural data is ubiquitous in various real-world application domains, including social networks [1], [2], [3], [4], [5], biological networks [6], [7], [8], [9], road networks [10], [11], [12], and computer networks [13], [14], [15]. In these diverse domains, complex relationships among nodes, intricately woven through edges, harbor valuable information within entities, graph structures, and overarching graph data patterns. In this case, graph learning [16] techniques have arisen as responses to better analyzing and understanding various graph types, serving a wide range of graph-related tasks with promising inference abilities, covering drug discovery [8], [17], knowledge graph exploration [18], [19], social network analysis [20], [21],

recommender systems [22], [23], and physical movement prediction[24], etc.

Despite the success of prevalent graph learning approaches, the presence of *distribution shifts* in graph data poses a substantial constraint on the capabilities of current methods [25]. This is due to the dynamic and evolving nature of real-world graph data. For example, social networks evolve with new users and shifting relationships over time, leading to significant variations on node features and edge connections, so that the performance of graph learning models would degrade on recommendation systems or trend analysis [26]. In financial networks, the relationships between entities (like stocks, commodities, or institutions) change due to market trends, economic policies, or global events [27], [28]. A graph learning model trained on historical market data might underperform when the underlying relationships between entities shift. In biology, networks representing interactions between proteins, genes, or species in an ecosystem can change due to mutations, environmental pressures, or disease outbreaks [29]. Models predicting disease spread or gene interactions must adapt to these shifts. In addition, transportation systems (like road networks, air traffic, or public transit systems) experience shifts due to factors like urban development, changes in travel patterns, or infrastructure modifications. These shifts impact models used for optimizing routes, predicting congestion, or planning new infrastructure [30]. These shifts in statistical distributions of graph data observed in nodes, edges, and different graphs considerably complicate the graph learning

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process, posing challenges for effective model deployment and application in real-world scenarios.

To this end, in this work, our focus is on engaging in **graph learning under distribution shifts**, specifically referring to the scenarios where the disparities of graph data probability distributions might encompass all aspects of graph components, including node features, graph structures, and label distributions. Consequently, graph learning models encounter difficulties in achieving precise generalization to previously unseen graph data distributions during the testing phase.

In recent years, there has been a growing interest in exploring the paradigms of graph learning under distribution shifts [31], [3], [4], [32], [25], [33], [34], [35], [36], [37], [38], [39], [40], to enable models to comprehend complex scenes, objects, and concepts in both static and dynamic scenarios for graph data. Concretely, the graph data distribution shift scenarios can be categorized based on *whether the test-stage distributions are observable* and *whether the available supervision information is sufficient*. Therefore, they can be classified into three main categories, as shown in Fig. 1:

- **Observed Shifts: Known test-stage data, variable supervision**, where observed test-stage graph data that may exhibit potential unknown distribution shifts from the training stage, available supervisions could be either sufficient or insufficient
- **Unobserved Shifts: Unknown test-stage data, limited supervision**, where unobserved test-stage graph data distributions with diverse and multiple shift types, available supervisions typically tend to be insufficient
- **Sequential Temporal Shifts: Time-dependent, unobserved data**, where unobserved test-stage graph data distributions that arrive sequentially with dynamic temporal shifts over time.

Based on these three types of graph data distribution shift scenarios, in this work, we conduct a comprehensive review and provide a systematic taxonomy of existing graph learning methods that deal with the challenges of distribution shift learning in graph data. Concretely, current graph learning methods can also be classified into three categories, with each category corresponding to a particular distribution shift scenario:

- **Graph Domain Adaptation Learning**, aims to transfer graph learning models from a training (source) domain to a test (target) domain and require their proficient performance on the target domain with differing graph data distributions [31], [41], [42], [3], [43], [4]. → *Observed Shifts*.
- **Graph Out-of-distribution Learning**, aims to empower the graph learning models to effectively learn test graph data with different distributions from the training data and potential new classes unseen in training [44], [25], enabling models' well generalization capabilities. → *Unobserved Shifts*.
- **Graph Continual Learning**, aims to enable graph learning models to assimilate new information contingent upon changes in the evolving graph data distributions, while concurrently refining pre-existing
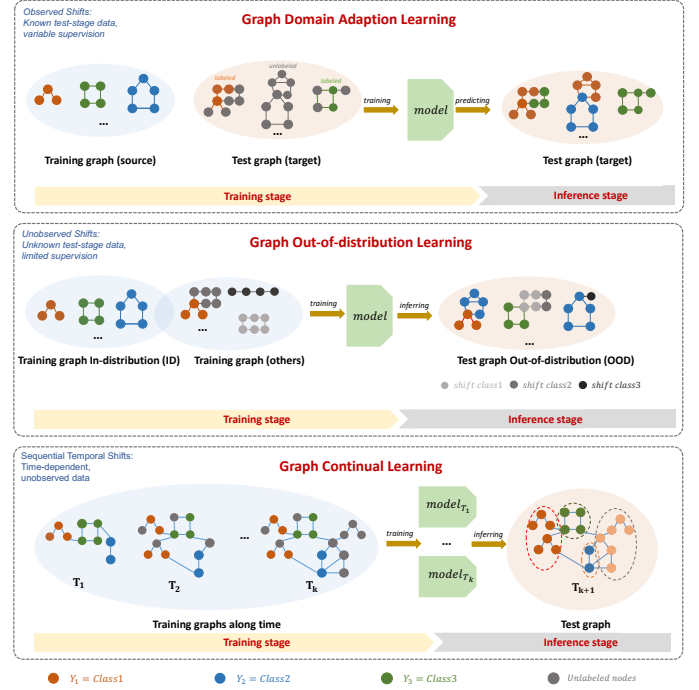

Fig. 1: Overview of graph data distribution shifts and corresponding graph learning methods.

knowledge and addressing nascent and previously unseen tasks [45], [46]. → *Sequential Temporal Shifts*.

Therefore, in this survey, our goal is to provide an in-depth understanding of graph data distribution shifts and delve into various graph learning models and approaches that tackle distribution shift challenges. We will examine key concepts, critical challenges, previous limitations, and evaluation protocols associated with graph learning under distribution shifts. Moreover, we will discuss the potential real-world applications and highlight the promising future directions within this research area. To the best of our knowledge, this is the first comprehensive survey on graph learning with general distribution shift scenarios. Nevertheless, it is worth establishing connections between our work and several prior studies that concentrate on specific aspects of graph distribution shift: Li et al. [25] reviewed the graph out-of-distribution generalization methods and Yang et al. [44] reviewed the graph out-of-distribution detection methods, which are two types of out-of-distribution tasks under the unobserved graph data shift scenario, respectively. Liu et al. [47] reviewed the graph out-of-distribution adaptation methods under the observed/unobserved graph data shift scenario. Yuan et al. [45] and Febrinanto et al. [46] reviewed the graph continual learning methods and benchmarks under the sequential temporal graph data shift scenario. In contrast, our emphasis is distinctly placed on a broader perspective of graph learning under distribution shifts. This encompasses a more extensive and fresh method review to furnish a more comprehensive research roadmap.

We envision that this survey will serve as an important resource for researchers and practitioners interested in graph learning under distribution shifts, provide insights into the latest developments and future research efforts, and

facilitate informed decision-making in the areas of model selection, architectural design, and evaluation strategies for the continuous development of graph learning models, with potential benefits for both academic and industrial applications.

In summary, the core contributions of this survey work can be presented as follows:

- **Broad-ranging Graph Distribution Shift Scenarios.** To the best of our knowledge, this is the first survey work in the field of graph learning covering broad-ranging graph distribution shift scenarios, facilitating in-depth understanding and analysis for dealing with diverse and complex graph data distribution shift cases.
- **Comprehensive Review and Taxonomy.** We provide a systematic taxonomy of existing graph learning advancements with various distribution shifts. This taxonomy includes three key categories: graph domain adaptation learning for observable shifts with known test-stage graphs, graph out-of-distribution learning for unobserved shifts with unknown test-stage graphs, as well as graph continual learning for sequential temporal shifts with time-evolving graphs.
- **Highlighted Practical Applications and Future Direction.** We highlight the practical utility of graph learning in addressing distribution shifts, spanning from applications in scientific discovery to personalized daily life recommendations. Additionally, we identify several promising future research directions, intending to inspire and propel the progress of this research field.

2 PROBLEM DEFINITION

In this section, we outline the background of graph neural networks, list commonly used notations, and define graph related concepts.

Given a graph $G = (V, E)$ where $V = \{v_1, \cdots, v_N\}$ is the node set with N nodes and $E = \{e_{i,j} | i, j = 1, \ldots, N\} \in V \times V$ is the edge set. The neighbor set of node v is denoted as $\mathcal{N}(v) = \{u : (v, u) \in E\}$. The node features are represented by a feature matrix $\mathbf{X} \in \mathbb{R}^{N \times d}$, where the i-th row $\mathbf{x}_i \in \mathbb{R}^d$ is the feature vector of node v_i and d is the number of feature dimensions. The topological structure of G is represented by the adjacency matrix $\mathbf{A} \in \{0, 1\}^{n \times n}$, where $\mathbf{A}_{i,j} = 1$ if the nodes v_i and v_j are connected, *i.e.*, $\exists e_{i,j} \in E$, otherwise $\mathbf{A}_{i,j} = 0$. $\mathbf{Y} \in \mathbb{R}^{N \times C}$ is the node label matrix of G, where C is the already-known classes used for training with $\mathcal{Y} = \{1, \cdots, C\}$. Therefore, a graph is composed of node features, topological structure, as well as node labels, denoted as $G = (\mathbf{X}, \mathbf{A}, \mathbf{Y})$.

Moreover, given a set of graphs with M graphs, we have $\mathbb{G} = \{(G_1, y_1), \ldots, (G_M, y_M)\}$, and $\mathbb{Y} = \{y_i \in \mathbb{R}^{1 \times K}\}_{i=1}^M$ is the label set of the graph set. Here, each label y_i corresponds to one of the K classes to which the graph G_i belongs. In this section, we primarily focus on illustrating the concepts of various graph distribution learning methodologies through the lens of node-level graph learning tasks. These principles can be readily extended to encompass edge-level and graph-level learning scenarios as well.

Definition 1 (Conventional Closed-set Graph Learning). *Given a graph $G = (\mathbf{X}, \mathbf{A}, \mathbf{Y})$, a GNN model $f_{\boldsymbol{\theta}}(\cdot)$ takes the node attributes $\mathbf{X}$ and graph structure $\mathbf{A}$ as inputs. With the assumption that test data distribution $\mathcal{P}_{te}$ and train data distribution $\mathcal{P}_{tr}$ share the same feature space and label space, for typical closed-set graph learning problem, the feature encoder and the classifier of the GNN model are optimized to minimize the expected risk [48] as*

$$f_{\boldsymbol{\theta}^*} = arg \min_{\boldsymbol{\theta}} \mathbb{E}_{G \sim \mathcal{P}_{tr}}[\mathcal{L}(f_{\boldsymbol{\theta}}(\mathbf{X}, \mathbf{A}), \mathbf{Y})] \qquad (1)$$

where $f_{\boldsymbol{\theta}^*}$ is the optimal GNN model trained on the training graph that achieves the minimal loss. And the loss function $\mathcal{L}(\cdot)$ measures the discrepancy between the output prediction $\hat{\mathbf{Y}} = f_{\boldsymbol{\theta}}(\mathbf{X}, \mathbf{A})$ and the ground-truth node labels $\mathbf{Y}$. Generally, $\mathcal{L}(\cdot)$ can be the cross-entropy function to discriminate between known classes.

In this case, on the test graph $G_{te} = (\mathbf{X}_{te}, \mathbf{A}_{te}) \sim \mathcal{P}_{te}$, we have $\hat{\mathbf{Y}}_{te} = f_{\boldsymbol{\theta}^*}(\mathbf{X}_{te}, \mathbf{A}_{te})$ for making inference of the test node labels.

Definition 2 (Graph Domain Adaptation Learning). *Given a graph $G_{src} = (\mathbf{X}_{src}, \mathbf{A}_{src}, \mathbf{Y}_{src}) \sim \mathcal{P}_{src}$ with sufficient labeled instances that are drawn from the source distribution $\mathcal{P}_{src}$ called the source domain, and a target graph $G_{tgt} = (\mathbf{X}_{tgt}, \mathbf{A}_{tgt}, \mathbf{Y}_{tgt}^\dagger) \sim \mathcal{P}_{tgt}$ with a small number of labels (subscript† denotes partially observed labels) or no labels $\mathbf{Y}_{tgt}^\dagger = \emptyset$ that are drawn from the target distribution $\mathcal{P}_{tgt}$ called the target domain, where $\mathcal{P}_{src} \neq \mathcal{P}_{tgt}$ but all nodes in G_{src} and G_{tgt} are constrained in the same C-classes as $\{\mathbf{Y}_{src}, \mathbf{Y}_{tgt}\} \in \mathcal{Y} = \{1, \cdots, C\}$.*

The goal of graph domain adaptation is to learn an optimal graph learning model $f_{\boldsymbol{\theta}^*}$ with both the source and target domains, so that it can achieve the minimal loss on the target domain, and the marginal distributions satisfy:

$$f_{\boldsymbol{\theta}^*} = \operatorname*{argmin}_{\boldsymbol{\theta}} \mathbb{E}_{G_{src} \sim \mathcal{P}_{src}, G_{tgt} \sim \mathcal{P}_{tgt}}[\mathcal{L}_{GDA}(f_{\boldsymbol{\theta}}(G_{src}, G_{tgt})].$$
$$(2)$$

In graph domain adaptation (GDA), both the source distribution $\mathcal{P}_{src}$ and the target distribution $\mathcal{P}_{tgt}$ are available during training. For different application scenarios of GDA research, the loss function $\mathcal{L}_{GDA}(\cdot)$ would show different formulations. For instance, in unsupervised GDA, the given target domain is totally unlabeled with $\mathbf{Y}_{tgt}^\dagger = \emptyset$, $\mathcal{L}_{GDA}(\cdot)$ would be an unsupervised learning objective without using the target domain labels. Moreover, in semi-supervised GDA, the given target domain contains a small number of labels with $\mathbf{Y}_{tgt}^\dagger \neq \emptyset$, $\mathcal{L}_{GDA}(\cdot)$ could use partial target domain labels to optimize graph machine learning models.

Definition 3 (Graph Out-of-distribution Learning). *Given a training graph $G_{tr} = (\mathbf{X}_{tr}, \mathbf{A}_{tr}, \mathbf{Y}_{tr}) \sim \mathcal{P}_{tr}$ where $\mathbf{Y}_{tr} \in \mathcal{Y}_{tr} = \{1, \ldots, C\}$, and a test graph $G_{te} = (\mathbf{X}_{te}, \mathbf{A}_{te}, \mathbf{Y}_{te}) \sim \mathcal{P}_{te}$ where $\mathbf{Y}_{te} \in \mathcal{Y}_{te} = \{1, \ldots, C, C + 1, \ldots\}$, denoting there exists unseen node classes from $\{C + 1, \ldots\}$ in the test graph, and $\mathcal{P}_{tr} \neq \mathcal{P}_{te}$, **open-world graph learning** aims to learn an optimal graph function $f_{\boldsymbol{\theta}^*}$ that can achieve the minimal loss on the training distribution P_{tr} and also achieve optimal performance on data from the test distribution P_{te} that may contain new label space $\overline{\mathcal{Y}} = \{1, \ldots, C, unknown\}$, where $\mathcal{Y}_{te} \supseteq \overline{\mathcal{Y}} \supset \mathcal{Y}_{tr}$ with the minimization of the expected risk [48]:*

$$f_{\boldsymbol{\theta}^*} = arg \min_{\boldsymbol{\theta}} \mathbb{E}_{G_{tr} \sim \mathcal{P}_{tr}, G_{te} \sim \mathcal{P}_{te}}[\mathcal{L}_{G-OOD}(f_{\boldsymbol{\theta}}(G_{tr})]. \quad (3)$$

TABLE 1: A summary of information used in graph domain adaption learning, graph out-of-distribution learning, and graph continual learning in both training and inference stages.

	Training	Inference	Labels
Graph Domain Adaption Learning	$G_{src}(tr), G_{tgt}(te)$	$G_{tgt}(te)$	$\mathbf{Y}_{tgt} \subseteq \mathbf{Y}_{src}$
Graph Out-of-distribution Learning	G_{tr}	G_{te}	$\mathbf{Y}_{tr} \subseteq \mathbf{Y}_{te}$
Graph Continual Learning	$G_{tr}^{(t)}\|_{t=t_0}^{t_k}$	$G_{te}^{(t')}\|_{t'=t_{k+1}}^{t_m}$	$\mathbf{Y}_{tr} \subseteq \mathbf{Y}_{te}$

Here, in open-world graph learning, only the training graph distribution $\mathcal{P}_{tr}$ is available during training, and the test distribution $\mathcal{P}_{te}$ is unavailable. The predicted class $unknown \in \overline{\mathcal{Y}}$ contains a group of novel categories, which may contain more than one class.

When only focusing on the detection of the unseen-class nodes, the problem degenerates into Graph OOD detection problem, i.e., a binary-class problem to learn whether a test example is from seen classes $\mathcal{Y}_{tr}$ or not. In addition, When $Y_{te} = Y_{tr}$, i.e. there is no unseen class during test, the model only concentrates on the feature distribution shift (i.e. the difference between the $\mathcal{P}_{te}$ and $\mathcal{P}_{tr}$), the problem will degenerate to **graph OOD generalization** *problem. We refer to* **graph OOD generalization, graph OOD detection** *and* **open-world graph learning** *collectively as* **graph out-of-distribution (G-OOD) learning**. *A more detailed taxonomy is illustrated in section 3.2 and Fig. 2.*

Both GDA and G-OOD aim to transfer the learned knowledge from a training set to a test set with a different data distribution. Differently, graph continual learning (GCL) aims to adapt to the dynamics in real-world applications by continually training the graph learning model on a sequence of training sets with evolving data distributions.

Definition 4 (Graph Continual Learning). *Given a sequence of training graphs $\mathcal{D}_{tr} = \{G_{tr}^{(t)}\}_{t=t_0}^{t_k}$ that are drawn from the training distribution $\mathcal{P}_{tr}$, where t is the index of the training task at the t-th time step. And when $\forall t \neq t'$, we have $\mathcal{P}_{tr}^{(t)} \neq \mathcal{P}_{tr}^{(t')}$. In this case, the goal of graph continual learning (GCL) is to learn an optimal graph learning model $f_{\boldsymbol{\theta}^*}$ incrementally from the sequential training graph set. At the learning session t, only the training graph $G_{tr}^{(t)} \sim \mathcal{P}_{tr}^{(t)}$ can be accessed as:*

$$f_{\boldsymbol{\theta}^{(t)*}} = \underset{\boldsymbol{\theta}^{(t)}}{\arg\min} \, \mathbb{E}_{G_{tr}^{(t)} \sim P_{tr}^{(t)}}[\mathcal{L}_{GCL}(f_{\boldsymbol{\theta}^{(t)}}(G_{tr}^{(t)}))]. \quad (4)$$

$f_{\boldsymbol{\theta}^{(t)*}}$ is expected to achieve the minimal loss on the data drawn from the test distribution $G_{te}^{(t')} \sim \mathcal{P}_{te}^{(t')}$ after any learning session $t' >= t$, as $f_{\boldsymbol{\theta}^{(t)*}}(G_{te}^{(t')}) = \mathbf{Y}_{te}^{(t')}$

Overall, the summary of the information used by these three research problems in both the training and inference stages is presented in Table 1. Specifically, graph domain adaptation learning (GDA) and graph out-of-distribution learning (G-OOD) are more concerned with the distribution shifts of static data. The main difference between them is that GDA deals with observed shifts, meaning it handles known test-stage data, whereas G-OOD tackles unobserved shifts, or unknown test-stage data. In contrast, graph continual learning (GCL) targets the distribution shifts of dynamic data, focusing on sequential temporal shifts.
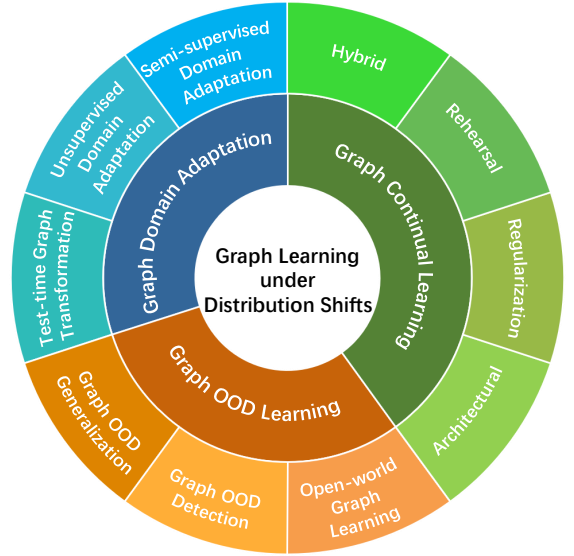

Fig. 2: Overview of the general taxonomy of graph learning under distribution shifts.

3 CATEGORIZATION AND FRAMEWORKS

Fig. 3 summarizes the general taxonomy of graph learning under distribution shifts and the related methods reviewed in this paper. The taxonomy is centered on the shifting scenarios and design details of the graph learning algorithms under distribution shifts. To begin with, according to the shifting scenarios of the explanations, methods for graph learning under distribution shifts can be classified into three categories: Graph domain adaptation, out-of-distribution graph learning and continual graph learning. We further consider the design details of different methods and classify them in a hierarchical manner for ease of understanding and comparative analysis.

3.1 Taxonomy of Graph Domain Adaptation Learning

Domain adaptation addresses the issue of declining model performance due to differences in data distributions across different domains, aiming to enhance the model's generalization capability on the target domain. Domain adaptation methods can be further categorized into three types: semi-supervised, unsupervised, and test-time graph transformation.

Semi-supervised Domain Adaptation. These approaches focus on training the model using labeled data from the source domain as well as unlabeled data from both the source and target domains, aiming to ensure a strong performance in the target domain.

Unsupervised Domain Adaptation. These methods concentrate on model transfer without the availability of labeled target domain data. The core idea is to reduce the feature distribution differences between the source and target domains through feature alignment, thereby enhancing the model's generalization ability to the target domain.

Test-time Graph Transformation (Adaptation). These approaches are centered around adjusting the graph data of the target domain during testing to match the characteristics
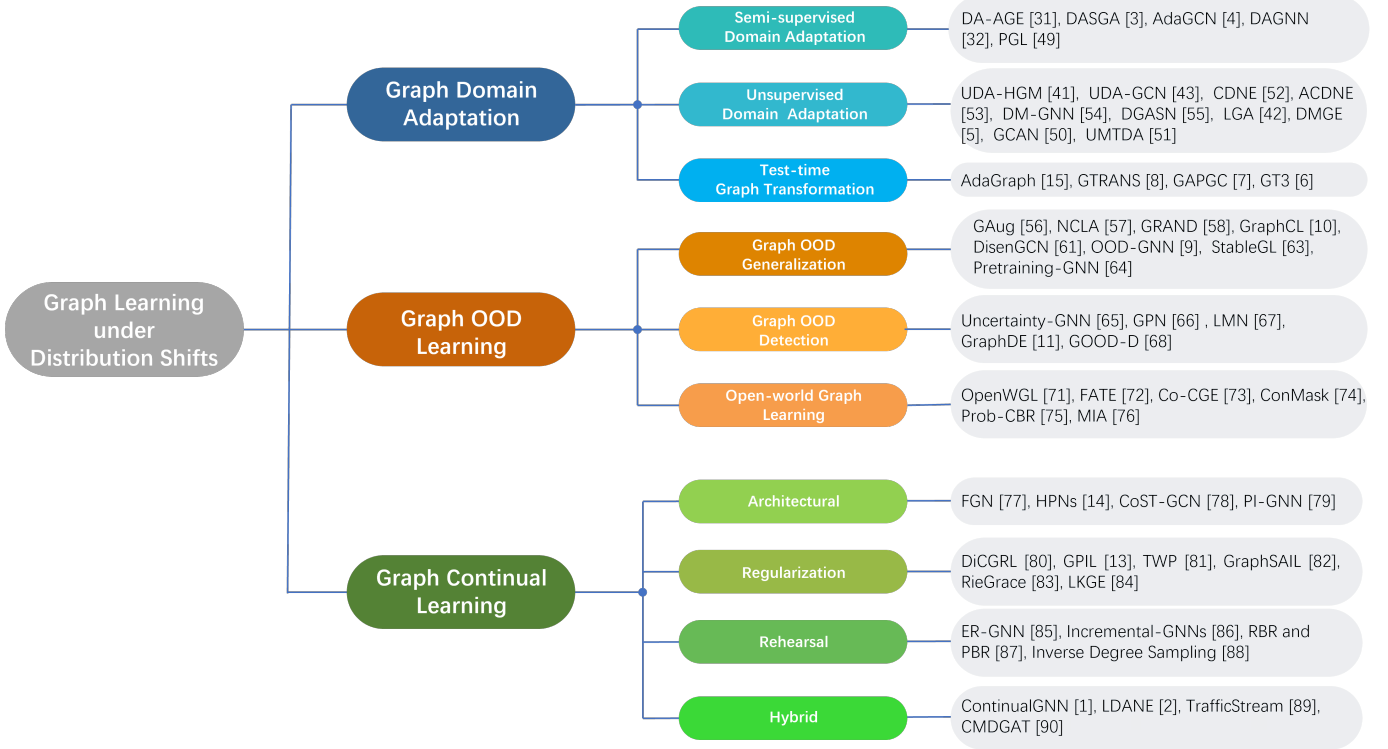
Fig. 3: Hierarchical classification of graph learning under distribution shifts.

of the target domain, enhancing the model's adaptability to the target domain.

3.2 Taxonomy of Graph Out-of-distribution Learning

Out-of-distribution (OOD) graph learning addresses the challenge of learning from graphs with different features than those seen during training. OOD graph learning can be further categorized into three types: Graph Out-of-Distribution Generalization, Graph Out-of-Distribution Detection, and Open-world Graph Learning.

Graph Out-of-distribution Generalization. This type of OOD graph learning focuses on developing models that can generalize well to graphs with different features than the ones seen in training. The goal is to ensure that the model's performance remains satisfactory even when confronted with graphs from previously unseen distributions.

Graph Out-of-distribution Detection. In this scenario, the focus is on identifying or detecting graphs that belong to out-of-distribution categories. The goal is to design models capable of flagging or distinguishing graphs that significantly deviate from the training data distribution, potentially indicating new or unfamiliar graph patterns.

Open-world Graph Learning. Open-world graph learning deals with the challenge of learning in situations where the set of possible graph classes is not known in advance. This means that the model must not only adapt to new graph classes but also make decisions about classifying data into known classes or identifying data as belonging to a novel class.

3.3 Taxonomy of Graph Continual Learning

Continual graph learning addresses the challenge of acquiring knowledge from a streaming of graph data that arrives over time and continuously evolves. The methods of continual graph learning can be further classified into four categories: architectural, regularization, rehearsal, and hybrid.

Architectural Approach. These approaches focus on modifying the specific architecture of networks, activation functions, or layers of algorithms to address a new task and prevent the forgetting of previous tasks.

Regularization Approach. These approaches consolidate the learned knowledge by adding a regularization item to the loss function, constraining the neural weights from updating in a direction that compromises performance on prior tasks.

Rehearsal Approach. These approaches maintain a memory buffer preserving the information of prior tasks and replay it when learning new tasks to mitigate catastrophic forgetting.

Hybrid Approach. These approaches combine more than one continual learning approach to take advantage of multiple approaches and improve the performance of models.

4 GRAPH DOMAIN ADAPTATION LEARNING

Domain adaptation is the task of transferring knowledge learned from a source domain to a target domain where the distribution of the data is different. In the context of graph learning, domain adaptation refers to the task of adapting graph-based learning models to new domains where the graph structure, node features, or edge features may be different. The requirement for domain adaptation in graph learning arises in many real-world applications where the graph data may change over time, or where
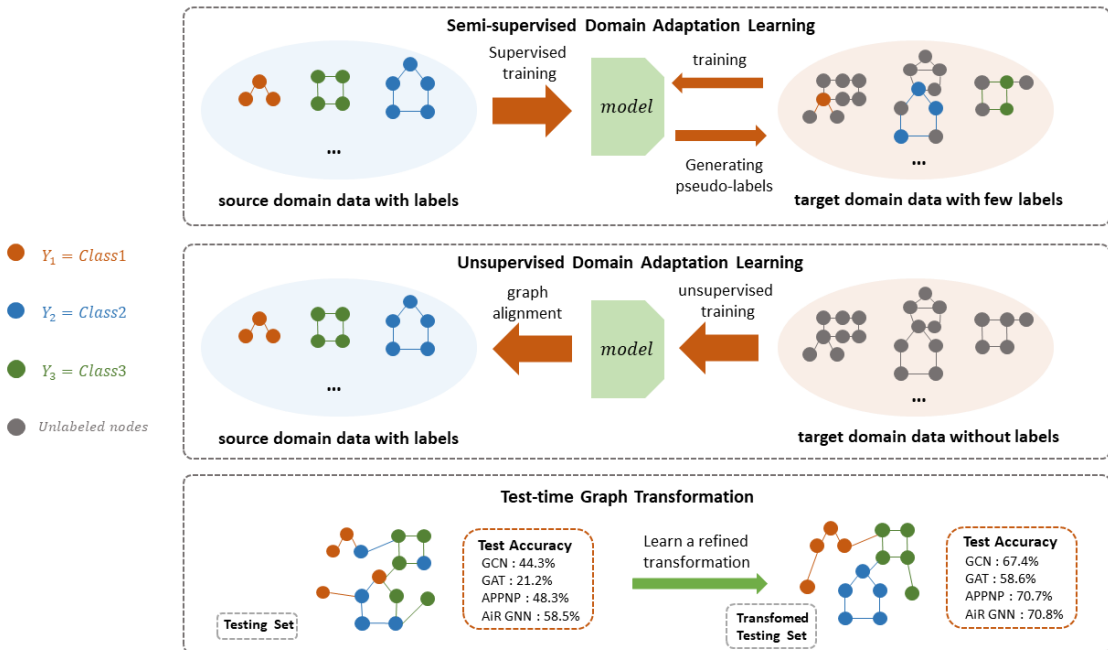
Fig. 4: The overview of graph domain adaptation learning.

models trained on one dataset need to be applied to a new dataset with different characteristics. For example, in social network analysis, models trained on one social network may not generalize well to a different social network due to differences in the graph structure and user behavior. In drug discovery, models trained on one set of molecules may not generalize well to a different set of molecules due to differences in the chemical properties of the molecules.

The methods for graph domain adaptation can be roughly divided into three groups: semi-supervised domain adaptation [31], [3], [4], [32], [49], unsupervised domain adaptation [41], [43], [42], [5], [50], [51], and test-time graph transformation (adaptation) [15], [8], [7], [6]. The categories of graph domain adaptation are shown in Fig. 4.

- **Semi-supervised Domain Adaptation**. These approaches involve adapting from a source domain to a target domain using a small amount of labeled data and unlabeled data from the target domain.
- **Unsupervised Domain Adaptation**. These approaches aim to enhance the model's cross-domain generalization performance by reducing the distribution discrepancy between the source and target domains through feature alignment, without relying on any labeled target data.
- **Test-time Graph Transformation (Adaptation)**. These approaches refer to adjusting the graph data of the target domain during testing to accommodate the characteristics of the target domain. This approach aims to enhance the performance of a model by fine-tuning its behavior based on the specifics of the target domain during the testing phase.

4.1 Semi-supervised Domain Adaptation

Semi-supervised domain adaptation denotes a circumstance wherein labeled data is accessible within the source domain,

whereas the target domain possesses a limited fraction of labeled data. The primary aim of this paradigm is to bolster the model's efficacy within the target domain through adept utilization of these labeled data instances from the source domain, along with any potentially available labeled data within the target domain. At its essence, this approach amalgamates the principles of supervised and unsupervised learning. This synergy is directed towards orchestrating a more potent adaptation to the data distribution inherent within the target domain. The ultimate aspiration is to engender robust predictive outcomes within this new domain context.

DA-AGE [31] is a model based on adversarial domain adaptation, designed to address distribution shift issues. It combines graph-based semi-supervised learning techniques within the framework of deep learning to leverage unlabeled data. This model is capable of training deep neural network (DNN) models using both labeled and unlabeled data, thereby tackling challenges arising from data distribution differences between the source and target domains.

DASGA [3] is a method used for graph domain adaptation. This algorithm is based on scenarios where the source graph has a larger number of annotated nodes. It achieves this by learning the label function spectrum in the source graph and transferring it to the target graph, even when the target graph has fewer labeled nodes. This process relies on transformations between Fourier bases to address the lack of one-to-one correspondence between Fourier basis vectors in two independently constructed graph domains, thus enabling flexible alignment between these two graphs.

AdaGCN [4] is a graph transfer learning framework that combines adversarial domain adaptation and graph convolution techniques. It consists of two main components: a semi-supervised learning part and an adversarial domain adaptation part. The former aims to utilize the label information available in both the source and target networks
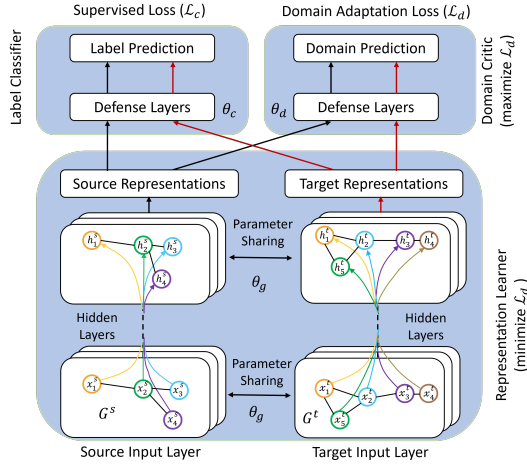
Fig. 5: AdaGCN incorporates adversarial domain adaptation and graph convolution methods.
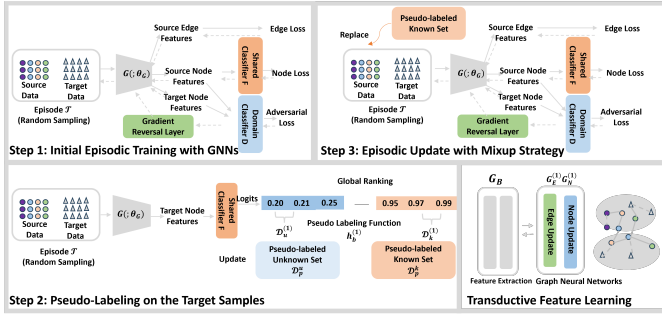

Fig. 6: PGL is an end-to-end progressive graph learning framework that integrates graph neural networks and episodic training.

to learn representations capable of distinguishing nodes of different categories. The role of the latter is to alleviate distribution differences between the source and target domains, thereby promoting the effectiveness of knowledge transfer.

DAGNN [32] is an end-to-end framework for cross-domain text classification. It models documents as graphs, employs domain-adversarial training for feature optimization, and captures non-consecutive semantics. By leveraging knowledge from different domains with hierarchical graph neural networks, DAGNN improves task performance by utilizing relationships and patterns across domains.

PGL [49] is an end-to-end progressive graph learning framework known for integrating graph neural networks with occasional training. This design helps mitigate potential mode collapse and employs adversarial learning to reduce the disparity between the source data distribution and the target data distribution. The framework is aimed at addressing more realistic open-set domain adaptation problems, where the target data may include additional categories not present in the source data.

Discussion. The success of semi-supervised domain adaption relies not only on the generalization capabilities of transfer models but also depends on the in-depth analysis and application of limited labeled data in the target domain. This integrated approach is key for future research and

practice.

4.2 Unsupervised Domain Adaptation

Unsupervised Domain Adaptation is centered on the task of transferring a model's knowledge when there exists an absence of labeled data within the target domain. The principal goal of this paradigm is to augment the model's efficacy within the target domain despite the unavailability of labeled target domain data. This is realized through the strategic alignment of the feature distributions inherent to both the source and target domains. The crux of this approach rests upon the harmonization of features, with the intention of mitigating the dissimilarities existing between the source and target domain features. This alignment is instrumental in empowering the model to adeptly adapt to the distinctive characteristics present within the target domain.

UDA-HGM [41] is an unsupervised domain adaptation method that focuses on unlabeled data in the target domain, emphasizing the correspondence between samples from the source and target domains. The research employs hypergraph representations of the source and target domains, utilizing first-order, second-order, and third-order similarities to achieve hypergraph matching with class regularization. To enhance computational efficiency, the research begins by selecting subsets of samples to construct graphs and then employs a customized optimization method for graph matching using conditional gradients and alternating direction method of multipliers for the matching process.

UDA-GCN [43] is an unsupervised domain adaptation graph convolutional network that focuses on domain adaptation learning for graph data. In its primary stage, it constructs a dual graph convolutional network component that operates on the basis of local and global consistencies to aggregate features. Further, an attention mechanism is applied to establish consistent representations for nodes across different graph domains. Additionally, a domain adaptation learning module is introduced to jointly optimize three different loss functions, facilitating cross-domain knowledge transfer.

CDNE [52] a cross-network deep network embedding model which incorporates domain adaptation into deep network embedding to learn label-discriminative and network-invariant node vector representations. For deep network embedding, CDNE leverages two stacked autoencoders to reconstruct the network proximity matrix of the source network and the target network respectively. Additionally, CDNE designs pairwise constraint to map more strongly connected nodes within each network closer in the embedding space. For domain adaptation, the marginal and class-conditional MMD constraints have been incorporated into CDNE to reduce the distribution shifts between the source and target networks.

ACDNE [53] is an adversarial cross-network deep network embedding model, which integrates adversarial domain adaptation with deep network embedding. On one hand, a deep network embedding module is designed by ACDNE, by utilizing two feature extractors to learn the embeddings from each node's own attributes and its neighbors' attributes respectively. On the other hand, an adversarial domain adaptation module is employed by ACDNE to make
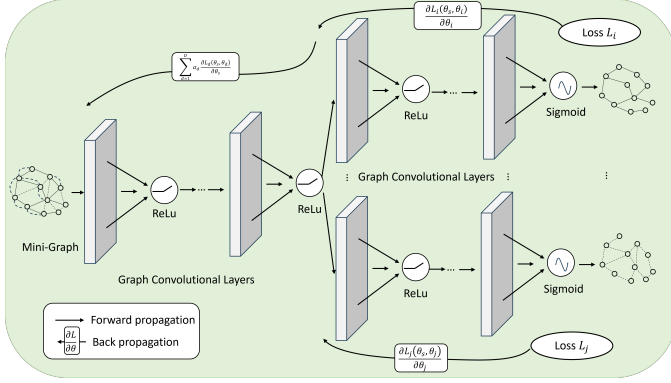
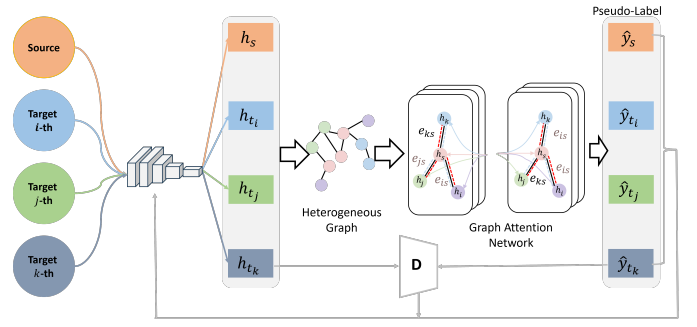Fig. 7: DMGE is a model that utilizes knowledge from different domains.

Fig. 8: UMTDA enables the learning of domain-invariant representations by sharing similar feature representations through heterogeneous graph attention networks.

a domain discriminator compete against the deep network embedding module, so as to learn network-invariant node embeddings.

DM-GNN [54] is a domain-adaptive message passing graph neural network which integrates graph neural network with conditional adversarial domain adaptation. DM-GNN separates ego-embedding learning from neighbor-embedding learning via dual feature extractors. DM-GNN devises a label-aware propagation scheme to promote intra-class propagation while avoiding inter-class propagation, making source embeddings more label-discriminative. To match the class-conditional distributions between the source and the target networks, DM-GNN adopts conditional adversarial domain adaptation.

DGASN [55] is a domain-adaptive graph attention-supervised network designed to address the cross-network homophilous and heterophilous edge classification problem. DGASN proposes to apply direct supervision on graph attention learning guided by the edge labels observed from the source network. Specifically, DGASN assigns lower (higher) attention weights to heterophilous (homophilous) edges during neighborhood aggregation, so as to guarantee more label-discriminative embeddings to separate nodes from different classes.

LGA [42] is a fresh model for enhancing distributional and structural similarities during the adaptation process. It involves embedding data from two domains into a latent space, aligning their distributions by minimizing the maximum mean discrepancy metric. Additionally, the transformed manifold is represented using graphs to maximize graphical structural similarities within the embedding space. This is accomplished by minimizing the spectrum distance between graph Laplacians of the embeddings. The spectrum retains intrinsic manifold information and remains unchanged under data reordering and eigenspace unitary transformations.

DMGE (Deep Multi-Graph Embedding) [5] is a model enhancing task performance by leveraging knowledge from different domains. It constructs a multi-graph based on the behaviors of users from different domains and utilizes a multi-graph neural network to learn cross-domain representation in an unsupervised manner. Particularly, a multiple gradient descent optimizer is used for efficiently training the model.

GCAN [50] is an end-to-end graph convolutional adversarial network that achieves unsupervised domain adaptation by jointly modeling data structures, domain labels, and class labels within a unified deep framework. Additionally, the model incorporates three effective alignment mechanisms: structure-aware alignment, domain alignment, and class centroid alignment. These alignment mechanisms aid in learning domain-specific features and semantic representations, thereby reducing disparities between different domains and enabling effective domain adaptation.

UMTDA [51] is a method designed for the scenario of multiple unlabeled target domains and one labeled source domain, aiming to perform deep semantic information propagation. Through a heterogeneous graph attention network, it strives to learn a shared unified subspace that allows all domains to share similar feature representations. In this process, attention mechanisms are used to optimize relationships between multiple domain samples, facilitating enhanced semantic propagation. Subsequently, by leveraging the graph attention network, it predicts pseudo-labels for the target domains. By aligning the centroids of the labeled source domain and the pseudo-label target domain, it achieves the learning of domain-invariant representations.

Discussion. A key challenge in unsupervised domain adaption is ensuring that models can generalize well from the source to the target domain without losing the critical information encoded in the graph structures. Future research should focus on enhancing these models to better handle the nuances of graph data, exploring more adaptive and flexible techniques that can account for varying degrees of distribution shifts.

4.3 Test-time Graph Transformation (Adaptation)

Test-time graph transformation (adaptation) aims to adapt models based on test samples in the presence of distributional shifts. Test time adaptation can be further subdivided into test time training and fully test time adaptation according to whether it can access the source data and alter the training of the source model. Here, we introduce several typical existing methods.

AdaGraph [15] presents the first deep architecture for Predictive Domain Adaptation. AdaGraph leverages metadata information to build a graph where each node represents a domain, while the strength of an edge models the

similarity among two domains according to their metadata. Then in order to exploit the graph for the purpose of DA and AdaGraph has a novel domain-alignment layers. This framework yields the new state of the art on standard PDA benchmarks.

GTRANS [8] which optimizes a contrastive surrogate loss to transform graph structure and node features, and provide theoretical analysis with deeper discussion to understand this framework. Experimental results on distribution shift, abnormal features and adversarial attack have demonstrated the effectiveness of GTRANS.

GAPGC (Graph Adversarial Pseudo Group Contrast) [7] is a test-time training method designed for GNNs with a contrastive loss variant as the self-supervised objective during testing. The framework of GAPGC is shown in Fig. 9. Recently, the effectiveness of test-time training has been validated to improve the performance on OOD test data, where some self-supervised auxiliary tasks are proposed. The authors argue that the simple augmentations in self-supervised training (e.g., randomly dropping nodes or edges) could harm the label-related critical information in graph representations. Therefore, GAPGC generates relatively reliable pseudo-labels, avoiding the severe shifts caused by the incorrect positive samples. The proposed adversarial learnable augmenter and group pseudo-positive samples can promote the relevance between the self-supervised task and the main task, to enhance the performance of the main task. The theoretical evidence is also derived to show that GAPGC can capture minimal sufficient information for the main task from an information theory perspective, which benefits the predictions on the OOD testing data.
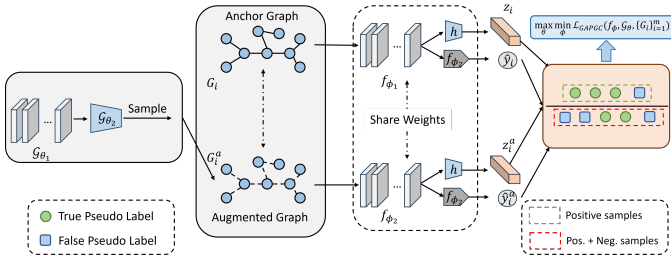

Fig. 9: GAPGC is a test-time training method designed for GNNs with contrast loss variants as self-supervised targets during testing.

GT3 (Graph Test-Time Training with Constraint) [6] is another test-time training method on graphs, which proposes a hierarchical self-supervised learning framework. Specifically, it first introduces the global contrastive learning strategy to encourage node representations to capture the global information of the whole graph. Global contrastive learning is based on maximizing the mutual information between the local node representation and the global graph representation. Then, it presents the local contrastive learning for distinguishing different nodes from different augmented views of a graph, so that the node representation can capture more local information. Besides, an additional constraint is proposed to encourage that the representations of testing samples are close to the representations of the training samples. The model's generalization capacity for

the graph classification task can be enhanced based on this test time training strategy with self-supervised learning.

Discussion. Test-time Graph Transformation (Adaptation) is a sophisticated approach aimed at enhancing the adaptability of graph-based machine learning models to new, potentially diverse target domains by adjusting the graph data during the testing phase.

TABLE 2: A summary of graph domain adaptation (GDA) learning methods.

Category	Method
Semi-supervised GDA Learning	DA-AGE [31]
	DASGA [3]
	AdaGCN [4]
	DAGNN [32]
	PGL [49]
Unsupervised GDA Learning	UDA-HGM [41]
	UDA-GCN [43]
	CDNE [52]
	ACDNE [53]
	DM-GNN [54]
	DGASN [55]
	LGA [42]
	DMGE [5]
	GCAN [50]
	UMTDA [51]
Test-time Graph Transformation (Adaptation)	AdaGraph [15]
	GTRANS [8]
	GAPGC [7]
	GT3 [6]

5 GRAPH OUT-OF-DISTRIBUTION LEARNING

Out-of-distribution (OOD) graph learning refers to the problem of learning from graphs that have different characteristics than those seen during training. Specifically, in graph-based machine learning, a common assumption is that the training and test data come from the same distribution. However, in many real-world scenarios, this assumption does not hold, and the test graphs may have different statistical properties than the training graphs. In such cases, a model trained on the training graphs may not generalize well to the test graphs. OOD graph learning addresses this problem by developing models that can handle the distribution shift between the training and test graphs. One way to achieve this is by learning representations that are invariant to the differences between the training and test distributions. Another approach is to explicitly model the distribution shift between the training and test graphs and adapt the model accordingly.

OOD graph learning has several applications, including social network analysis, recommender systems, and drug discovery. In these applications, the graphs may have different characteristics depending on the population or context, and it is important to develop models that can handle

these differences to achieve good performance in the target application.

Fig. 10 depicts an overview of the mentioned domains, in which the differences are shown visually.

5.1 Graph Out-of-distribution Generalization

To tackle the challenges brought by unknown distribution shifts and solve the graph OOD generalization problem, considerable efforts have been made in literature, which can be divided into three categories. We select some typical examples for each category to introduce.

5.1.1 Data Augmentation

This category of methods aims to manipulate the input graph data, i.e., graph augmentation. By systematically generating more training samples to increase the quantity and diversity of the training set, graph augmentation techniques are effective in improving the OOD generalization performance.

GAug (Graph Augmentation) [56] is a method for feature-wise graph augmentation. It utilizes a differentiable edge predictor to generate augmented graphs by encoding class-homophilic structure, which promotes intra-class edges and reduces inter-class edges to enhance prediction accuracy and generalization ability. GAug modifies the input graph using an edge prediction module and learns to generate new possible edges.

NCLA (Neighbor Contrastive Learning on Learnable Graph Augmentation) [57] is an end-to-end automatic graph contrastive learning method, applying neighbor contrastive learning on learnable graph augmentation. NCLA automatically generates multiple graph augmented views with adaptive topology by the multi-head graph attention mechanism, where each attention head corresponds to each augmented view. The attention-based learnable graph augmentation avoids improper modification of the original topology and can be compatible with various graph datasets without prior domain knowledge.

GRAND (Graph Random Neural Network) [58] is a framework for enhancing generalization in GNNs by combining feature-wise graph augmentation methods. First, it randomly drops node features and propagates perturbed features. Then in accordance with the graph homophily assumption[59], stochastic augmentation is employed to generate diverse augmented representations for individual nodes.

GraphCL (Graph Contrastive Learning) [10] GraphCL is a mixed-type graph data augmentation method, which provides four data augmentations, including node dropping, edge perturbation, attribute masking, and subgraph sampling. As depicted in Fig. 11, two categories of augmentations are randomly sampled from a pool of augmentations and implemented on the input graph. A GNN encoder and a projection head are trained with the objective of maximizing the consensus between their respective representations[60].

5.1.2 Model Develoment

This category of methods aims to propose new graph models for learning OOD generalized graph representations.

DisenGCN [61] is a method that utilizes the DisenConv, a disentangled multichannel convolutional layer, to learn disentangled representations of nodes. Within DisenConv, a dynamic process determines the neighboring nodes that are influenced by specific latent factors and directs them to the corresponding channels for information extraction and convolution. The disentangled nature of these latent factors contributes to improved generalization performance when dealing with out-of-distribution data.

OOD-GNN [9] is a GNN designed backed by confounder balancing theory[62] in causality. It is designed for poor generalization on unseen testing graphs with different distributions. It utilizes a nonlinear graph representation decorrelation method using random Fourier features to encourage independence between relevant and irrelevant graph representations, eliminating spurious correlations. OOD-GNN optimizes sample graph weights and the graph encoder to enhance discriminative graph representations, resulting in improved predictions.

5.1.3 Learning Strategy

This category of methods focuses on exploiting the training schemes with tailored optimization objectives and constraints to enhance the OOD generalization capability.

StableGL [63] is a framework for Graph Invariant Learning in GNNs that addresses unstable inference in different test environments caused by distribution shifts. It consists of two essential components: Locally stable learning captures stable node properties by reweighting the neighborhood aggregation process, while globally stable learning reduces training losses in different environments, ensuring the generalization of GNNs.

Pretraining-GNN [64] refers to a self-supervised technique employed in the pre-training of GNNs. The crux of this approach lies in the pre-training of a highly expressive GNN on both individual nodes and complete graphs, enabling the simultaneous acquisition of valuable local and global representations. Consequently, this method effectively sidesteps negative transfer phenomena and substantially enhances the model's generalization capabilities across various downstream tasks.

Discussion. In the graph OOD generalization, while the Data Augmentation addresses graph OOD generalization by diversifying the training graph data, Model Development focuses on building inherently more adaptable models, and Learning Strategy emphasizes the training schemes with tailored optimization objectives and constraints that enhance the model's ability to generalize to new distributions. Each approach tackles the challenge of Graph OOD Generalization from a different angle, offering a comprehensive capability for improving model performance on unseen graph data.

5.2 Graph Out-of-distribution Detection

Graph Out-of-Distribution detection (Graph OOD detection) aims to identify test-times samples that are semantically different from the training data categories, and therefore should not be predicted into the known classes. Here, we select some typical examples for the introduction.
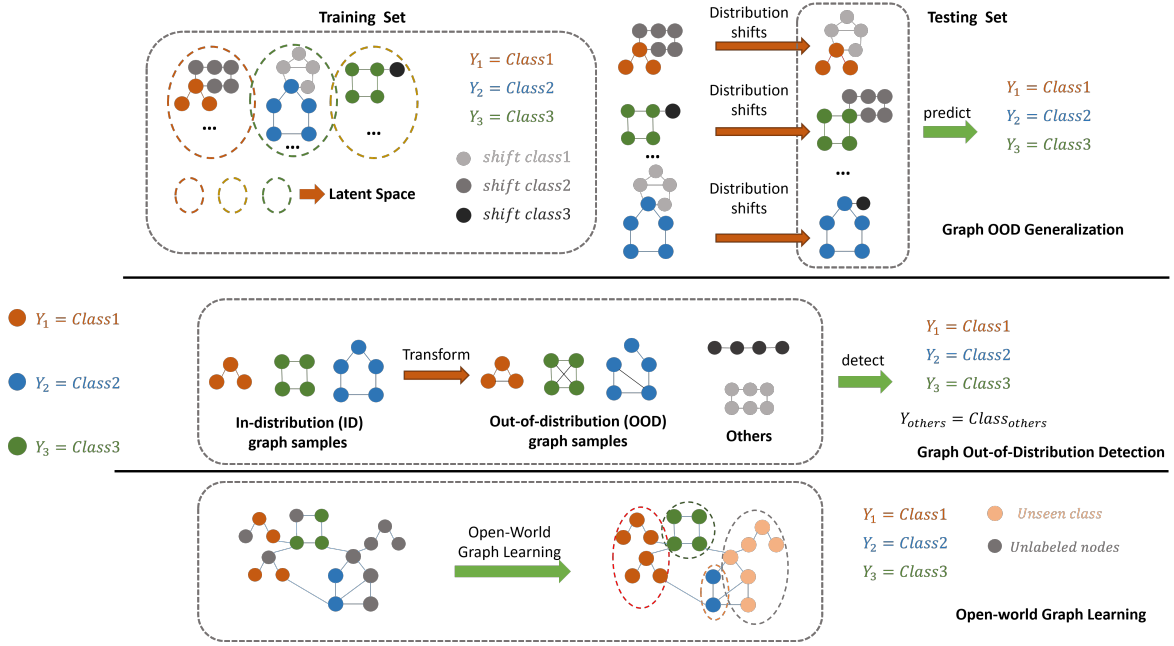
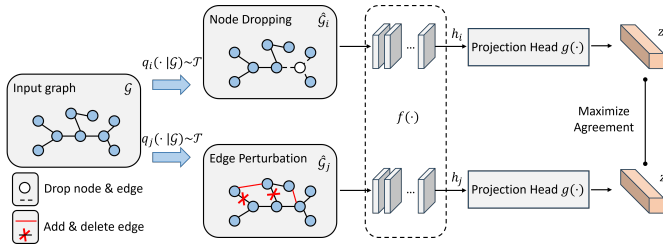Fig. 10: The overview of graph out-of-distribution learning.

Fig. 11: A framework of GraphCL. GraphCL is a mixed-type graph data augmentation method, which provides four data augmentations, including node dropping, edge perturbation, attribute masking, and subgraph sampling.

Uncertainty-GNN [65] is an innovative framework that integrates multiple uncertainty sources to enhance the performance of GNNs in semi-supervised node classification tasks. It effectively improves predictions and accuracy by leveraging deep learning-based and belief/evidence theory-based uncertainties. Uncertainty-GNN improves GNN performance in node classification tasks by effectively addressing misclassification and out-of-distribution detection.

GPN (Graph Posterior Networks) [66] is a model that combines node classification and OOD detection, using variational inference and a latent variable to approximate the true posterior distribution and differentiate between in-distribution and OOD nodes. LMN mitigates cross-distribution mixing, learns from neighboring nodes without explicit OOD labels, and reduces overfitting with bi-level optimization. Overall, LMN provides a comprehensive solution for accurate node classification and reliable OOD detection.

LMN [67] is a model that combines node classification and OOD detection, using variational inference and a latent variable to approximate the true posterior distribution and differentiate between in-distribution and OOD nodes. LMN mitigates cross-distribution mixing, learns from neighboring nodes without explicit OOD labels, and reduces overfitting with bi-level optimization. Overall, LMN provides a comprehensive solution for accurate node classification and reliable OOD detection.

GraphDE [11] is a unified framework for graph OOD detection and debiased learning. It utilizes a latent environment variable and generative models to address outliers in the training data. An OOD detector is also included to distinguish between in-distribution and OOD samples, enhancing the robustness of graph representation learning. Overall, GraphDE is a promising solution for reliable graph representation learning in real-world applications.

GOOD-D (Graph Out-Of Distribution Detection) [68] is an unsupervised method for detecting OOD graphs. It utilizes a hierarchical graph contrastive learning framework to capture attributive and structural patterns from in-distribution (ID) training data. By maximizing agreement between feature and structure graph views at multiple levels, GOOD-D effectively detects OOD graphs. It incorporates a self-adaptive mechanism to balance learning objectives and OOD scores.

Discussion. Graph OOD Detection aims to equip models with the ability to identify and detect graphs that represent new, unknown, or significantly different patterns from those seen during training. This capability is essential in numerous fields where understanding and reacting to evolving or novel graph structures is crucial.

5.3 Open-world Graph Learning

Open-world Graph Learning is a task where models are trained in a setting without prior knowledge of the number of classes or their training samples. The challenge lies in distinguishing unseen classes without labeled samples from existing classes. This applies to both graph structures and
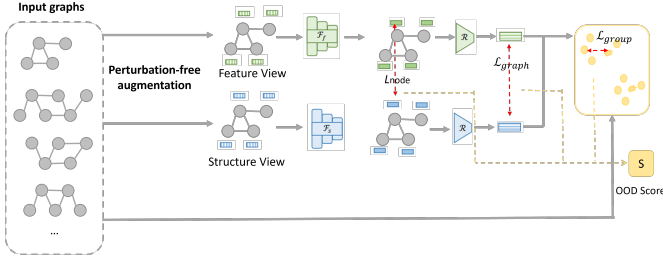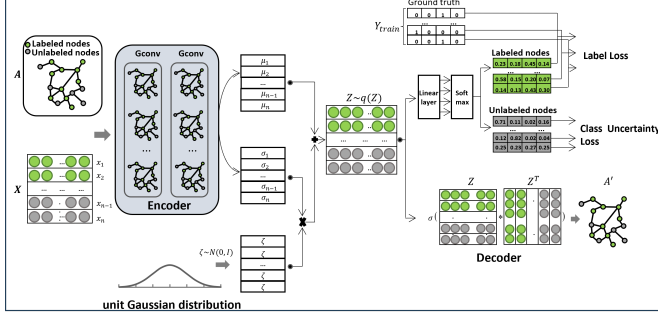
Fig. 12: The framework of GOOD-D.

Fig. 13: The framework of OpenWGL. OpenWGL captures uncertainty using a graph variational autoencoder for node embeddings and differentiates between seen and unseen class nodes through label and class uncertainty loss minimization with an automatic threshold.

knowledge graphs. The literature can be categorized into graph structure and knowledge graph studies.

5.3.1 Graph Structure

In the open-world learning of graph structure, the model needs to better learn the feature representation of graph data, classify nodes belonging to known classes into correct groups through threshold judgment or classifier output, etc., and also classify nodes not belonging to existing classes into invisible classes [69], [70], [71].

OpenWGL [71] tackles open-world graph learning with two key components: Node Uncertainty Representation Learning and Open-world Classifier Learning. As shown in Fig. 13, it captures uncertainty using a graph variational autoencoder for node embeddings and differentiates between seen and unseen class nodes through label and class uncertainty loss minimization with an automatic threshold. This approach provides a comprehensive solution for accurate classification in open-world scenarios.

FATE (Federated Learning via Adapted Transformer) [72] is a federated learning framework that handles open-world feature extrapolation using graph representation and learning. It utilizes a backbone network and a graph neural network to handle new features without retraining. FATE includes two training strategies for better extrapolation and reduced overfitting. The framework is effective and scalable, supported by theoretical analysis and experiments.

Co-CGE [73] is an approach for Compositional Zero-Shot Learning (CZSL) in an open-world setting that aims to recognize unseen compositions of known state-object primitives. It utilizes a graph convolutional neural network to model dependencies between states, objects, and compositions. By incorporating feasibility scores, Co-CGE enhances CZSL performance by considering the feasibility of unseen compositions.

5.3.2 Knowledge Graph

Knowledge graph completion (KGC) aims to fill in missing relationships in a Knowledge Graph (KG). Traditional closed-world approaches for KGC are limited in their ability to address a small number of missing relations. However, recent advancements in KGC involve incorporating knowledge from open-world resources, like online encyclopedias and newswire corpus, to enhance completion capabilities.

ConMask [74] is a model specifically designed for open-world Knowledge Graph Completion (KGC) tasks. It consists of Relationship-Dependent Content Masking, Target Fusion, and Target Entity Resolution components. By masking irrelevant information, extracting entity embeddings, and generating similarity rankings, ConMask effectively connects new entities to knowledge graphs, improving their completeness in an open-world setting.
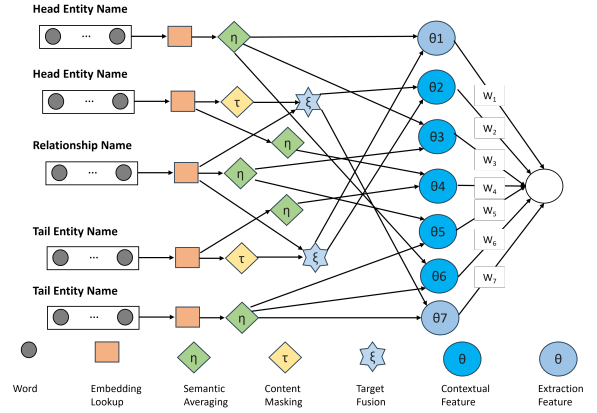

Fig. 14: The framework of ConMask. It consists of Relationship-Dependent Content Masking, Target Fusion, and Target Entity Resolution components.

Prob-CBR (Probabilistic Case-based Reasoning) [75] is an approach for open-world graph completion. It combines probabilistic and case-based reasoning principles to handle uncertainty in knowledge graphs. By retrieving similar cases, Prob-CBR predicts attributes using reasoning paths. Its probabilistic model estimates query effectiveness with simple path statistics. It dynamically grows with new entities and outperforms other approaches.

MIA [76] is an open-world KGC model that utilizes a word-level attention mechanism to simulate interactions between entity descriptions, names, relationship names, and candidate tail entity descriptions. As shown in Fig. 15, it improves representations by incorporating additional textual features from head entity descriptions. However, its effectiveness in predicting the tail entity relies on the availability of relationship-related information in entity descriptions.

Discussion. Open-world Graph Learning is a dynamic and challenging research area, requiring models to go beyond traditional classification tasks to recognize and categorize previously unseen classes. In graph structures, it
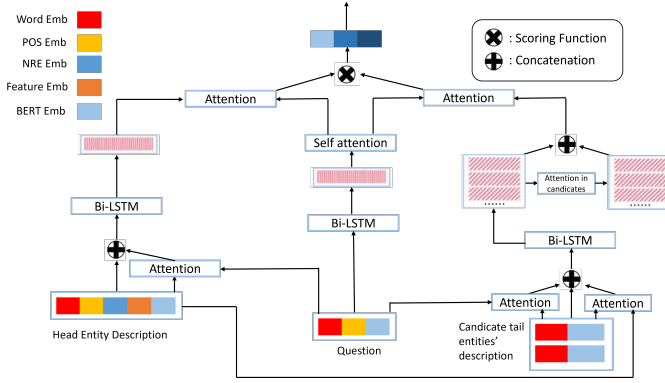
Fig. 15: The framework of MIA. MIA improves representations by incorporating additional textual features from head entity descriptions.

involves advanced feature representation learning and the innovative classification of nodes into both known and unseen classes. In the realm of knowledge graphs, the shift towards leveraging open-world resources for KGC marks a significant advancement in making these graphs more complete and reflective of the ever-changing real world. Both areas highlight the need for models that are adaptable, flexible, and capable of handling the complexities and uncertainties inherent in real-world data.

TABLE 3: A summary of graph out-of-distribution (OOD) learning methods.

Category	Subcategory	Method
Graph OOD Generalization	Data Augmentation	GAug [56]
		NCLA [57]
		GRAND [58]
		GraphCL [10]
	Model Development	DisenGCN [61]
		OOD-GNN [9]
	Learning Strategy	StableGL [63]
		Pretraining-GNN [64]
Graph OOD Detection	-	Uncertainty-GNN [65]
		GPN [66]
		LMN [67]
		GraphDE [11]
		GOOD-D [68]
Open-world Graph Learning	Graph Structure	OpenWGL [71]
		FATE [72]
		Co-CGE [73]
	Knowledge Graph	ConMask [74]
		Prob-CBR [75]
		MIA [76]

6 GRAPH CONTINUAL LEARNING

Graph continual learning refers to the problem of learning from a stream of graph data that arrives over time and continuously evolves. In this setting, the goal is to develop models that can learn from new graphs as they arrive, without forgetting what has been learned from previous graphs. The graph continual learning problem is particularly challenging because the distribution of graphs can change over time, and the model must adapt to these changes without degrading its performance as previously.

Graph continual learning has applications in various fields, such as social network analysis, recommendation systems, and biological network analysis. In these fields, the graph data can arrive in a stream, and it is essential to have models that can adapt to the evolving graph data.

The categorization of graph continual learning methods is based on how these methods consider graph structure data in the incremental learning process. Thus, the existing graph continual learning works can be divided into four categories: architectural, regularization, rehearsal, and hybrid, which are as shown in Fig. 16 and follows:

- **Architectural Approach**. These approaches focus on modifying the specific architecture of networks, activation functions, or layers of algorithms to address a new task and prevent the forgetting of previous tasks.
- **Regularization Approach**. These approaches consolidate the learned knowledge by adding a regularization item to the loss function, constraining the neural weights from updating in a direction that compromises performance on prior tasks.
- **Rehearsal Approach**. These approaches maintain a memory buffer preserving the information of prior tasks and replay it when learning new tasks to mitigate catastrophic forgetting.
- **Hybrid Approach**. These approaches combine more than one continual learning approach to take advantage of multiple approaches and improve the performance of models.

We summarize the methods of graph continual learning in Table 4.

6.1 Architectural Approach

In the general continual learning setting, the architectural approaches mainly pay attention to altering the specific architecture of networks, activation functions, or layers of algorithms to address new tasks to prevent catastrophic forgetting of already seen tasks [38], [39], [40]. In graph continual learning scenario, the architectural approaches solve problems by techniques such as graph structure evolution, unit expansion, and compression.

FGN (Feature Graph Networks) [77] is a framework that converts graph architectures into a format compatible with learning structures. Illustrated in Fig. 17, it allows independent processing of graph nodes during knowledge acquisition and has implications for graph relationships. In feature graphs, the fixed node count corresponds to unchanging feature dimensions in standard graphs.

HPNs (Hierarchical Prototype Networks) [14] extract abstract knowledge from expanding graphs using prototypes. They encode attributes and relationships, generating prototypes at different levels. These prototypes capture shared attributes and relationships among nodes. HPNs enable the adaptive selection and composition of prototypes, facilitating the extraction of hierarchical knowledge.

CoST-GCN [78] is a variant of ST-GCN [24] designed for graph-based human action recognition. It introduces
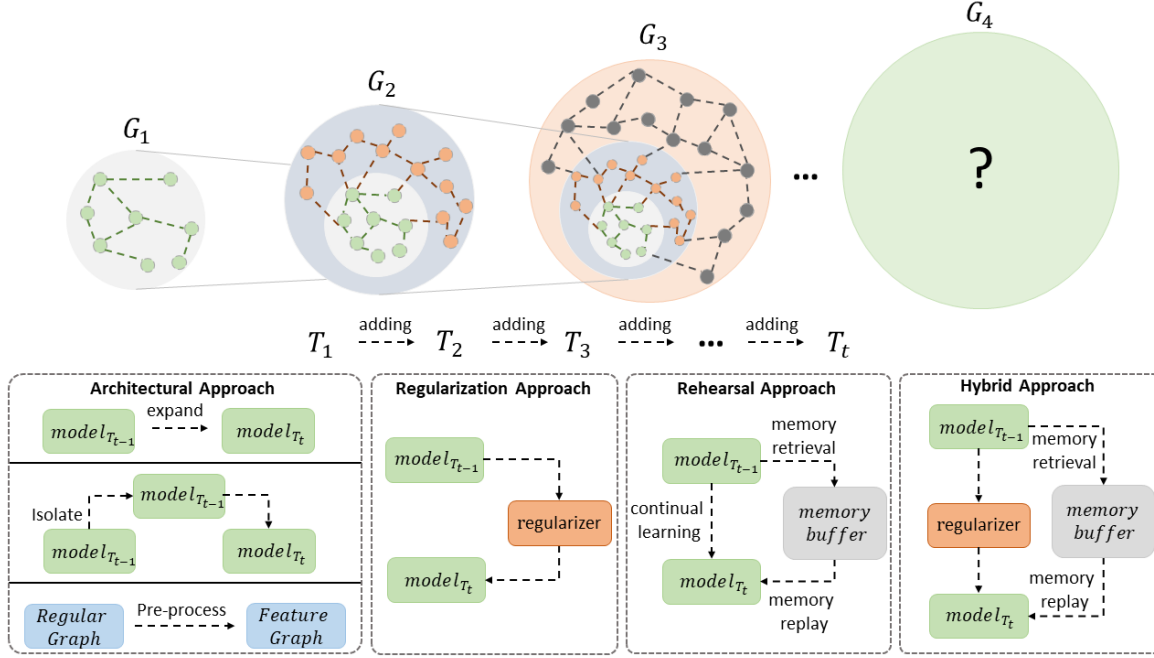
Fig. 16: Graph evolution and graph continual learning categorization. Graph lifelong learning aims to accommodate a new task T_t based on the graph $G_t = G_{t-1} + \Delta G_t$ while maintaining the performance in solving previous tasks $T_1, T_2, ..., T_{t-1}$. the existing graph continual learning works can be divided into four categories: architectural, regularization, rehearsal, and hybrid.

TABLE 4: A summary of graph continual learning (GCL) methods.

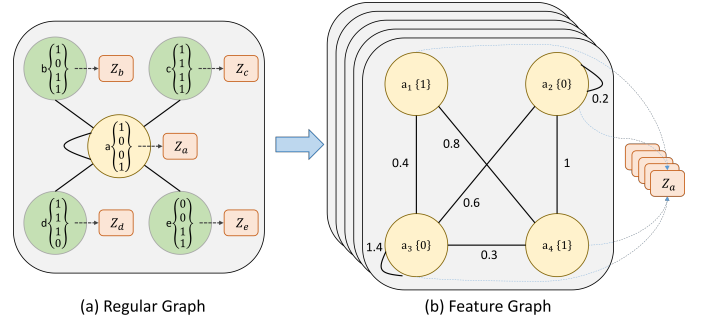| Category	Method
Architectural (Arch.)	FGN [77]
	HPNs [14]
	CoST-GCN [78]
	PI-GNN [79]
Regularization (Reg.)	DiCGRL [80]
	GPIL [13]
	TWP [81]
	GraphSAIL [82]
	RieGrace [83]
	LKGE [84]
Rehearsal (Reh.)	ER-GNN [85]
	Incremental-GNNs [86]
	RBR and PBR [87]
	Inverse Degree Sampling [88]
Hybrid	ContinualGNN (Reg.& Reh.) [1]
	LDANE (Arch.& Reg.& Reh.) [2]
	TrafficStream (Reg.& Reh.) [89]
	CMDGAT (Arch.& Reh.) [90]

Fig. 17: The framework of FGN. FGN allows independent processing of graph nodes during knowledge acquisition and has implications for graph relationships.

a Continual Inference Network that enables step-by-step predictions without redundant frame processing. CoST-GCN reduces time complexity, accelerates on-hardware, and decreases memory usage during online inference while maintaining predictive accuracy.

PI-GNN (Parameter Isolation GNN) [79] is a model for continual learning on dynamic graphs. The method employs a strategy by using parameter isolation and expansion. The underlying rationale is rooted in the observation that distinct parameters play varying roles in learning diverse graph patterns. Building upon this insight, the approach expands model parameters to enable the assimilation of emerging graph patterns.

Discussion. Both in general continual learning and graph continual learning scenarios, architectural approaches are key to managing the balance between learning new tasks

and retaining old information. While the general continual learning setting often focuses on network-level adaptations, graph continual learning requires specific techniques tailored to the unique nature of graph-based data, such as evolving graph structures or managing graph complexity through expansion and compression. These approaches underscore the necessity for adaptable and flexible models capable of handling the dynamic nature of continuous learning environments.

6.2 Regularization Approach

This approach implements a single model and has a fixed capacity by leveraging the loss function using the loss term to help consolidate knowledge in the learning process for new tasks and retain previous knowledge [91], [92]. Prior knowledge of graph structures and tasks will be maintained to achieve stable performance while learning novel knowledge.

(a) The disentangle module of DiCGRL.
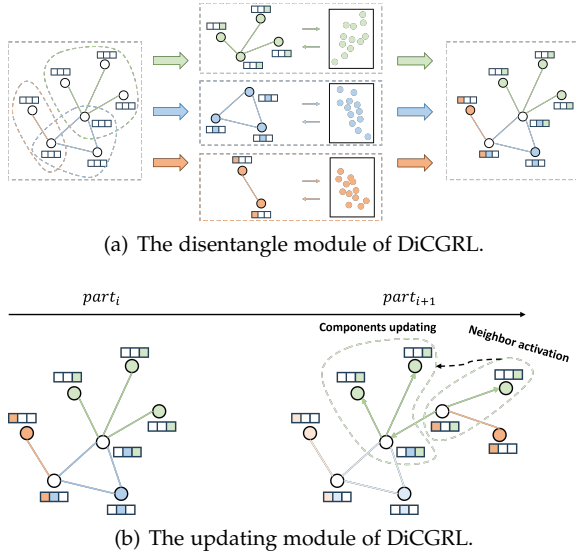

(b) The updating module of DiCGRL.

Fig. 18: The framework of DiCGRL. DiCGRL takes two approaches to continuously learn a new graph embedding whilst preventing the forgetting of old knowledge.

DiCGR [80] is an approach designed to support continual learning on graph data. It addresses the challenge of preserving previously acquired knowledge while learning new information. DiCGRL achieves it by breaking down relational triplets into individual components, refining the embeddings to better capture the graph structure, and incorporating a regularization mechanism to prevent forgetting of previously learned knowledge. DiCGRL takes two approaches to continuously learn a new graph embedding whilst preventing the forgetting of old knowledge, respectively the disentangle module shown in Fig. 18(a) and the updating module shown in Fig. 18(b).

GPIL [13] is a framework that aims at acquiring proficiency in different classes. It utilizes a recurrent strategy, pretraining the encoder on base classes and maintaining it during pseudo incremental learning. To mitigate catastrophic forgetting, this approach introduces a Hierarchical Attention Graph Meta Learning framework with augmented loss function using regularization techniques.
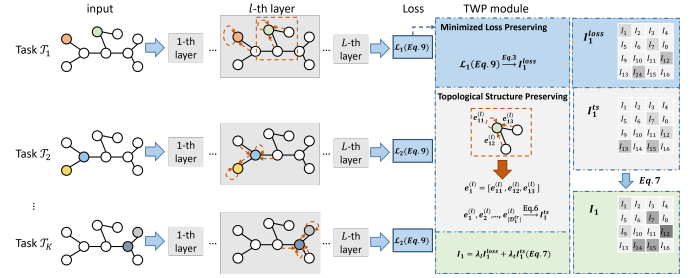

Fig. 19: The framework of TWP. TWP leverages the gradients of task-specific objectives alongside topological preservation in relation to each parameter.

TWP [81] is a framework designed to bolster continual learning while mitigating the risk of catastrophic forgetting within GNNs. As shown in Fig. 19, TWP computes the importance score for each network parameter, rooted in its contribution to both the graph's topological architecture and its effectiveness in task execution. TWP leverages the gradients of task-specific objectives alongside topological preservation in relation to each parameter.

GraphSAIL [82] is an Incremental Learning framework for GNN-based recommender systems. It enables efficient updates, reducing computation time for more frequent recommendations. GraphSAIL implements inter-distillation to evaluate the agreement of high-level node encoding between the teacher and student models, enhancing the performance of its recommendation system.

RieGrace [83] is a self-supervised Riemannian Graph Continual Learner. It incorporates an Adaptive Riemannian GCN that shapes the Riemannian space using learned curvature adaptive to each graph. Additionally, it utilizes a Label-free Lorentz Distillation approach with teacher-student AdaRGCN models for the graph sequence. Overall, RieGrace enables graph continual learning in adaptive Riemannian spaces through self-supervision.

LKGE [84] is a model for lifelong learning in expanding knowledge graphs. It utilizes a masked KG autoencoder, embedding transfer strategy, and embedding regularization to efficiently transfer and retain knowledge. It streamlines the process of incorporating new data while preserving existing knowledge in KG embeddings.

Discussion. The regularization approach in continual learning, particularly for graph-based models, is a strategy that emphasizes the importance of retaining prior knowledge while acquiring new information. By carefully modifying the loss function, this approach seeks to maintain stable performance across a series of tasks without expanding the model's capacity. This is particularly crucial in graph-based applications where the relationships and structures in the data are complex and evolving.

6.3 Rehearsal Approach

This approach regulates retraining processes for previous tasks to strengthen the relationship between memory and performance on previously learned tasks [93]. This graph learning approach enables the selection of appropriate samples of graph representation, such as nodes and edges, for

retraining purposes. The number of samples is carefully considered to minimize the computational complexity.

ER-GNN [85] is a framework that implements a graph-based experience replay mechanism. This framework's core principle involves preserving historical knowledge within an experience buffer, drawn from the preceding task learning phases. ER-GNN prevents catastrophic forgetting by retaining previously learned knowledge using an experienced buffer. It selects and stores relevant nodes in the buffer using an experience node strategy.

Incremental-GNNs [86] is a model specifically designed for incremental training on graph data. The model utilizes prior knowledge to enhance the learning process across a sequence of tasks. This acquired knowledge can be explicitly stored as historical data or implicitly encoded within the model's parameters. The model then evaluates the impact of this accumulated knowledge, leveraging it to improve the performance of the network.

RBR and PBR (Random-Based Rehearsal and Priority-Based Rehearsal) [87] are methods for training GNNs on streaming graph data. They use experience replay with a node sampling strategy that prioritizes higher loss samples. This allows for continuous learning and adaptation to changing dynamic graph streams, aiming for faster training, low latency, and high accuracy.

Inverse Degree Sampling [88] is an approach in graph-based recommender systems that focuses on selecting interaction subsets using an inverse degree experience sampling strategy. By redirecting the model's attention to interactions involving users with infrequent interactions, this strategy enhances the applicability of reservoir sampling in continual sampling contexts.

Discussion. In graph continual learning, the rehearsal approach offers a viable method for reinforcing the model's memory of previous tasks while learning new ones. By judiciously retraining on selected graph samples, this approach helps maintain a balance between retaining past knowledge and acquiring new information, ensuring sustained performance across a series of evolving tasks. This strategy is particularly relevant in dynamic environments where graph data continuously changes or expands.

6.4 Hybrid Approach

The hybrid approach combines more than one continual learning approach to take advantage of each approach and maximize the performance of models [94], [95].

ContinualGNN [1] is a framework that combines two distinct strategies: a replaying strategy and a regularization approach, functioning synergistically to mitigate catastrophic forgetting and maintain the established learned patterns. It identifies and incorporates novel patterns in the evolving graph structure while solidifying knowledge to maintain acquired insights throughout the network.

LDANE [2] is a framework that acquires low-dimensional representations for nodes in an expanding network. Underpinned by an architectural paradigm known as Dynamic Expandable Networks [96], LDANE advances the field by integrating attribute constraints. As shown in Fig. 20, it incorporates attribute constraints to align learned embeddings with specific attributes, adapting to changes in node attributes.
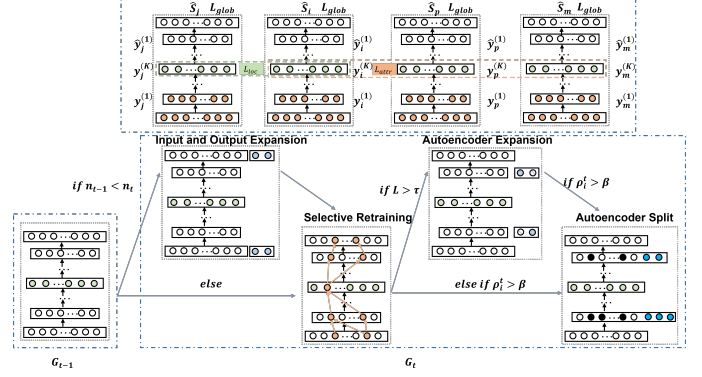

Fig. 20: The framework of LDANE. LDANE incorporates attribute constraints to align learned embeddings with specific attributes, adapting to changes in node attributes.

TrafficStream [89] is a framework that captures patterns for new graph structures and consolidates knowledge between previous and new ones. It uses a traffic flow forecasting model (SurModel) to represent intelligent transportation system data. It efficiently updates current network patterns through processes that consider network structure changes caused by factors like the addition of new sensors or stations.

CMDGAT [90] is a model that enhances the descriptive capacity of point clouds by using a novel graph continual network architecture. The architecture includes an attention mechanism that leverages knowledge from previous point cloud pairs to associate and aligns points in the current pair. By utilizing insights from past associations, the network optimally registers points, improving the overall representation of the point clouds.

Discussion. The hybrid approach in graph continual learning offers a versatile and effective way to tackle the challenges of learning in dynamic and evolving environments. By combining the strengths of various continual learning methods, it aims to achieve robust performance, adaptability, and efficient use of computational resources. This approach is particularly relevant in complex learning scenarios where no single method can adequately address all challenges.

7 APPLICATIONS

7.1 AI-aided Drug Discovery.

AI-aided drug discovery [17] is becoming increasingly prevalent when it offers the great potential to accelerate the development of new pharmaceuticals, making the process faster, more cost-effective, and more efficient. It has wide application scenarios across various domains, including generative chemistry [97], protein structure prediction [98], [99], virtual screening [100], [101], drug repurposing for emerging diseases [102], and many others. Due to the distribution shift issues of graph data, the compatibility assumption between training and test sets does not usually hold in the drug discovery-related fields, especially when the learned knowledge from the training set may not smoothly provide accurate predicting signals for test samples [6], [17], [8], [7], [9], [11].

For instance, when performing virtual screening for hit finding [17], the prediction model is typically trained on known target proteins. However, a 'black swan' event like COVID-19 can occur, resulting in a new target with unseen data distribution. The performance on the new target will significantly degrade. Moreover, for molecular prediction [9], the GNN models trained on molecules with one group of scaffolds, i.e., the two-dimensional structural frameworks of molecules, might learn the spurious correlations between the scaffolds and labels, so that the GNN models would make incorrect predictions on real-world out-of-distribution testing molecules with different scaffolds.

Hence, dealing with distribution shifts on graph data is a critical way to address the performance degradation for practical AI-aided drug discovery. The potential solutions contain but are not limited to designing robust and generalizable graph learning models through domain adaption, OOD modeling, and continuing graph learning; Meanwhile, developing curated distribution shifted graph datasets and benchmarks to better understand distribution shift cases and characteristics for facilitating and promoting the development of drug discovery.

7.2 Personalized Intelligent Recommendation Systems.

In the recommender system, the training samples with nodes and relations are usually observed and collected with a certain selection bias [63], that is, the logged interactions collected from current undergoing systems may warp (graph) recommenders biased towards popular items, leading to potential distribution shifts on the deployed environment with caused unfairness towards less exposed items. Moreover, considering male users often have fewer logged interactions on e-commerce platforms, the graph recommenders may be trained with a bias towards female users and thus deteriorate the experience of male users.

Hence, explicitly reducing the performance variances across different deployment environments with distribution shifts is the key to the graph learning based recommender system, for confronting the inconsistencies between the training and testing distributions, and achieving fairness for different groups of users. Moreover, due to the continuous and frequent updating characteristic of recommender systems, tackling the catastrophic forgetting problem that occurs when training a model in an incremental pattern would benefit modeling a user's long-term preference (or an item's long-term property) under the evolving distribution shifts [82], [14], [13], [88].

In this way, various graph learning models dealing with distribution shifts would benefit real-world recommender systems to make more adaptive and stable predictions of practical unseen users' preferences, leading to more accurate and intelligent recommendation [5], [8], [63].

7.3 Open-world Knowledge Exploration and Learning.

Real-world information representation and related applications usually rely on knowledge-driven approaches that utilize knowledge graphs (KGs) with comprehensive knowledge exploration and learning. Throughout the whole lifecycle of KG, new facts, unseen entities, and unseen relations continually emerge, evolve, and grow alongside the development, leading to inevitable dynamic distribution shifts [75], [84]. In this case, conducting open-world knowledge exploration and investigating lifelong KG learning under such temporal distribution shifts, would facilitate the learning and updating from growing new knowledge, facts, and relations, meanwhile, preserving the previously learned useful old knowledge and serving for various KG-related application scenarios [103], covering KG representation learning, KG question and answering, KG completion [104].

Moreover, such knowledge exploration in open-world KG under distribution shifts also provides a great chance to collaborate existing KG learning with the recent prevalent large language models (LLMs) [105], [106], considering LLMs and KGs are inherently interconnected and can mutually enhance each other. For instance, DAGNN [32] conducts cross-domain text classification by modeling documents as graph data structure, and combining the hierarchical structure and domain labels into a unified deep model. And ChatRule [107] unleashes the power of LLMs for mining logical rules over knowledge graphs for enhancing the reasoning ability. It can be anticipated that open-world knowledge exploration and learning with KG related temporal shift graph learning would be capable of sophisticated reasoning and decision-making based on a deep understanding of real-world knowledge, ultimately driving forward the frontiers of AI research and its practical applications.

7.4 Intelligent Transportation System Forecasting.

Traffic flows typically show high-quantity, long-term streaming evolution, and gradual expansion characteristics in traffic networks. Accurately forecasting traffic flows plays an important role in improving the efficiency of intelligent transportation systems [89]. Considering the traffic networks would change flows of nodes and expanding structures in a long-term period indicated by spatial-temporal graphs [108], [109], the distribution shift in the inconsistency between patterns (context attribute shift and the spatial structure shift) of new data and historical data would negatively affect the accuracy of forecasting. Hence, the key to conducting graph learning on intelligent transportation system forecasting under such distribution shifts is to jointly incorporate long-term stable patterns and temporarily disappearing patterns, for efficiently capturing patterns from new data while consolidating historical knowledge using graph continual learning approaches.

Hence, the ongoing development of graph learning models under distribution shifts with continual learning holds great promise for the future of transportation management and optimization. It can be anticipated that we can enhance the accuracy of traffic flow predictions and ultimately contribute to the efficiency and effectiveness of intelligent transportation systems.

8 FUTURE DIRECTIONS

8.1 Graph Data-centric Learning under Distribution Shifts.

Very recently, there has been a growing interest in data-centric graph machine learning (DC-GML) for the recognition and prioritization of the importance of graph data [110].

Modeling graph data shifts in cross-domains and various distributions [111] is an important aspect of DC-GML, as the domain and distribution shifts of graph data would significantly affect the generalization ability and robustness of graph learning algorithms. For one thing, there is some recent research focusing on exploiting the distinct graph distribution characteristics, emphasizing invariance, stability, evolution, etc. [112], [113], [8]. For another thing, a very young research topic graph learning model evaluation problem [114] is explored to observe and predict the GNN model performance under various graph data distribution shifts (e.g., domain changes) without test-time ground truth labels.

Therefore, emphasizing the investigation of distribution shifts in graph data-centric characteristics, while also tackling the co-development of distribution-shifted graph data and models, holds great potential as a future research avenue. This approach ensures that optimization and customization are applied to both elements, catering to a wide range of practical scenarios in graph learning and analysis. Consequently, it facilitates a comprehensive understanding of graph data distribution shifts and enhances the design and learning process of graph models, ultimately resulting in improved performance in data-centric graph machine learning.

8.2 Cross-modality Distribution Shift Exploration on Graph Learning.

Data types in the real world exhibit various modalities and scales, e.g., images, texts, tabular data, audios, and graphs, which are crucial for the advancement of artificial intelligence and machine learning communities [115]. Considering the complexity of cross-modal data, learning algorithms are used to make inferences for test data they have not encountered during training, leading to inevitable inductive bias. Meanwhile, there are natural and more general distribution shifts among modalities used during model training and deployment. In such cases, as an important and commonly used structural data type, graph data might not be explicitly given for training and inference in real-world multi-modal model development [116].

Hence, constructing graphs from multi-modal data with different node representations, relationships, and attributes, can be a promising future research direction under potentially more complex distribution shifts, such as scene graph construction from images [117], and knowledge graph construction from texts [106], [118], [32]. Meanwhile, another crucial future problem lies in conducting effective graph learning on these constructed graphs under distribution shifts. This involves thoroughly incorporating cross-modal dependencies. For example, this could entail learning about structural shifts using flexible message propagation strategies and adaptively transferring learned node or graph representations across various distributions and downstream tasks.

8.3 Comprehensive Graph Learning Task-driven Evaluation Protocols.

Given the complex and diverse nature of graph data distribution shifts, there is still potential to enhance the evaluation protocols used in various downstream tasks of graph learning for future exploration. These improved protocols should focus on two key aspects: at the model level, to measure performance across different tasks, and at the graph data level, to assess data distribution driven by both the graph learning models and the tasks they are applied to. For instance, in terms of OOD generalization baselines, graph learning models should be evaluated on both near and far out-of-distribution graph datasets, which may originate from different domain sources. An instance of this would be training models on citation networks and then evaluating their performance on social networks [119].

Therefore, future research should concentrate on developing effective metrics to evaluate the distance or discrepancy among various graph data, considering both node-level analysis in a single graph and collective graph-level analysis in an entire dataset. Additionally, it is also important to focus on establishing fair and uniform methods to compare and evaluate graph learning models under varying degrees of distribution shifts [114]. This should encompass diverse scenarios including graph domain adaptation, OOD generalization, detection, prediction, etc.

8.4 Trustworthy Graph Learning Under Distribution Shifts.

Graph data distribution shifts impose significant challenges to various aspects of trustworthiness in graph learning [120], including adversarial robustness under graph distribution related attacks, model explainability to diverse and complex graph distributions, as well as privacy and fairness guarantee under different distribution transfer or domain adaption learning.

From the *adversarial robustness* point of view [121], when small but intentional adversarial perturbations are imposed on the input graphs, these alterations can lead to even more significant and unpredictable shifts in graph data distributions [122], [123]. As a result, this makes graph learning models more vulnerable and less resistant to adversarial attacks. Hence, enhancing the robustness of graph learning models under adversarial attacks on graph data distributions could be a valuable direction to explore for future research.

Moreover, considering the *explainability* [124], future graph learning models are expected to have the ability to interpret or explain their decisions or outputs when models are dealing with different graph distributions with diverse characteristics [125].

Furthermore, in terms of the *privacy and fairness* [126], [127], when graph data comes from sensitive personal sources or a certain graph learning model is trained on one specific distribution domain, how to maintain privacy across different domains within different graph data distributions is still a challenging aspect for privacy-guaranteed graph learning. Besides, how to ensure that the predictions of graph learning models do not systematically disadvantage any particular group or distribution with fairness is another promising future research question when deployed across varied graph data domains.

9 CONCLUSION

In this work, we present an in-depth review and synthesis of the forefront approaches and methodologies in graph

learning under distribution shifts. We categorized graph learning methods into graph domain adaptation learning, graph out-of-distribution learning, and graph continual learning, based on their observability of distributions and the availability of supervision information, where each with a detailed taxonomy and discussion of the current advancements. The comprehensive analysis, along with the highlighted discussions on potential applications and future research directions, not only provides a clear road map of the state-of-the-art approaches, but also help shed light on the effective development of graph learning techniques with diverse and complex distribution shifts.

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