## Graph Data Augmentation for Graph Machine Learning: A Survey

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### **Abstract**

Data augmentation has recently seen increased interest in graph machine learning given its ability of creating extra training data and improving model generalization. Despite this recent upsurge, this area is still relatively underexplored, due to the challenges brought by complex, non-Euclidean structure of graph data, which limits the direct analogizing of traditional augmentation operations on other types of data. In this paper, we present a comprehensive and systematic survey of graph data augmentation that summarizes the literature in a structured manner. We first categorize graph data augmentation operations based on the components of graph data they modify or create. Next, we introduce recent advances in graph data augmentation, separating by their learning objectives and methodologies. We conclude by outlining currently unsolved challenges as well as directions for future research. Overall, this paper aims to clarify the landscape of existing literature in graph data augmentation and motivate additional work in this area. We provide a GitHub repository with a reading list that will be continuously updated.

### 1 Introduction

Data driven inference has received a significant boost in generalization capability and performance improvement in recent years from data augmentation (DA) techniques. The DA techniques increase the amount of training data by creating plausible variations of existing data without additional ground-truth labels, and have seen widespread adoption in fields such as computer vision (CV) [Cubuk *et al.*, 2019] and natural language processing (NLP) [Feng *et al.*, 2021]. These techniques allow inference engines to learn to generalize across those variations and attend to signal over noise.

In recent years, with the rapid development of graph machine learning (GML) methods such as graph neural networks (GNNs) [Kipf and Welling, 2016; Hamilton *et al.*, 2017],

there has been increased interest and demand for data augmentation techniques on graph data [Zhao et al., 2021b]. Due to the irregular and non-Euclidean structure of graph data, graph data augmentation (GDA) techniques could hardly be directly analogized from the DA techniques used in CV and NLP. Moreover, GML faces unique challenges such as feature data incompleteness, structural data sparsity brought by power-law distributions, lack of labelled data due to costly annotations, and over-smoothing caused by message passing in GNNs. To address these challenges, there has been a growing number of works on GDA. GML researchers design graphspecific augmentation techniques for these unique challenges on graphs. On graph-level tasks, GDA techniques aim at generating extra data for training with known labels from the input training data to improve generalization. On node-level tasks, GDA techniques have enhanced GML models from a variety of perspectives. For example, Rong et al. [2019] randomly removes edges during training to alleviate the over-smoothing problem. Zhao et al. [2021b] enhanced graph structure to promote graph homophily. Kong et al. [2020] modified or added node attributes via adversarial training.

This paper aims to sensitize the GML community towards this growing area of work, when data augmentation has already drawn much attention in CV and NLP. As interest and work on this topic continue to increase, this is an opportune time for a paper of our kind to (i) give a bird's eye view of existing GDA techniques, and (ii) identify key challenges to effectively motivate and orient interest in this area. To the best of our knowledge, this is the first comprehensive survey on the topic of graph data augmentation. We hope this survey can serve as a guide for researchers and practitioners who are new to or interested in studying this topic.

This paper is structured as follows. Section 2 gives background on GNNs and data augmentation. It categorizes GDA techniques based on their modified components of graph data. Section 3 describes GDA techniques for (semi-)supervised GML – which we separate by the task levels: node-level tasks (Section 3.1), graph-level tasks (Section 3.2), and edge-level tasks (Section 3.3). Section 4 introduces GDA techniques that are used with self-supervised learning objectives, i.e., contrastive learning (Section 4.1) and consistency learning (Section 4.2). Within these subsections, we introduce the GDA techniques grouping by their methodologies. Finally, Section 5 discusses challenges and future directions for GDA.

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<sup>&</sup>lt;sup>1</sup>https://github.com/zhao-tong/graph-data-augmentation-papers

### 2 Background

### 2.1 Graph Neural Networks

Graph neural networks (GNNs) enjoy widespread use in modern graph-based machine learning due to their flexibility to incorporate node features, custom aggregations, and inductive operation, unlike earlier works which were based on embedding lookups [Perozzi et al., 2014; Grover and Leskovec, 2016]. Following the initial idea of convolution based on spectral graph theory [Bruna et al., 2013], many spectral GNNs have since been developed and improved by [Defferrard et al., 2016; Kipf and Welling, 2016; Levie et al., 2018; Klicpera et al., 2018; Ma et al., 2021]. As spectral GNNs generally operate (expensively) on the full adjacency, spatial-based methods which perform graph convolution with neighborhood aggregation became prominent [Hamilton et al., 2017; Veličković et al., 2017; Xu et al., 2018], owing to their scalability and flexibility [Ying et al., 2018].

### 2.2 Data Augmentation

Data augmentation (DA) encompasses techniques of increasing/generating training data without directly collecting or labeling more data. Most DA techniques either add slightly modified copies of existing data or generate synthetic based on existing data. The augmented data act as a regularizer and reduce overfitting when training data-driven models [Shorten and Khoshgoftaar, 2019]. DA techniques has been commonly used in CV and NLP [Feng et al., 2021], where augmentation operations such as cropping, flipping, and backtranslation are commonly used in machine learning model training. In graph machine learning, in contrast to regular data such as grids (e.g., images) and sequences (e.g., sentences), the graph structure is encoded by node connectivity, which is non-Euclidean and irregular. Most structured augmentation operations used frequently in CV and NLP cannot be easily analogized to graph data. Therefore, how to generate effective augmented data examples on graph data is less obvious.

### 2.3 Graph Data Augmentation

Similar to DA techniques for CV and NLP, GDA creates data objects via modification or generation. However, as graphs are connected data, unlike images or texts, the data objects in graph machine learning are often non-i.i.d. Hence, for nodelevel and edge-level tasks, GDA techniques modify the entire dataset (graph) instead of some data objects (nodes or edges). Based on the graph data components that are modified or created, we define four categories of GDA operations as follows.

**Node Augmentations** are the GDA operations that create or remove nodes from the graph. For example, Mixup-based methods [Wang *et al.*, 2021b] created new nodes by combining two existing nodes. Feng *et al.* [2020] proposed the DropNode operation that removed nodes by masking of the features of selected nodes.

**Edge Augmentations** are the GDA operations that modify the graph connectivity via adding/removing edges. The modifications can be either deterministic (e.g., GDC [Klicpera *et al.*, 2019] and GAug-M [Zhao *et al.*, 2021b]

both modified the graph structure and used the modifed graph for training/inferencing) or stochastic (e.g., Rong *et al.* [2019] proposed to randomly drop edges during each training epoch).

**Feature Augmentations** are the GDA operations that modify or create raw node features. For example, You *et al.* [2020] used Attribute Masking that randomly masked off node features; FLAG [Kong *et al.*, 2020] augmented node features with gradient-based adversarial perturbations.

**Subgraph Augmentation** refers to the GDA operations that operate at the graph level, such as cropping out subgraphs or creating new graphs. As the subgraph augmentation operations usually affect multiple nodes in the subgraph, they are mostly used for graph level tasks. For example, JOAO [You *et al.*, 2021] used subgraph cropping; ifMixup [Guo and Mao, 2021] created new graphs by mixing up two graphs.

### 3 Graph Data Augmentation Techniques for Supervised Learning

In this section, we discuss GDA techniques that are used for supervised graph learning. We categorize the GDA techniques by their task levels (node, graph, or edge).

### 3.1 Node-level Tasks

Edge Dropping Edge dropping methods stochastically remove a certain amount of edges from the graph data during each training epoch. Rong *et al.* [2019] first proposed DropEdge which randomly dropped a fixed fraction of edges in each epoch, in a way similar to Dropout. By showing the GNN model different part of the graph in each training epoch, DropEdge significantly improved the model's generalization and alleviates the over-smoothing problems of GNNs, especially for deeper GNNs. Although DropEdge efficiently augmented the edges, it is often criticized for also removing task-relevant signals and corrupting informative graph structures.

Following DropEdge, Zheng et al. [2020] proposed NeuralSparse that utilized a MLP-based graph sparsification model that learned to remove only the potentially task-irrelevant edges. The graph sparsification model is supervised and trained jointly with GNN on the node classification loss. PTDNet [Luo et al., 2021] further applied the nuclear norm regularization loss to impose the low-rank constraint on the modified graph by the graph sparsification model. Gao et al. [2021] proposed TADropEdge that leveraged the graph spectrum to generate edge weights that represent the edges' criticality for the graph connectivity. TADropEdge dropped the edges using the edges weights as the probabilities.

Other than node classification, Spinelli *et al.* [2021] proposed FairDrop for the task of fair graph representation learning, which biasedly dropped edges with a sensitive attribute homophily mask to protect against unfairness.

**Graph Diffusion** Klicpera *et al.* [2019] first proposed generalized graph diffusion that modeled a "future" state of the graph where the signals were more spread out. By utilizing commonly used graph diffusion such as personalized PageRank (PPR) or heat kernal along with graph sparsification, GDC [Klicpera *et al.*, 2019] generates a diffused version

Table 1: A summary of graph data augmentation techniques for graph machine learning. Task levels: V: node-level; G: graph-level; E: edge-level. Augmented data categories: V: node; E: edge; X: feature; G: subgraph.

†Although GRAND and NodeAug are semi-supervised methods, they used GDA operations with only self-supervised learning objectives (i.e, consistency loss). Therefore, we categorize their GDA techniques as designed for self-supervised learning objectives.

		Tas V	sk Le G	evel E	Aug V	gmer E	ited I X	Oata G	Augmentation Methodology
GDA for Supervised Objective	DropEdge [Rong et al., 2019] NeuralSparse [Zheng et al., 2020] TADropEdge [Gao et al., 2021] FairDrop [Spinelli et al., 2021]	\ \langle \langle \ \langle \langle \ \langle \l				√ √ √ √			Edge dropping
	GDC [Klicpera et al., 2019] MV-GCN [Yuan et al., 2021]	<b>/</b>				<b>√</b>			Graph diffusion
	AdaEdge [Chen et al., 2020] Pro-GNN [Jin et al., 2020] GAug-M [Zhao et al., 2021b] GAug-O [Zhao et al., 2021b] Eland [Zhao et al., 2021c] MH-Aug [Park et al., 2021]	\ \ \ \ \ \ \				> > > > > > > > > > > > > > > > > > >			Structure prediction
	FLAG [Kong et al., 2020] LA-GNN [Liu et al., 2021] SR+DR [Song et al., 2021]	<b>✓</b> ✓	✓	✓			√ √ √		Feature generation
	AutoGRL [Sun et al., 2021a]	<b>✓</b>			✓	✓	✓		AutoML
	GraphMix [Verma et al., 2019] Graph Mixup [Wang et al., 2021b] ifMixup [Guo and Mao, 2021] Graph Transparent [Park et al., 2022]	1	√ √ √		1			√ √ √	Mixup
	GraphCrop [Wang et al., 2020a]		✓					✓	Subgraph cropping
	MoCL [Sun et al., 2021b]		/					<b>✓</b>	Substructure substitution
	M-Evolve [Zhou et al., 2020]		<b>✓</b>			✓			Motif-similarity mapping
	CFLP [Zhao et al., 2021a]	<u>.                                      </u>		/		✓			Counterfactual augmentation
	MeTA [Wang et al., 2021a]			<b>✓</b>					Edge perturbation
GDA for Self-supervised Objective	DGI [Velickovic et al., 2019] GraphCL [You et al., 2020] GRACE [Zhu et al., 2020] SUBG-CON [Jiao et al., 2020] InfoGCL [Xu et al., 2021] BGRL [Thakoor et al., 2022] GRAND <sup>†</sup> [Feng et al., 2020]	1 1111	1		\frac{1}{\sqrt{1}}	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	\ \ \	Corruption
	MVGRL [Hassani and Khasahmadi, 2020] MV-CGC [Yuan <i>et al.</i> , 2021]	1				<b>√</b> ✓			Graph diffusion
	JOAO [You et al., 2021] GCA [Zhu et al., 2021] LG2AR [Hassani and Khasahmadi, 2022] FairAug [Kose and Shen, 2022] AD-GCL [Suresh et al., 2021]	\ \ \ \ \ \ \ \	1		\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	\ \ \ \ \ \ \	\ \ \ \ \ \ \	√ √	Automated augmentation
	NodeAug <sup>†</sup> [Wang et al., 2020b]	1				✓	✓		Biased perturbation

of the observed graph. The generated graph is then used for both training and inferencing. While message passing-based GNNs are only capable of aggregating one hop information in each layer, GDC allows GNNs to learn from multi-hop information without specifically re-designing the model.

To further utilize the information given by different graph diffusions, MV-GCN [Yuan et al., 2021] generates two complementary views with PPR and heat kernal and learns from both created views and the original graph. MV-GCN uses a consistency regularization loss to reduce the distribution distance of the representations learned from the three views.

Structure Prediction Prediction-based GDA techniques update the graph structure to enhance task-relevant information in the graph. For example, Zhao et al. [2021b] showed the correlation between graph structural homophily and node classification performance. Then they proposed GAug-M and GAug-O to update the graph structure by neural link predictors. Similar to GDC [Klicpera et al., 2019], GAug-M deterministically modifies the graph structure and use the updated graph for training and inferencing. To allow inductive learning on graphs, GAug-O samples graph structure from learned probabilities in each training epoch. Chen et al. [2020] also proposed AdaEdge that iteratively add/remove edges according to the node classification prediction. In each iteration, AdaEdge adds edges between nodes that are predicted to be in the same class with high confidence, and vice versa. Pro-GNN [Jin et al., 2020] updates the graph structure with constrains on the low-rank property and feature smoothness.

MH-Aug [Park *et al.*, 2021] creates an "explicit" target distribution, with controlled strength and diversity, to sample augmented graphs. As sampling from the complex target distribution is infeasible, MH-Aug adopts the Metropolis-Hastings algorithm to obtain the augmented samples.

Zhao et al. [2021c] proposed Eland for the task of anomaly detection on time-stamped user-item bipartite graphs. Eland first transforms the user-item graph into users' action sequences and adopts seq2seq model for future action prediction. The predicted user actions are added back into the graph to generate the augmented graph data. As the augmented graph contains richer user behavior information, Eland enhances the anomaly detection performance and detects anomalies at an early stage.

**Feature Augmentation** For (semi-)supervised graph learning, feature augmentation methods usually try to improve the node feature quality by learning additional task-relevant features. FLAG [Kong et al., 2020] utilizes adversarial training to iteratively augment the node features with gradient-based adversarial perturbations. Being a free training approach, FLAG improves the performances of GNNs on the tasks of node classification, link prediction, and graph classification. LA-GNN [Liu et al., 2021] enhances the locality of node representations by generating additional node features based on the conditional distribution of local neighborhoods. The generated feature is directly used together with the raw node features. Similarly, SR+DR [Song et al., 2021] generates topology features with DeepWalk [Perozzi et al., 2014], and uses a dual GNN model with topology regularization to jointly train with both raw and topology features.

**Mixup** Mixup [Zhang et al., 2018] merges two images to generate a new images with a weighted label. Given the dependent and non-Euclidean structure of graph, the direct analog of Mixup on graph data is not obvious. Verma et al. [2019] proposed GraphMix that augmented the training of a GNNs with a Fully-Connected Network. As GraphMix is more of a regularization method than the analog of Mixup on graphs, Wang et al. [2021b] proposed Graph Mixup, which analogized Mixup with a two-branch graph convolution module. Given a pair of nodes, Graph Mixup mixes the raw features of them, feeds the them into the two-branch GNN layer, and mixes their hidden representations of each layer. Mixing up the nodes on features and hidden states avoids re-assembling the local neighborhoods of the two nodes.

**AutoML** With the rapid development of AutoML, automated graph learning method were proposed to automate the design of GNN architecture as well as the choice of GDA operations. Sun *et al.* [2021a] proposed AutoGRL for the task of node classification. Though training process, AutoGRL learns the best combination of GDA operations, GNN architecture, and hyperparameters. The searching space of AutoGRL includes four GDA operations implemented by random masking and GAug-M [Zhao *et al.*, 2021b]: drop features, drop nodes, add edges, and remove edges.

### 3.2 Graph-level Tasks

For graph-level tasks, where data objects are independent graphs, certain augmentation operations in CV and NLP can be transferred to graph data. For example, similar to image cropping, GraphCrop [Wang et al., 2020a] crops a contiguous subgraph from each of the given graph object. GraphCrop adopts a graph diffusion-based node-centric strategy to maintain the topology characteristics of original graphs.

M-Evolve [Zhou et al., 2020] utilizes motifs to augment the graph data. M-Evolve first finds and selects the target motif in the graph, then adds or removes edges within the selected motifs based on a sampling weight calculated with Resource Allocation index. Similarly, MoCL [Sun et al., 2021b] utilizes biomedical domain knowledge to augment the molecular graphs on the substructures such as functional groups. MoCL selects a substructure from each molecular graph and replaces it with another substructure.

Mixup Several Mixup methods were also proposed for graph classification. For example, the aforementioned Graph Mixup [Wang et al., 2021b] also works for graph classification. Graph Mixup mixes the latent representations of the pair of graphs. On the other hand, ifMixup [Guo and Mao, 2021] directly applies Mixup on the graph data instead of the latent space. As the pair of graphs are irregular and the nodes from two graphs are not aligned, if Mixup arbitrarily assigns indices to the nodes in each graph and matches the nodes according to the indices. Following ifMixup, Graph Transparent [Park et al., 2022] also mixes graph in data space. Unlike ifMixup that randomly matches nodes during mixing, Graph Transparent uses substructures as mixing units to preserve the local structural information. Graph Transparent employs the node saliency information to select one meaningful substructure from each graph, where the saliency information is defines as the  $l_2$  norm of the gradient of the classification loss.

### 3.3 Edge-level Tasks

We note that very few GDA techniques were proposed for edge level tasks such as link prediction. Zhao *et al.* [2021a] proposed a counterfactual data augmentation method CFLP. CFLP asks the counterfactual question of "would the link still exist if the graph structure became different from observation?" To answer the question, Zhao *et al.* [2021a] proposed counterfactual links that approximates the unobserved outcome in the question. CFLP trains the link prediction model with both the given training data and the generated counterfactual links (as augmented data).

Wang et al. [2021a] proposed MeTA for link prediction on temporal graphs. MeTA contains a multi-level module that processes the augmented graphs of different magnitudes on separate levels. MeTA adopted three augmentation operations for the temporal graphs: perturb time that modifies the time-stamp on edges, remove edge that is similar to DropEdge [Rong et al., 2019], and add edges that repeats existing edges with a different time-stamp. During training and prediction, MeTA performs message passing across levels to provide adaptively augmented input graphs.

# 4 Graph Data Augmentation Techniques for Self-supervised Learning Objectives

In this section, we cover the GDA techniques that are used for self-supervised learning objectives, i.e., contrastive learning and consistency learning. Self-supervised objectives learn representations that are robust to noise and perturbations by maximizing the (dis)agreements of learned representations. Therefore, unlike the above presented GDA techniques that aim to enhance the task-relevant information in the data, most of the GDA techniques for self-supervised learning are stochastic augmentations that aims to corrupt the given graph data. Moreover, most self-supervised graph representation learning methods tend to use a combination of several simple GDA operations.

### 4.1 Contrastive Learning

In the past few years, with the rapid development of contrastive learning, several graph contrastive learning methods [You et al., 2021] have been proposed. Contrastive learning aims to maximize the distance between representations of different objects and minimize the distance between representations learned from different views of the same object. Data augmentation is commonly used for generating the different views for contrastive learning.

**Corruption** To efficiently generate different augmented data for graph contrastive learning, the most commonly used GDA operations are the corruption-based ones. For example, DGI [Velickovic *et al.*, 2019] adopts feature corruption where it conducts a row-wise shuffling on the raw node feature matrix **X**. The feature corruption by DGI can also be viewed as randomly swapping the nodes in the graph.

GraphCL [You et al., 2020] and InfoGCL [Xu et al., 2021] adopt four GDA operations: node dropping that randomly removes nodes along with its edges, edge perturbation

that randomly adds or drops edges, attribute masking that randomly masks off certain node attributes, and subgraph sampling that samples a connected subgraph. Similar to the subgraph sampling operation used in GraphCL, SUBGCON [Jiao et al., 2020] utilizes a subgraph sampler to sample the augmented subgraph. GRACE [Zhu et al., 2020] and BGRL [Thakoor et al., 2022] use only the basic random edge dropping and attribute masking for creating different views of the graph.

Graph diffusion As an efficient GDA operation that can naturally creates a "future view" of the given graph, graph diffusion is used in graph contrastive learning. MV-GRL [Hassani and Khasahmadi, 2020] adopts the diffusion graph proposed by GDC [Klicpera et al., 2019] as the second view. Interestingly, Hassani and Khasahmadi [2020] showed that using three views (original graph, diffusion graphs by PPR and heat kernal) would not result with better performance than using two views (original graph and one diffusion graph), and concluded "increasing the number of views does not improve the performance." However, Yuan et al. [2021] later proposed MV-CGC that adopted a similar contrastive learning framework with three views: original graph, diffusion graph, and their proposed feature similarity view. Empirically, the node representations learned by MV-CGC outperformed those learned by MVGRL on node classification.

**Automated GDA** As aforementioned, most contrastive learning methods adopt a combination of several simple augmentation operations. The selection among the operations and their magnitudes significantly increases the number of hyperparameters. Therefore, automated solutions that can learn the augmentation strategies are developed.

JOAO [You et al., 2021] models the selection of GDA for GraphCL [You et al., 2020] as a bilevel optimization problem, where the outer level learns the augmentation strategy and the inner level learns graph representations with the given augmentations. AD-GCL [Suresh et al., 2021] utilizes an adversarial graph augmentation strategy to avoid redundant information brought by random augmentation. LG2AR [Hassani and Khasahmadi, 2022] learns a probabilistic policy that contains a set of distributions over different augmentation operations, and samples augmentation strategy from the policy in each training epoch. GCA [Zhu et al., 2021] designs adaptive augmentations based on the node centrality measures. Unlike the above-mentioned that finds the best augmentation strategy for the dataset, the adaptive augmentation of GCA gives different augmentation to nodes according to their importance. Similarly, FairAug [Kose and Shen, 2022] utilizes adaptive augmentation for fair graph representation learning.

### 4.2 Consistency Learning

Similar to contrastive learning, consistency learning learns representation from different views of data and maximizes their agreement. However, unlike contrastive learning that compares between data objects, the consistency loss compares the distributions of a batch of representations via metrics like KL-divergence. Therefore, the consistency loss is rarely used itself, but often used along with super-

vised losses in the semi-supervised learning. For example, NodeAug [Wang et al., 2020b] uses three local structure-based augmentation operations: replace attributes, remove edges, and add edges. NodeAug minimizes the KL-divergence between the node representations learned from the original graph and augmented graph. GRAND [Feng et al., 2020] creates multiple different augmented graphs with node dropping and feature masking. The consistency loss then minimizes the distances of the representations learned from the augmented graphs.

### 5 Challenges and Directions

### 5.1 Automation and Domain Adaptation

As GDA is a relatively new topic, many GDA techniques (as shown in Table 1) have been proposed and used independently. However, an ideal GDA solution would have to select and tune many data augmentation techniques prior to deployment. This challenge has been observed in CV. For example, over ten independent augmentation operations exist for image data [Cubuk et al., 2019], each with its own magnitude parameter. CV researchers then developed automated augmentation solutions to adaptively customize augmentation strategies for each (batch of) object. Although several automated augmentation solutions exist for graph contrastive learning, automated augmentation methods for (semi-)supervised graph learning are still needed. Moreover, the automated augmentation solutions should be transferable. That is, domain adaptation is a desired characteristic for automated GDA techniques. When the automated augmentation method trained on one dataset could only be used on that dataset, the method would just automate the hyperparameter training process and lose the generalizability [You et al., 2021]. Therefore, for an ideal automated GDA method, it should be able to be trained on one dataset and used for many, ideally cross domain. Automated GDA methods that can be transferable across domains are still missing.

### 5.2 Scalability for Large-Scale Graphs

Many GDA techniques used global structural information during the augmentation process as those were hard to learn by message passing GNNs. However, learning global information often requires the method to learn from the entire graph, which can cause the scalability issue. The scalability issue is especially severe for node-level tasks where the graph size can be very large. While the complex GDA techniques bring significant performance improvements, the scalability of the methods are still worthy of attention. For example, in order to enable end-to-end training, GAug-O [Zhao et al., 2021b] required back-propagating on the entire adjacency matrix, resulting the extra need of memory on GPU cards. To improve the performance of DropEdge [Rong et al., 2019], TADropEdge [Gao et al., 2021] required the pre-calculation of a score for each edge in the graph prior to the training of GNNs. Therefore, to be applicable in real life applications, efficiency is also a necessity for GDA techniques. As mentioned in the previous subsection, an automated solution that combines the fast and simple augmentation operations may be solution. Nonetheless, how to design an efficient automated GDA framework is still an open question.

### 5.3 Generalization and Regularization

On certain types of graph data such as molecule graphs, most commonly used GDA operations would change the underlying semantic of the graph. For example, dropping a carbon atom from the phenyl ring of aspirin breaks the aromatic system and results in a alkene chain [Lee *et al.*, 2021], which is an entirely different chemical compound. Therefore, domain-based regularization should be used in such situation. So far, only Sun *et al.* [2021b] proposed MoCL that considers the semantic information brought by local substructures when augmenting the molecule graphs, leaving the domain-specific regularization for GDA rather under-explored. Moreover, as a generalization improving technique, GDA should be naturally good for out-of-distribution (OOD) data. GDA techniques for OOD graph learning are still missing.

### **5.4** Theoretical Foundation

GDA is a powerful technology to improve the performance of data-driven inference on graphs without the need of extra labeling effort or complex models. GDA is also known for improving the generalization of graph learning and alleviating the over-smoothing problem of GNNs. Yet, there is little rigorous understanding of how and why GDA achieves those, especially for (semi-)supervised learning. Although several works [Zhao et al., 2021b; Chen et al., 2020] have analyzed the relation between graph homophily and classification performance or the over-smoothing problem, we are facing lack of a rigorous proof or theoretical bounds on those relations.

Recently, several works provided theoretical insights of data augmentation in CV. For example, Wu et al. [2020] theoretically analyzed the generalization effect of data augmentation on images. They interpreted the effect of data augmentation from bias and variance, where data augmentation adds new information to model while also serving as a regularization. Due to the irregular characteristics of graph data, these theoretical analysis cannot be directly used for GDA. Other than the perspective of generalization, several recent works have studied the certified robustness of GNNs [Zügner and Günnemann, 2020]. Improved robustness bounds would be a desired property of GDA techniques. Recent studies [Topping et al., 2022] on the topology bottleneck and over-squashing of GNNs provide theoretical guides for edge-based GDA techniques. Counterfactual augmentation methods on graphs such as CFLP [Zhao et al., 2021a] can also bring insights for analyzing GDA from the perspective of causality.

### 6 Conclusions

In this paper, we presented a comprehensive and structured survey of data augmentation techniques for graph machine learning. We categorized existing GDA techniques, introduced recent GDA approaches based on their methodologies, and outlined current challenges as well as directions for future research. We showed that there was much room for further exploration on GDA. In conclusion, we hope this paper serves as a guide for GML researchers and practitioners to study and use GDA techniques, and inspire additional interest and work on this topic.

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