Data Augmentation for Deep Graph Learning: A Survey

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Abstract

Graph neural networks, as powerful deep learning tools to model graph-structured data, have demonstrated remarkable performance on numerous graph learning tasks. To counter the data noise and data scarcity issues in deep graph learning (DGL), increasing graph data augmentation research has been conducted lately. However, conventional data augmentation methods can hardly handle graph-structured data which is defined on non-Euclidean space with multi-modality. In this survey, we formally formulate the problem of graph data augmentation and further review the representative techniques in this field. Specifically, we first propose a taxonomy for graph data augmentation and then provide a structured review by categorizing the related work based on the augmented information modalities. Focusing on the two challenging problems in DGL (i.e., optimal graph learning and low-resource graph learning), we also discuss and review the existing learning paradigms which are based on graph data augmentation. Finally, we point out a few directions and challenges on promising future works.

1 Introduction

Graphs have been widely used for modeling a plethora of structured and relational systems, such as social networks, knowledge graphs, and academic graphs, where nodes represent the entities and edges denote the relations between entities. As a powerful deep learning tool to model graph-structured data, graph neural networks (GNNs) which generally follow a recursive message-passing scheme, have drawn a surge of research interests lately. Owing to their state-of-the-art performance in various graph analytical tasks, GNNs nowadays have become the prevailing backbone of modern deep graph learning (DGL) models.

Despite the superb power of GNNs, their effectiveness on real-world graphs tends to be delicate, mainly because of two problems: (1) real-world graphs are usually extracted from complex interaction systems which inevitably contain uncertain, redundant, wrong, and missing features or connections. However, most existing DGL models rely on a fundamental assumption that the observed graph is clean and consistent with the properties of GNNs, and thus directly training them on such suboptimal graphs might lead to serious performance degradation [Dai *et al.*, 2021]; and (2) many prevailing DGL models are designed for a supervised or semi-supervised setting where sufficient ground-truth labels are available. Nonetheless, data labeling is time-intensive and resource-expensive, especially when considering the high-dimensional features and complex structure of real-world graphs. Similar to other neural endeavors, DGL models may easily overfit and lose their efficacy when labeled training data is extremely limited [Sun *et al.*, 2020; Ding *et al.*, 2022].

To enhance the quantity and/or the quality of training data, data augmentation is proposed as an effective tool to augment the training data by either slightly modifying existing data or generating synthetic instances from existing data. The importance of data augmentation has been well recognized in the field of computer vision and natural language processing due to its effectiveness in improving model performance in noisy and low-resource settings [Zhao *et al.*, 2021b]. More recently, data augmentation techniques have also been explored in the graph domain to push forward the frontier of DGL and demonstrated promising results. Apart from i.i.d. data such as images or text, graph-structured data is known to be far more complicated with different information modalities and graph properties, yielding a broader design space for data augmentation on graphs. Though an increasing number of graph data augmentation (GraphDA) methods have been actively conducted, this problem has not been well formulated and it is challenging for researchers to grasp the techniques behind and further leverage them to solve different DGL problems. Therefore, a systematic review of GraphDA is of great benefit to be aware of existing research in this field and what the challenges are.

Contributions. To this end, in this work, we present a forward-looking and up-to-date survey for GraphDA. Our major contributions are summarized as follows:

- To the best of our knowledge, this is the first survey for GraphDA. We provide a formal formulation for this emerging research area and review the related recent advances, which can facilitate the understanding of important issues for future research.
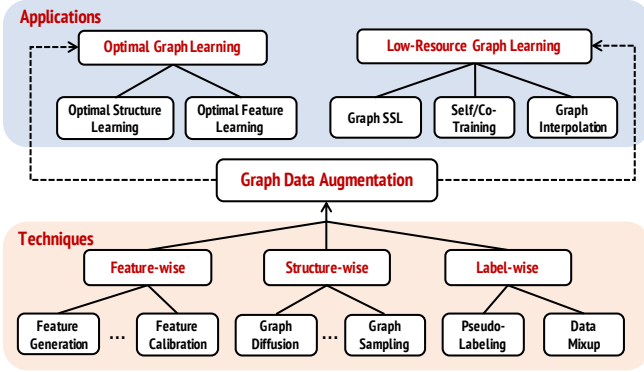- We present a taxonomy of GraphDA which categorizes

Figure 1: Taxonomy of Graph Data Augmentation (GraphDA).

the existing techniques in terms of the target augmentation modality (i.e., feature-wise, structure-wise, and label-wise) and provides a clear design space for developing and customizing new GraphDA methods.

- We discuss the applications of GraphDA in solving two representative DGL problems (i.e., optimal graph learning and low-resource graph learning) and review the prevalent learning paradigms. We also outline the open issues and promising future directions in this area.

2 Techniques of Graph Data Augmentation

For general purpose, in this survey we focus on attributed graphs, which can be represented as $\mathcal{G} = (\mathbf{A}, \mathbf{X})$, where $\mathbf{A} \in \{0,1\}^{n \times n}$ denotes the adjacency matrix and $\mathbf{X} \in \mathbb{R}^{n \times d}$ denotes the node feature matrix. Here n is the number of nodes, m is the number of edges, and d is the feature dimension. In addition, a node/graph label vector $\mathbf{y} \in \mathbb{R}^n$ could be provided depending on the specific target tasks.

In general, the goal of graph data augmentation (GraphDA) is to find a mapping function $f_\theta : \mathcal{G} \rightarrow \tilde{\mathcal{G}}$ such that the augmented graph(s) $\{\tilde{\mathcal{G}} = (\tilde{\mathbf{A}}, \tilde{\mathbf{X}})\}$ enrich or change the information from the given graph(s). Particularly, this paper concentrates on the GraphDA efforts which boost and empower the efficacy of DGL models. In this survey, we provide a systematic taxonomy to cover mainstream GraphDA techniques (Section 2) and two influential DGL problems (Section 3) where GraphDA is of fundamental significance. Figure 1 summarizes our proposed taxonomy.

As attributed graphs are consisted by multiple information modalities, graph data augmentation can be broken down based on the augmentation modality, including: *feature-wise*, *structure-wise*, and *label-wise* augmentations. We summarize the basic techniques in terms of each augmentation modality and clearly illustrate the explored design space for GraphDA.

In terms of the optimization objectives, most, if not all, of the augmentation strategies can also be classified as: *task-independent* and *task-dependent* augmentations, whose mathematical presentations are Eq. (1a) and Eq. (1b):

$$\min_{\theta} \quad \mathcal{L}_{\text{aug}}(\{\mathcal{G}_i\}, \{f_\theta(\mathcal{G}_i)\}), \tag{1a}$$

$$\min_{\theta, \phi} \quad \mathcal{L}_{\text{all}}(\{\mathcal{G}_i\}, \{f_\theta(\mathcal{G}_i)\}, \phi), \tag{1b}$$

where θ and ϕ are the parameters of augmentation task and downstream task, $\mathcal{L}_{\text{aug}}(\cdot)$ is the augmentation objective, and $\mathcal{L}_{\text{all}}(\cdot)$ is the merged objective for both augmentation and downstream tasks. Notice that (1) some of the task-independent augmentations are not parameterized (e.g., randomly dropping edges), and the augmentation strategy selection θ is mainly based on heuristics; (2) according to specific tasks, $\mathcal{L}_{\text{all}}(\cdot)$ can be instantiated as either a joint optimization or a bi-level optimization objective.

2.1 Feature-wise Augmentation

In this subsection, we summarize the feature-wise augmentation strategies as three operations: (1) feature generation, (2) feature perturbation, and (3) feature calibration/denoising.

Feature Generation. Feature generation is commonly used to (1) initiate node features on plain graphs to smoothly incorporate into DGL models (e.g., GNNs) and (2) supplement additional node features which are hard to be captured by downstream models. Among all the feature-wise augmentations, feature generation is the only manner to change the feature dimension. A simple yet effective solution is to encode proximate/topological information into the generated features such as one-hot encoding of node index or node properties, etc. If the original node feature $\mathbf{X}$ is missed, the generated node feature can be fed directly into the downstream tasks. Otherwise, a popular choice is to concatenate the generated and the original node features (i.e., $\{\tilde{\mathbf{X}}, \mathbf{X}\}$). Note that the above augmentation strategies are all *task-independent* which can be precomputed before model learning.

Besides, a popular line of research is to generate features based on the given node features. A straightforward strategy is named Mixup [Zhang *et al.*, 2018] which generates node features based on the interpolation of given node features. We will introduce Mixup with more details in Sec. 2.3 as it includes but is not limited to the augmentation on node features. Also, incorporating generative modules into an end-to-end model is established and such strategies are all *task-dependent*. For example, [Liu *et al.*, 2021a] augments the node feature through a generative model whose input is the local neighborhood information of the target node, and naturally the optimization of the augmenter (i.g., generator) falls into the formulation of Eq. (1b).

Feature Perturbation. Feature perturbation aims to augment the input graph by partially perturbing the node features. In general, there are two popular feature perturbation methods: *feature shuffling* and *feature masking*. Specifically, as the i-th row of the matrix $\mathbf{X}$ represents the node feature of the i-th node, shuffling the rows of the node feature matrix is equivalent to obtaining an alternative graph with the same topology but permuted nodes. Since only the node feature is shuffled but the topology structure is kept, it will lead to the discrepancy between the above two distributions, which is implemented to generate negative samples in multi-view learning [Velickovic *et al.*, 2019]. Random shuffling is the most typical way and it is *task-independent*. For feature masking, its core operation is to set a part of the entries in the node feature matrix $\mathbf{X}$ to zero. This technique is popular in contrastive learning [Zhu *et al.*, 2020; You *et al.*, 2020a;

You et al., 2021] to generate augmented graph pairs and almost all works conduct that randomly which are *task-independent*. Aside from the above works, efforts such as (virtual) adversarial training on graphs [Feng et al., 2019] perturb the node feature to regularize the downstream models. As they fall into the domain of *adversarial attack and defense* on graphs, we do not discuss them in detail here and refer readers to a comprehensive survey [Sun et al., 2018] on this topic.

Feature Calibration/Denoising. The given node features are hardly optimal for specific downstream tasks due to various reasons such as noise, the precision of sensors, and so on. Minor calibrations on the node features are promising to show advantages and at the same time keep the majority of the initial node property. An instinctive strategy [Xu et al., 2021] is to compute the gradient of specific objective functions w.r.t. the node feature matrix and calibrate the node feature matrix based on the computed gradient. A special case of noisy features is that part of the features is missing whose corresponding solution is feature imputation. It is a reverse operation of the feature masking and has not been well-studied on graph-structured data due to the difficulties to incorporate topology information into the imputation models. Representative works include GCNMF [Taguchi et al., 2021] and Feature Propagation [Rossi et al., 2021]. The former represents the missing data by Gaussian mixture models; the latter diffuses the features from known features to unknown features based on the heat diffusion equation.

2.2 Structure-wise Augmentation

Different from i.i.d. data, graphs are inherently relational where the connections (i.e., edges) between data instances (i.e., nodes) are critical in understanding and analyzing graph data. Hence, many efforts are raised on augmenting the graph structure. We categorize them into: (1) edge addition/dropping, (2) node addition/dropping, (3) graph diffusion, and (4) graph sampling.

Edge Addition/Dropping. Manipulating the structure on given node sets (i.e., adding and dropping edges, a.k.a., *graph rewiring*) is widely adopted by DGL tasks. Mathematically it keeps the original node order and rewrites a part of the entries in the given adjacency matrices. Based on that, the augmented adjacency matrix $\tilde{\mathbf{A}}$ shares the same size as the initial one (i.e., $\mathbf{A}$). This augmentation method is also related *graph sparsification* [Zheng et al., 2020; Luo et al., 2021] (with special focus on dropping), *graph sanitation* [Xu et al., 2021], *graph sampling*, to name a few. It not only can be *task-independent* such as randomly dropping edges [You et al., 2020a; You et al., 2021; Zhu et al., 2021] but also can be *task-dependent* by formulating the topology (e.g., as a learnable distribution) into the downstream objectives [Zheng et al., 2020; Luo et al., 2021; Xu et al., 2021; Suresh et al., 2021b].

Node Addition/Dropping. Compared with adding/deleting edges, the augmentation operations on node sets are significantly more complicated. If we aim to add a node into the given graph, as an example, we need to (1) insert a row and a column into the given adjacency matrix $\mathbf{A}$, (2) insert a row

into the given node feature matrix $\mathbf{X}$, and may need to (3) expand the node label vector $\mathbf{y}$ depending on the specific downstream tasks. A typical application is to improve the propagation/connectivity of the whole graph by inserting a supernode into the given graph [Gilmer et al., 2017]. The supernode is connected with all the existing nodes in the graph. Its feature can be the aggregation of all the existing node features or can be learned through the downstream tasks. To alleviate the imbalanced label distribution, GraphSMOTE [Zhao et al., 2021a] insert nodes to enrich the minority classes. Dropping nodes from given graphs is an essential part of *graph sampling* technique which will be discussed later. Common goals of dropping nodes for DGL tasks are to generate perturbed graph samples [You et al., 2020a; You et al., 2021; Zhu et al., 2021] and extract informative subgraphs [Yu et al., 2020].

Graph Diffusion. As a structural augmentation strategy, graph diffusion can generate an augmented graph by providing the global views of the underlying structure. Graph diffusion injects the global topological information to the given graph adjacency by connecting nodes with their indirectly connected neighbors with calculated weights. The generalized graph diffusion can be formulated as:

$$\mathbf{S} = \sum_{k=0}^{\infty} \gamma_k \mathbf{T}^k, \tag{2}$$

where $\mathbf{T} \in \mathbb{R}^{N \times N}$ is the generalized transition matrix derived from the adjacency matrix $\mathbf{A}$ and θ is the weighting coefficient which determines the ratio of global-local information. Imposing $\sum_{k=0}^{\infty} \gamma_k = 1, \gamma_k \in [0, 1]$ and $\lambda_i \in [0, 1]$ where λ_i are eigenvalues of $\mathbf{T}$, guarantees convergence. Two popular examples of graph diffusion are personalized PageRank (PPR) [Page et al., 1999] (i.e., $\gamma_k = \alpha(1 - \alpha)^k$) and the heat kernel [Kondor and Lafferty, 2002] (i.e., $\gamma_k = e^{-t} \frac{t^k}{k!}$). where α denotes teleport probability in a random walk and t is diffusion time. Closed-form solutions to heat kernel and PPR diffusion are formulated in Eq. (3) and (4), respectively:

$$\mathbf{S}^{\text{heat}} = e^{-(\mathbf{I} - \mathbf{T})t}, \tag{3}$$

$$\mathbf{S}^{\text{PPR}} = \alpha(\mathbf{I} - (1 - \alpha)\mathbf{T})^{-1}. \tag{4}$$

Graph Sampling. Graph sampling or subgraph sampling is a commonly used data augmentation techniques for graphs. It can be used for different purposes, such as scaling up GNNs [Hamilton et al., 2017], enabling contrastive learning [Qiu et al., 2020], and so on. The augmented graph is obtained via a sampler SAMPLE:

$$\tilde{\mathcal{G}} = \texttt{SAMPLE}(\mathcal{G}), \tag{5}$$

where SAMPLE can be vertex-based sampling [Jiao et al., 2020], edge-based sampling [Zheng et al., 2020], and traversal-based sampling [Qiu et al., 2020], and other advanced methods such as Metropolis-Hastings sampling [Park et al., 2021]. For all the above samplers, they commonly return a connected subgraph induced from the sampled nodes. The induction step adds more connections into the sampled subgraph and empirically helps improve convergence. Generally speaking, the goal of graph sampling is to find augmented graph instances from input graphs that best preserve

desired properties by sampling a portion of nodes and their underlying linkages.

Graph Generation. Graph generation has a longstanding history. Classic methods on this topic are mostly based on reproducing some priori properties of given graphs, which are *task-independent*. Most modern graph generation techniques are also *task-independent* whose generators are expected to automatically learn from observed graphs. Representative works include GraphRNN [You *et al.*, 2018b] and NetGAN [Bojchevski *et al.*, 2018] where the former models a graph in an autoregressive manner and the latter trains a generator using the Wasserstein generative adversarial net objective. In addition, *task-dependent* graph generation plays a crucial role in many areas. A tractable implementation is applying reinforcement learning to encode desired molecule properties into the generated graphs [You *et al.*, 2018a]. LDS [Franceschi *et al.*, 2019] jointly learns an edge discrete probability distribution and the parameters of a node classifier. Aside from the above works, problems named *graph coarsening* [Cai *et al.*, 2021] and *graph condensation* [Jin *et al.*, 2021] can also be categorized into this field whose goals are to generate refined graphs from initial large graphs. The former pays more attention to finding a surjective mapping from original nodes to aggregated nodes, and the latter generates condensed graphs from scratch.

2.3 Label-wise Augmentation

Due to the shortage of human-annotated labels on graphs, label-wise augmentation is another important line of research in GraphDA to augment the limited labeled training data. In general, it can be categorized into two classes: (1) pseudo-labeling and (2) data mixup.

Pseudo-Labeling. Pseudo-labeling is a semi-supervised learning mechanism that aims to obtain one (or several) augmented labeled set(s), based on their most confident predictions on unlabeled data. Its learning process starts with a base teacher model trained on the labeled set $\mathcal{D}^L$, and then the teacher model is applied to the unlabeled data $\mathcal{D}^U$ to obtain pseudo labels (hard or soft) of unlabeled data. Finally, a subset of unlabeled data $\mathcal{D}^P$ will be used to augment the training data, and the combined data $\mathcal{D}^L \cup \mathcal{D}^P$ can be used to train a student model. In this sense, the label signals can be "propagated" to the unlabeled data samples via the learned teacher model. Note that this learning process could go through multiple rounds until converges by iteratively updating the teacher model with the current student model.

It is known that deep neural nets are error-prone to fitting and memorizing label noise given their high model capacity, while the pseudo labels computed with low confidence often have severe label noise, posing a great threat to the success of pseudo-labeling algorithms. In general, the key of pseudo-labeling is to mitigate the label noise by either selecting which subset of samples $\mathcal{D}^P$ in unlabeled data or re-weighting the pseudo-labeled instances in each round.

Data Mixup. Instead of leveraging unlabeled data, there is another simple and data-agnostic augmentation routine, termed Mixup [Zhang *et al.*, 2018], which directly interpo-lates the training samples. Generally, Mixup constructs virtual training samples:

$$\begin{aligned}
\tilde{\mathbf{x}} &= \lambda \mathbf{x}_i + (1-\lambda)\mathbf{x}_j, \\
\tilde{\mathbf{y}} &= \lambda \mathbf{y}_i + (1-\lambda)\mathbf{y}_j
\end{aligned} \tag{6}$$

$(\mathbf{x}_i, \mathbf{y}_i)$ and $(\mathbf{x}_j, \mathbf{x}_j)$ are two labeled samples randomly sampled from the training set, and $\lambda \in [0,1]$. In this way, mixup methods extend the training distribution by incorporating the prior knowledge that linear interpolations of feature vectors should lead to linear interpolations of the associated targets. Similarly, Manifold Mixup [Verma *et al.*, 2019] performs mixup on the intermediate representations learned from two training samples. However, how to explicitly mix the structure information between nodes remains an understudied problem.

3 Applications of Graph Data Augmentation in Deep Graph Learning

In this section, we review and discuss how GraphDA techniques can be leveraged to solve the two representative DGL problems, i.e., *optimal graph learning* and *low-resource graph learning* that are related to data quality.

3.1 GraphDA for Optimal Graph Learning

To mitigate the negative impacts from the given suboptimal graph, GraphDA has been widely used in optimal graph learning. Overall, optimal graph learning has two sub-problems:

Optimal Structure Learning. We summarize optimal structure learning works into three lines of work: (1) computing node similarities via metric learning (i.e., *metric-based* methods), (2) optimizing adjacency matrices as learnable parameters (i.e., *optimization-based* methods), and (3) learning probabilistic distributions of graph structure (i.e., *probabilistic modeling* methods). Specifically, the core idea of metric-based methods is to estimate node-wise similarity by different metric functions (i.e., edge predictors). A straightforward instantiation is GAUG [Zhao *et al.*, 2021b] which trains an edge predictor based on the given graph topology. In addition, such metric functions can be updated iteratively with the training of downstream tasks (e.g., GNNs-based node classification). For example, AdaEdge [Chen *et al.*, 2020a] iteratively adds or removes edges to the graph topology based on the classification results (from GNNs-based classifier) and trains GNNs classifier on the updated graphs to overcome the over-smoothing issue. IDGL [Chen *et al.*, 2020b] shares a similar idea with AdaEdge but updates the graph topology based on the learned node embeddings to enhance the robustness of the downstream model.

Optimization-based methods straightforwardly include the topology (e.g., adjacency matrix) as an optimization variable. Generally, differentiable heuristics of graph topology (e.g., smoothness) are integrated into the optimization objectives. For example, TO-GNN [Yang *et al.*, 2019] adopts the label smoothness and Pro-GNN [Jin *et al.*, 2020] adopts the feature smoothness and topology sparsity. Aside from graph topology constraints, Gasoline [Xu *et al.*, 2021] updates the initial graph through the feedback from the evaluation performance (e.g., classification loss) on the validation nodes.

Probabilistic modeling methods assume graphs are sampled from certain distributions and parameters of such distributions are learnable. For instance, LDS [Franceschi *et al.*, 2019] models the edges between each pair of nodes by sampling independent parameterized Bernoulli distributions and learning the model according to the feedback from classification loss. Since modeling every pair of nodes tend to be computationally expensive, an efficient solution is to estimate the dropping probability on existing edges. NeuralSparse [Zheng *et al.*, 2020] and PTDNet [Luo *et al.*, 2021] follow this strategy. The former one models the edge dropping probability as a categorical distribution on edges connecting to a target node, and the latter models every existing edge as a Bernoulli distribution. Both of them formulate their concrete instantiations based on the Gumbel-Max trick. In addition, the technique *Stochastic Block Model* (SBM) is useful to formulate the random graph from which the observed graph is realized. Bayesian-GCNN [Zhang *et al.*, 2019] and GEN [Wan and Kokel, 2021] both formulate the optimal graph distribution based on the SBM. The former infers the optimal SBM based on the observed initial graphs and corresponding node labels; the latter infers the optimal distribution based on a set of k-NN graphs constructed according to the hidden representations from GNNs layers.

Optimal Feature Learning. Compared to structure optimization, the research of graph feature optimization remains in its infancy, and recently there are some representative works have been proposed. AirGNN [Liu *et al.*, 2021b] aims to regularize the l_{21} norm between the input node features and convoluted node features such that the model is more tolerant against abnormal features. To handle missing node features, a special case of suboptimal initial node features, Feature Propagation [Rossi *et al.*, 2021] diffuses the features from known features to unknown features based on the heat diffusion equation; in other words, it replaces the missing node features with aggregated features from the neighborhood of the target nodes. GCNMF [Taguchi *et al.*, 2021] explicitly formulate the missing node features as Gaussian mixture models and learn model parameters with the downstream tasks in an end-to-end fashion.

3.2 GraphDA for Low-Resource Graph Learning

As one of the most effective solutions for addressing data scarcity issues on graphs, GraphDA has drawn much attention in the following topics of low-resource graph learning.

Graph Self-Supervised Learning. Recently data augmentation has been widely used for graph self-supervised learning (SSL). Inspired by the idea of AutoEncoders, graph generative modeling methods perform data augmentation on the input graphs and then learn the model by recovering feature/structure information from the augmented graphs. For an input graph, the features of nodes and/or edges are masked with zero or certain tokens. Then, the objective is to recover the masked features/structure according to the unmasked information via GNNs. For example, GPT-GNN [Hu *et al.*, 2020] proposes an auto-regressive framework to perform reconstruction on input graphs. Given a graph with its nodes and edges randomly masked, GPT-GNN generates one

masked node and its edges at a time and optimizes the likelihood of the node and edges generated in the current iteration. [You *et al.*, 2020b] define the Graph Completion pretext which aims to recover the masked feature of target node based on its neighbors' features and connections. Denoising Link Reconstruction [Hu *et al.*, 2019] randomly drops existing edges to obtain the perturbed graph and try to recover the discarded connections with a pairwise similarity-based decoder trained by a cross-entropy loss. GraphBert [Zhang *et al.*, 2020] leverages node feature reconstruction and graph structure recovery to pre-train a graph transformer model.

On the other hand, motivated by recent breakthroughs in contrastive visual feature learning, data augmentation is also widely used for Graph Contrastive Learning (GCL) methods. Generally, GCL methods try to generate augmented examples from the input and view two augmented examples that are from the same original sample as a positive pair, while those from different original samples are negatives. For instance, GCC [Qiu *et al.*, 2020] proposes to use subgraphs as contrastive instances to pre-train the graph encoder, which can be used for different downstream tasks with either freezing or full fine-tuning strategy. GraphCL [You *et al.*, 2020a] considers four graph-level augmentations: node dropping, edge perturbation, feature masking, and subgraph sampling. GRACE [Zhu *et al.*, 2020] adapts two augmentation strategies, removing edges and masking node features, to generate augmented views of graph data. It jointly considers both intra-view and inter-view negative pairs for contrast purposes. CSSL [Zeng and Xie, 2021] augments graphs with the different graph alteration operations (nodes/edges addition/deletion), and studies the performance under three types of training schemes. Note that there are more recent works in GCL, we will not cover all of them due to the space limit.

Graph Self/Co-Training. To alleviate the small data issue, one effective solution is to leverage the unlabeled data to augment the scarce labeled data. Following the idea of pseudo-labeling, self-training [Yarowsky, 1995] imputes the labels on unlabeled data based on a teacher model trained with limited labeled data, and it has become a prevailing paradigm to solve the problem of semi-supervised node classification when training data is limited. Among those methods, [Li *et al.*, 2018] first combines GCNs and self-training to expand supervision signals. CGCN [Hui *et al.*, 2020] generates pseudo labels by combining variational graph auto-encoder with Gaussian mixture models. Furthermore, M3S [Sun *et al.*, 2020] propose the multi-stage self-training and utilize a clustering method to eliminate the pseudo labels that may be incorrect. Similar ideas can also be found in [Dai *et al.*, 2021]. In addition, recent researches [Dong *et al.*, 2021; Ding *et al.*, 2022] also try to decouple the transformation and propagation operations in GNN layers and adopt label propagation as the teacher model to further enhance the generation of pseudo labels.

Similar to Self-training, Co-training [Blum and Mitchell, 1998] has also been investigated for augmenting the training set with unlabeled data. It learns two classifiers with initial labeled data on the two views respectively and lets them label unlabeled data for each other to augment the training

data. [Li *et al.*, 2020] develop a novel multi-view semi-supervised learning method Co-GCN, which unifies GCN and co-training into one framework.

Graph Interpolation. Another way of augmenting training data is using interpolation-based data augmentation, such as Mixup [Zhang *et al.*, 2018]. While unlike images or natural sentences which embrace a grid or linear sequence format, graphs have arbitrary structure and topology, rendering the use of interpolation-based data augmentation inapplicable. Although we can create additional nodes by interpolating the features and corresponding labels, it remains unclear how these new nodes must be connected to the original nodes via synthetic edges such that the structure of the whole graph is preserved. Meanwhile, due to the cascading effect of graph data, even simply deleting or adding one edge from a graph can dramatically change its semantic meanings.

To address those challenges, GraphMix [Verma *et al.*, 2021] applies manifold Mixup [Verma *et al.*, 2019] to graph node classification which jointly trains a fully-connected network and a GNN with shared parameters, for graph node classification in semi-supervised learning. Similarly, [Wang *et al.*, 2021] also follows the manifold mixup method and interpolates the input features of both nodes and graphs in the embedding space as data augmentation. Those methods leverage a simple way to avoid dealing with the arbitrary structure in the input space for mixing a graph pair, through mixing the graph representation learned from GNNs. GraphMixup [Wu *et al.*, 2021] performs semantic-level feature mixup by constructing semantic relation spaces and edge mixup with an edge predictor trained on two well-designed context-based self-supervised tasks, which is effective to solve class-imbalanced node classification tasks. To get rid of the manifold intrusion issue, [Guo and Mao, 2021] propose an input-level Mixup method to augment training data for graph classification. Graph Transplant [Park *et al.*, 2022] is another input-level Mixup graph augmentation method that can mix two dissimilar-structured graphs by replacing the destination subgraph with the source subgraph while preserving the local structure.

4 Future Directions

GraphDA is an emerging and fast-developing field. Although substantial progress has been achieved, many challenges remain. In this section, we discuss some promising research directions as follows.

Data Augmentation beyond Simple Graphs. Most of the aforementioned works develop the augmentation strategies on homophilic (i.e., assortative) graphs where edges tend to connect nodes with the same properties (e.g., labels, features). However, heterophily (i.e., disassortativity) also exists commonly in networks such as heterosexual dating networks. Many existing augmentation approaches [Suresh *et al.*, 2021a] on heterophilic graphs focus on improving the assortativity of the given graphs or dropping/deweighting the existing disassortative edges [Ye and Ji, 2021]. The augmentation on node features, labels, and non-existing edges of heterophilic graphs remains understudied.

Besides, existing GraphDA efforts are mainly developed for either plain or attributed graphs, while principled augmentation approaches for other types of graphs (e.g., heterogeneous graphs, hypergraphs, multiplex graphs) remain largely unexplored. Those complex graphs provide broader design space for augmentation but also challenge the effectiveness of existing GraphDA methods greatly, which is vital to explore in the future.

Data Augmentation for Graph Imbalanced Training. The graph data is inherently imbalanced which follows the power-law distribution. As an example, on the benchmark Pubmed dataset, nodes are labeled into three classes but the minority class only contains 5.25% of the total nodes. Such imbalanced data will lead to the suboptimal performance of downstream tasks especially classification tasks and one of the effective solutions is to augment the minority to alleviate the imbalance. Some initial attempts for this problem are proposed. GraphSMOTE [Zhao *et al.*, 2021a] augments the minority by mixing up the minority nodes; GraphMixup [Wu *et al.*, 2021] constructs semantic relation spaces for the augmentation of minority nodes. However, many challenges on this topic are still under-explored. For example, if the size of minority nodes is extremely small, such as few-shot or even 1-shot per class, how to transfer knowledge from the majority classes to augment the minority classes is worth studying.

Learnable and Generalizable Graph Augmentation. Unlike images, designing effective and semantic-preserving data augmentation for graphs is challenging due to their non-Euclidean nature and the dependencies between data samples. Most graph data augmentation methods adopt arbitrary augmentations on the input graph, which may unexpectedly change both structural and semantic patterns of the graph, leading to degraded performance [Park *et al.*, 2021]. For instance, perturbing the structure of a molecular graph might generate a molecule of totally different properties. Hence, proposing a principled and noise-free graph augmentation function is necessary. In the meantime, as different graphs have different properties, how to make the augmentation methods generalizable across different datasets. Also, since different graphs usually have different graph properties, developing generalizable data augmentation without learning from scratch arbitrary is important to improve the practical usage of GraphDA methods.

5 Conclusion

In this paper, we present a forward-looking and structured survey of graph data augmentation (GraphDA). In order to inspect the nature of GraphDA, we give a formal formulation and a taxonomy to facilitate the understanding of this emerging research problem. Specifically, we frame GraphDA methods into three categories according to the target augmentation modalities, i.e., feature-wise, structure-wise, and label-wise augmentations. We further review the application of GraphDA methods to address two data-centric DGL problems (i.e., optimal graph learning and low-resource graph learning) and discuss the prevailing GraphDA-based algorithms. Finally, we outline current challenges as well as opportunities for future research in this field.

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