Data Augmentation on Graphs: A Survey

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In recent years, graph representation learning has achieved remarkable success while suffering from low-quality data problems. As a mature technology to improve data quality in computer vision, data augmentation has also attracted increasing attention in graph domain. For promoting the development of this emerging research direction, in this survey, we comprehensively review and summarize the existing graph data augmentation (GDAug) techniques. Specifically, we first summarize a variety of feasible taxonomies, and then classify existing GDAug studies based on fine-grained graph elements. Furthermore, for each type of GDAug technique, we formalize the general definition, discuss the technical details, and give schematic illustration. In addition, we also summarize common performance metrics and specific design metrics for constructing a GDAug evaluation system. Finally, we summarize the applications of GDAug from both data and model levels, as well as future directions.

CCS Concepts: • Theory of computation → Graph algorithms analysis; • Computing methodologies → Machine learning.

Additional Key Words and Phrases: Graph Data Augmentation, Survey, Graph Representation Learning

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1 INTRODUCTION

Graphs or networks are important data structures widely used to model a variety of complex interaction systems in real-world scenarios. For example, the interactions of users on Facebook can be modeled as a social network, where nodes represent accounts and edges represent the existence of a friend relationship between two users; the structure of a compound can be modeled as a molecular graph where nodes represent atoms and edges represent the chemical bonds connecting the atoms; a literature database can be modeled as a heterogeneous citation network, where nodes represent authors and papers, and edges can represent collaboration relationships between authors, attribution relationships between authors and literature, and citation relationships between papers. At present, graphs have emerged as one of the fundamental techniques supporting relational data mining. On this basis, various graph representation learning (GRL) methods [10, 12, 28] have been...
continuously proposed and optimized, and have achieved excellent performance on various graph analysis tasks.

As a data-driven study, GRL relies on sufficient high-quality data to characterize the underlying information of graphs. However, modeling real-world interaction systems often suffers from several data-level challenges that negatively affect the learning of graph models and the performance of downstream tasks: 1) Obtaining data labels is expensive and time-consuming, which limits the effectiveness of graph learning methods based on supervised or semi-supervised settings. For example, the anonymity of blockchain makes account identity labeling information scarce in cryptocurrency transaction networks, which leads to a higher risk of account identification models falling into over-fitting and low generalization [94]. Moreover, there are far fewer anomalous accounts and transaction behaviors in the transaction network than normal ones, and this label imbalance problem [45, 72, 90] will limit the performance of graph models on downstream tasks. 2) Complex interaction systems in real world usually encounter problems such as information loss, redundancy, and errors [37, 91, 93]. For example, due to the privacy restrictions of transaction data, we usually have no access to some private sensitive attribute information; malicious association of bot accounts in social networks will interfere with recommendation systems to accurately characterize user features; malicious data tampering introduces adversarial noise. These phenomena lead to suboptimal, untrustworthy, and vulnerable graph representation learning.

Inspired by the remarkable success of data augmentation in computer vision and natural language processing, a range of problems caused by low-quality data in the graph domain can also be alleviated by developing data augmentation on graphs. Data augmentation can increase the limited amount of training data by slightly modifying existing data or synthesizing new data, helping machine learning models reduce the risk of over-fitting during the training phase [50]. Unlike image and text data, graph-structured data are non-Euclidean and discrete, and their semantics and topological structure are dependent, making it challenging to transfer existing data augmentation techniques or design new ones. Despite recent advances in graph augmentation techniques, this fledgling research field is still not sound, lacking: 1) Systematic taxonomies; 2) Generalized definitions; 3) Scientific evaluation system; 4) Clear application summary. This makes it difficult for researchers to have a clear and inductive understanding of graph data augmentation (GDAug), and cannot use or design GDAug techniques well in graph learning.

Recently there have been some surveys related to GDAug, as listed in Table 1. These surveys review existing GDAug techniques according to different taxonomies, such as graph tasks (node-level, edge-level, graph-level) in [39, 88], graph elements (structure-oriented, features-oriented, labels-oriented) in [7, 36, 71, 74, 99], and scales (micro-level, meso-level, macro-level) in [81]. However, these GDAug-related surveys seldom generalize general definitions, describe design details, and summarize evaluation system for GDAug. Meanwhile, these surveys related to graph self-supervised learning [36, 71, 74, 99] only investigate GDAug as a module in graph contrastive learning, and lack a comprehensive summary on evaluation system, application, and technical perspectives. Therefore, this paper comprehensively summarizes the contents related to GDAug, and the main contributions can be summarized as follows:

- We summarize existing multiple taxonomies for GDAug and review representative methods using a taxonomy based on fine-grained graph elements (i.e., feature, node, edge, subgraph, graph and label), which facilitates researchers understand GDAug from various design perspectives.
- We generalize general definition, discuss technical details, and provide clear schematic illustration for each specific GDAug method. To the best of our knowledge, this is the most exhaustive summary of GDAug from a technical perspective.
Table 1. Emphasizing the contribution of this paper in contrast to related surveys.

| Context for GDAug | Related Survey | Ours | [39] | [7] | [88] | [81] | [71] | [36] | [74] | [99] |
|------------------|---------------|------|------|------|------|------|------|------|------|------|
| Topic conformity | ✓             | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    |
| Summary of taxonomies | ✓          | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    |
| Generalized definitions | ✓         | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    |
| Technical details | ✓             | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    |
| Schematic illustration | ✓         | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    |
| Summary of evaluation systems | ✓        | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    |
| Summary of application | ✓         | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    |
| Technical perspective | ✓           | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    |
| Summary of open resources | ✓        | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    | ✓    |

- We summarize the available evaluation metrics for GDAug, including common performance metrics and specific design metrics.
- We summarize the applications of GDAug to graph learning, and discuss the challenges and future direction.

2 PRELIMINARIES

2.1 Graph

A graph that contains all the necessary and optional graph elements can be represented as $G = (\mathcal{V}, \mathcal{E}, X_v, X_e, \mathcal{Y}_v, \mathcal{Y}_e)$, where $\mathcal{V} = \{v_1, v_2, \ldots, v_{|\mathcal{V}|}\}$ and $\mathcal{E} = \{e_1, e_2, \ldots, e_{|\mathcal{E}|} | e = (v_i, v_j) ; v_i, v_j \in \mathcal{V} \}$ are the sets of nodes and edges respectively, $X_v \in \mathbb{R}^{|\mathcal{V}| \times F_v}$ and $X_e \in \mathbb{R}^{|\mathcal{E}| \times F_e}$ are the feature matrices of nodes and edges respectively, $\mathcal{Y}_v = \{(v_i, y_i) | v_i \in \mathcal{V}\}$ is the set of node labels and $\mathcal{Y}_e$ is the graph label. For the sake of simplicity, the subscript of feature matrix is ignored when there is no need to specify what kind of features. The necessary structure elements $(\mathcal{V}, \mathcal{E})$ can also be represented alternatively as adjacency matrix $A \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{V}|}$, where $A_{ij} = 1 \left[ (v_i, v_j) \in \mathcal{E} \right]$ for $1 \leq i, j \leq |\mathcal{V}|$. A diagonal matrix $D \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{V}|}$ defines the degree distribution of $G$, and $D_{ii} = \sum_{j \neq i} A_{ij}$.

2.2 Data Augmentation

Data augmentation can increase training data without collecting or labeling more data. Instead, it enriches the data distribution by slightly modifying existing data or synthesizing new data. Data augmentation serves as a regularizer to help machine learning models reduce the risk of over-fitting during the training phase, and has been widely applied in CV and NLP, such as rotation, cropping, scaling, flipping, mixup, back translation, synonym substitution. In graph domain, data augmentation can be regarded as a transformation function on graphs: $f: G = (A, X) \rightarrow \hat{G} = (\hat{A}, \hat{X})$, where $\hat{G}$ is the generated augmented graph. However, due to the non-Euclidean data nature and the dependencies between the semantics and topology of samples, it is challenging to transfer existing data augmentation techniques onto graphs or design effective graph augmentation techniques.
techniques. Therefore, research and investigations on data augmentation techniques on graphs are urgently needed and valuable.

3 TAXONOMIES OF GRAPH DATA AUGMENTATION

In this section, we briefly summarize the feasible taxonomies of data augmentation on graph structured data. GDAug methods can be categorized into different types based on different graph elements, target tasks, model dependence and augmentation strategies. We try to give a clear overview on the main taxonomies of GDAug.

3.1 Graph Element

The GDAug algorithms can be executed on different graph elements, i.e., graph feature, graph structure and graph label. The available graph element associated with GDAug generally depends on the graph types and tasks.

- **Feature-wise Augmentation:** Graph features are available in attributed graphs and can be categorized into node features, edge features, as well as other relevant features such as position features (in molecular graphs). More broadly, the latent and hidden features learned by neural networks (or other models) on graphs also belong to graph features. Feature-wise augmentation mainly augments graph data by modifying, creating, or fusing raw graph features, e.g., feature masking and feature completion.

- **Structure-wise Augmentation:** A granularity-based partitioning on graph structure can be represented as node, edge, path, subgraphs (motif, community), and full graph. Structure-wise augmentation mainly augments graph data by modifying the raw graph structure or generating new graph structures, e.g., node dropping, edge rewiring and graph diffusion.

- **Label-wise Augmentation:** A labeled graph carries labels associated with nodes, edges or the full graph. To alleviate the data-hungry problem, label-wise augmentation generally augments the limited labeled training data by assigning pseudo labels for unlabeled data or synthetic samples.

3.2 Target Task

The GDAug algorithms can be designed for different graph tasks, yielding three schemes:

- **Node-level Augmentation** augments graph entities by removing nodes from graphs (e.g., node dropping), creating nodes for graphs (e.g., virtual node generation), or manipulating node features (e.g., node feature masking).

- **Edge-level Augmentation** augments graph entities by reconstructing the graph connectivity (e.g., edge rewiring) or manipulating edge features.

- **Graph-level Augmentation** augments graph entities by manipulating local/global graph structure (e.g., subgraph cropping and graph coarsening) or creating synthetic graph views (e.g., graph mixup).

The micro-level augmentation (node and edge) can generally serve for multiple graph tasks such as node classification, link prediction and graph classification, while graph-level augmentation is mainly designed for graph-level tasks like graph classification.

3.3 Model Dependency

According to the degree of dependence between the GDAug algorithm and the graph model, we can divide the GDAug into the following two categories:

- **Model-agnostic Augmentation** does not rely on the information of graph models and generally augments graph entities in a trival manner (e.g., arbitrary, heuristic and rule-based).

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• **Model-based Augmentation** is coupled with graph models and relies on the information provided by the models (e.g., model parameters and training signals) to augment graph entities. It can also be regarded as learnable augmentation and generally accepts the training signals like gradient information to optimize augmentors.

3.4 Augmentation Mechanism

The GDAug algorithm can be designed via different mechanisms. In most instances, designers will focus on manipulating the existing graph entities or generating new ones. Based on the augmentation mechanism, we have:

- **Manipulation-based Augmentation** manipulates (e.g., masking and rewiring) the feature or structure in the existing graph instances to augment graph entities, similar to imposing perturbations on existing graph elements.
- **Generation-based Augmentation** augments graph entities by creating brand-new graph features or structures based on existing graph information.
- **Sampling-based Augmentation** typically samples the graph elements from the existing graph instances as the augmented graphs, following a graph sampling pattern.

4 TECHNIQUES OF GRAPH DATA AUGMENTATION

For the given graph data and related tasks, we hope to assist researchers to quickly find or design appropriate graph augmentation strategies. Referring to the above taxonomies, we will review the representative algorithms for graph data augmentation according to graph elements (or graph scales), followed by several reasons: 1) The design freedom of augmentation strategies is limited by the diversity of graph elements, e.g., a graph without attributes generally cannot apply feature-level augmentations; 2) Augmentations based on different graph elements are usually suitable for different graph tasks, e.g., node-level augmentations are generally suitable for graph tasks at multiple scales (node, edge, graph), while subgraph-level augmentations are generally only suitable for graph-level tasks; 3) Taxonomy based on graph elements (or graph scales) is easier and clearer to organize than other taxonomies. To sum up, we will first divide these algorithms into feature-level, node-level, edge-level, subgraph-level, graph-level and label-level, and then further group them into different strategies for each category.

4.1 Feature-level Augmentation

Features are usually composed of multiple graph attributes, which are often derived from the real physical properties of the data and play an important role in graph representation learning. Graph features are available in attribute graphs and weighted graphs, and can be attached by different structure elements, such as nodes in point clouds carrying position features, edges in knowledge graphs carrying relationship information, and molecular graphs with global-level toxicological or catalytic properties. More broadly, graph embeddings or hidden features generated by graph representation learning are also graph features. Existing feature-level augmentations mainly concentrates on feature shuffling and feature masking.

4.1.1 Feature Shuffling. This strategy shuffles the graph features especially node features to generate augmented samples. Without loss of generality, we define feature shuffling as follows:

Definition 4.1. Feature Shuffling. For a given attributed graph \( G = (A, X_v) \), feature shuffling executes row-wise shuffle on the node features, yielding an augmented graph \( \hat{G} = (A, \hat{X}_v) \) with the same topology but rearranged nodes, i.e.,

\[
\hat{X}_v = X_v[\text{idx}, :] \quad \text{with} \quad \text{idx} = \text{Randperm}(|V|)
\]
where \texttt{Randperm}(n) function returns a random permutation of integers from 0 to \(|V| – 1\).

This augmentation is typically applied in contrastive learning to generate a diverse set of isomorphic negative samples, where the topological structure is preserved but the nodes are located in different locations and receive different contextual information, as schematically depicted in Fig. 1. DGI [61] considers feature shuffling as a corruption function to generate negative samples for the first time, and plenty of related work [23, 33, 38, 48, 64] followed suit. STDGI [41] extends the DGI method to spatio-temporal graphs and applies feature shuffling to randomly permute the node features at each time step.

### 4.1.2 Feature Masking

This augmentation is also named feature perturbation and is commonly used to generate augmented graphs with masked or perturbed features. Without loss of generality, we define the generalized feature masking as follows:

**Definition 4.2. Feature Masking.** For a given attributed graph \( G = (A, X) \), feature masking performs attribute-wise masking on graph features, by making the \( j \)-th attribute of feature vector \( x_i \) masked as \( m_{ij} \) with probability \( p_{ij}^m \), finally yielding an augmented graph \( \hat{G} = (A, \hat{X}) \) with the same topology but masked features, i.e.,

\[
\hat{X} = X \circ (1 - \mathbb{1}_m) + M \circ \mathbb{1}_m
\]

with \( \mathbb{1}_m[i,j] \sim \text{Bernoulli}(p_{ij}^m) \), \( M[i,j] = m_{ij} \)

where \( \circ \) is the Hadamard product, \( \mathbb{1}_m \) is the masking location indicator matrix, each element of \( \mathbb{1}_m \) is drawn from a Bernoulli distribution with parameter \( p_{ij}^m \), and \( M \) is the masking value matrix.

### Table 2. Summary of different feature masking augmentations.

| Reference | Strategy (custom) | Feature Masking Setting | Model Dependency |
|-----------|-------------------|-------------------------|------------------|
| [1, 21, 25, 58, 59, 86, 94, 100] | uniform zero masking | constant \( m_{ij} \) \( = 0 \) | model-agnostic (random) |
| [79, 80] | noise masking | \( \mathcal{N}(0, \Sigma) \) | model-agnostic (random) |
| [66] | noise masking | \( \mathcal{N}(X, \Sigma) \) | model-agnostic (random) |
| [101] | importance-based masking | node centrality | model-agnostic (heuristic) |
| [69] | importance-based masking | attribute weight | more relevant attributes | model-agnostic (heuristic) |
| [30] | gradient-based masking | constant \( m_{ij} \) \( = 1 \) | adversarial perturbation | model-based (learnable) |

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Note that the elements of masking matrix \( \mathbf{1}_m[i, j] \) are set to 1 individually with a probability \( p_{ij}^m \) and 0 with a probability \( 1 - p_{ij}^m \). Different types of masking probabilities \( p_{ij}^m \) and masking values \( m_{ij} \) specify different masking strategies, as schematically depicted in Fig. 2. For example, \( p_{ij}^m \) and \( m_{ij} \) can be set to fixed constants, yielding uniform zero masking, which means uniformly masking a fraction of the dimensions with zeros in the graph features and has been widely used in [1, 21, 25, 58, 59, 94, 100] to generate contrastive graph views. GraphCL [80] utilizes a noise masking with \( p_{ij}^m = 1 \) and \( M \sim \mathcal{N}(0, \Sigma) \) to replace the whole node feature matrix with Gaussian noise. MeTA [66] performs timestamp perturbation by adding Gaussian noise to time attribute in edges, yielding augmented timestamps. NodeAug [69] introduces an importance-based masking that replaces the uninformative attributes with more relevant ones, and computes the mask probabilities through attribute weights. Similarly, GCA [101] uses multiple node centralities to compute the mask probabilities. FLAG [30] introduces a learnable gradient-based masking and iteratively augments node features with adversarial perturbation during training. Finally, it’s worth noting that feature masking can be applied to different graph features like node features, edge features or other relevant features. For example, Ethident [94] uniformly masks the edge features in the Ethereum interaction graph, and SMICLR [46] focuses on molecular graph representation learning and designs the ‘XYZ mask’ augmentation to add tiny perturbations in the atoms’ coordinates (i.e., node position features).

### 4.2 Node-level Augmentation

Node-level augmentation mainly focuses on manipulating graph nodes to generate data diversity, and is generally applied to both node-level tasks (node interpolation, node masking) and graph-level tasks (node dropping).

#### 4.2.1 Node Dropping

This augmentation is also named node removing, node deletion or node masking and can be regarded as a cross-class method. Without loss of generality, we define node dropping as follows:
Definition 4.3. **Node Dropping.** For a given graph $G = (A, X_v)$, node dropping first selects a certain proportion of nodes $V_d$, and then uses a corruption function $C$ to deactivate them in the graph, finally yielding an augmented graph $\hat{G}$. According to the mechanism of the corruption function, node dropping can be further divided into two modes. One is to discard the selected nodes and their respective connections from the graph, i.e.,

$$\hat{A}, \hat{X}_v = C(A, X_v) = A[\hat{V}, \hat{V}], X_v[\hat{V}, :]$$

where $\hat{V} = V \setminus V_d$. And the other is to ignore the features of the selected nodes, i.e.,

$$\hat{X}_v = C(X_v) = X_v \odot (1 - 1_m) \quad \text{with} \quad 1_m[V_d, :] = 1, \quad 1_m[\hat{V}, :] = 0$$

where $1_m$ is a masking location indicator matrix.

In mode one, node dropping is essentially a node-level graph pruning that completely removes features and structures associated with selected nodes from the graph, eventually yielding a subgraph of the original graph as an augmented sample, as schematically depicted in Fig. 3. This augmentation mode is generally applied in the graph classification task [46, 79, 80, 84, 94], and can also be regarded as GDAug of subgraph sampling (as discussed in Sec. 4.4.1). As for mode two, node dropping is essentially the local node feature masking, which masks messages from selected nodes by setting their features to all-zero vectors. For example, this mode can enable a node to aggregate messages only from a subset of its neighbors, achieving an augmentation in the receptive field of the target node, and is thus widely applied in node-level tasks [8, 43, 53, 65].

4.2.2 **Node Interpolation.** This is a generative augmentation strategy that creates synthetic nodes by combining the existing nodes. Existing work based on node interpolation is mainly inspired by Mixup [62, 85] and SMOTE [4]. Mixup is a recently proposed image augmentation method based on the principle of Vicinal Risk Minimization (VRM), which can generate new synthetic images via linear interpolation. Incorporating the prior knowledge that linear interpolation of features should
lead to linear interpolation of the associated targets, Mixup can extend the training distribution as follows \[85\]:

\[
\hat{x} = (1 - \lambda) \cdot x_i + \lambda \cdot x_j \\
\hat{y} = (1 - \lambda) \cdot y_i + \lambda \cdot y_j
\]

(5)

where \((x_i, y_i)\) and \((x_j, y_j)\) are two labeled samples sampled from training set, and \(\lambda \in [0, 1]\). Similarly, Manifold Mixup \[62\] performs mixup on the intermediate embedding space. As for SMOTE \[4\], the most popular over-sampling method, it generates new samples by performing interpolation between samples in minority classes and their nearest neighbors. In some ways, SMOTE can be regarded as a special case of Mixup. After reviewing their applications in graph domain, we define the generalized node interpolation as follows:

**Definition 4.4. Node Interpolation.** For a given attributed graph \(G = (A, X_v, Y_v)\) and an anchor node \((v_a, y_a) \sim D_a\), node interpolation first samples a target node \((v_t, y_t)\) from data distribution \(D_t\), and then combines the two nodes in the feature space \(F\) via generalized linear interpolation, yielding new synthetic node \((\hat{v}, \hat{y})\), i.e.,

\[
\hat{h} = (1 - \Lambda) \circ h_a + \Lambda \circ h_t \\
\hat{y} = (1 - \lambda) \cdot y_a + \lambda \cdot y_t
\]

(6)

where \(\Lambda = \lambda \cdot (1 - \mathbb{1}_m)\), \(h_a, h_t \in F\), \((v_t, y_t) \sim D_t\)

We show the general process of node interpolation in Fig. 4. Note that this definition has a slightly different form than Mixup, but is easier to encapsulate existing related work, as summarized in Table 3.

### Table 3. Summary of different node interpolation augmentations.

| Reference | Node Interpolation Setting | Adjoint edge generation? |
|-----------|-----------------------------|---------------------------|
| [68]      | \(V\)                       | False                     |
| [63]      | \(V_a, V_U\)                | False                     |
| [75]      | \(V\)                       | True                      |
| [45]      | target minority class \(V_a, V_U\) \(\| m \in (0, 1)^F\) | True                      |
| [72, 90]  | target minority class \(v_t = \arg\min_{v_i \in (V \setminus V_a), y_i=y_a} \|h_i-h_a\|\) \(\| m \in (0, 1)^F\) | True                      |
Table 3. Node interpolation is mainly proposed to alleviate low generalization, especially for class imbalance problem. For example, to improve class-imbalanced node classification, existing work [45, 72, 90] utilizes node interpolation to generate synthetic samples for minority classes. In data selection, the anchor nodes are sampled from the target minority class, and the target nodes vary for different approaches. GraphMixup [72] and Graphsmote [90] consider the nearest neighbor of the anchor node with the same label as the target node, i.e.,

\[ v_t = \arg \min_{v_i \in \{V \setminus V_a\}, \ y_i = y_a} \| h_i - h_a \| \]  

(7)

In contrast, GraphENS [45] argues that selecting similar neighbors as target nodes in a highly imbalanced scenario will lead to information redundancy, so it selects target nodes from all classes, even unlabeled nodes. Regardless of the class imbalance issue, other work [63, 68, 75] usually does not restrict the selection of node pairs, that is, sampling node pairs randomly from the training set.

In addition, it is worth noting that node interpolation can only generate isolated synthetic nodes, so it generally relies on an edge generation module to connect the generated nodes to the graph. For example, Graphsmote [90] employs a weighted inner product predictor and jointly trains it via edge reconstruction task, finally yielding binary or soft edges for synthetic nodes. Similarly, GraphMixup [72] also adopts the same edge generator but optimizes it with three self-supervised tasks: edge reconstruction, local-path prediction and global-path prediction. Moreover, GraphENS [45] first generates the adjacent node distribution for the synthetic node by mixing those of the anchor node and the target node, and then connects the synthetic node to the graph by sampling neighbors from the distribution. Two-stage Mixup [68] does not construct an edge generator to connect synthetic nodes, but indirectly uses the adjacency information of anchor nodes and target nodes to aggregate messages for synthetic nodes. As an exception, GraphMix [63] trains a fully-connected network jointly with GNN via weight sharing, which can avoid message aggregation while performing interpolation-based regularization, thus eliminating edge generation.

Lastly, as a generalized definition, we perform feature interpolation using a composite parameter \( \Lambda \), in which \( 1_m \) usually serves for masking class-specific attributes of target nodes from introducing noise, as mentioned in [45]. When mask is not used (i.e., \( 1_m = 0 \)), \( \Lambda \) degenerates to \( \lambda \).

4.3 Edge-level Augmentation

Edge-level augmentation mainly focuses on manipulating the connection structure of graphs to generate data diversity, and is generally applied to node-level tasks and graph-level tasks. Existing edge-level augmentations include edge removing, edge additions and their hybrids, which we unify as edge rewiring.

Table 4. Summary of different edge rewiring augmentations.

| Reference | Strategy (custom) | Rewiring Setting | Model Dependency |
|-----------|-------------------|------------------|------------------|
| [46, 59, 79, 80, 84, 94] | uniform rewiring | constant | model-agnostic (random) |
| [1, 21, 58, 61, 100] | | | |
| [51, 69, 93, 95, 96, 101] | importance rewiring | weighted by feature and structure information | model-agnostic (heuristic) |
| [29, 33, 53, 89] | prediction rewiring | generated by edge predictor and binarized by threshold or topk | model-agnostic (heuristic) |
| [25, 57] | gradient-based rewiring | binarized by gradient information | model-based (learnable) |
| [43] | probabilistic rewiring | sampled from specific distribution | model-based (learnable) |
4.3.1 Edge Rewiring. It is a widely used augmentation that can modify the graph structure without affecting the graph size. Edge rewiring is also named edge perturbation and consists of two parts, edge removing and edge addition. Without loss of generality, we define it as follows:

**Definition 4.5. Edge Rewiring.** For a given graph $G = (A, X)$ without considering edge features, edge rewiring removes or adds a portion of edges in $G$, by applying masks parameterized by two probabilities $p_{ij}^{-}$ and $p_{ij}^{+}$ to the adjacency matrix $A$, finally yields an augmented graph $\hat{G} = (\hat{A}, X)$, i.e.,

$$\hat{A} = A \circ (1 - 1_r) + (1 - A) \circ 1_r$$

with $1_r[i, j] \sim \begin{cases} \text{Bernoulli} (p_{ij}^{-}) & \text{if } A_{ij} = 1 \\ \text{Bernoulli} (p_{ij}^{+}) & \text{if } A_{ij} = 0 \end{cases}$

where $1_r$ is the rewiring location indicator matrix, $p_{ij}^{-}$ represents the probability of removing edge $e_{ij}$ and $p_{ij}^{+}$ represents the probability of connecting nodes $v_i$ and $v_j$.

Note that elements in $1_r$ with edge locations ($A_{ij} = 1$) are set to 1 individually with probability $p_{ij}^{-}$ and 0 otherwise, while elements in $1_r$ with non-edge locations ($A_{ij} = 0$) are set to 1 individually with probability $p_{ij}^{+}$ and 0 otherwise. The first term implies edge removing where $\circ (1 - 1_r)$ drops edges $e_{ij}$ if $1_r[i, j] = 1$, and the second term performs edge addition where $1 - A$ represents the non-edge location indicator matrix and $\circ 1_r$ links node pair $(v_i, v_j)$ if $1_r[i, j] = 1$. In addition, when the removing probability $p_{ij}^{-}$ (or addition probability $p_{ij}^{+}$) equals to 0 for all $v_i, v_j \in V$, the edge rewiring degrades into edge addition (or edge removing).

Furthermore, different types of rewiring probabilities ($p_{ij}^{-}$ and $p_{ij}^{+}$) specify different rewiring strategies, as summarized in Table 4 and illustrated in Fig. 5. A large number of studies [1, 21, 46, 58, 59, 61, 79, 80, 84, 94, 100] related to graph contrastive learning typically use **uniform edge rewiring** to generate contrastive graph views, in which the rewiring probabilities are generally set as fixed constants. Rong et al. [49] proposed DropEdge and its layer-wise version to alleviate over-smoothing.
in node representation learning. The former generates perturbed adjacency matrix via random edge removing and shares it with all layers in the GNN models, while the latter independently generates perturbed adjacency matrix for each layers. Similar to feature masking, rewiring strategies can also be designed in an importance-based manner. The rewiring probabilities can be weighted according to different information such as node centrality [69, 101], node similarity [93, 95, 96], hop count [69], sensitive attribute [51], etc. For example, NodeAug [69] considers that nodes with larger degree values and closer distance to the target node contain more information, and further weights the rewiring probabilities by node degree and hop count. In addition, several studies first compute the edge probability matrix via different edge prediction strategies like node similarity [33], graph diffusion [29] and graph auto-encoder (GAE) [53, 89], and further achieve edge rewiring via threshold-$\epsilon$ [29] or top-$k$ [29, 33, 53, 89]. For example, GAUG [89] considers graph auto-encoder (GAE) as the edge predictor to generate the edge probability matrix, and then removes the top-$k$ existing edges with least edge probabilities and adds the top-$k$ non-edges with largest edge probabilities.

The above studies are generally regarded as model-agnostic methods, and this augmentation can also be coupled with specified task models, yielding the learnable edge rewiring. GROC [25] uses gradient information to guide edge rewiring, yielding an adversarial transformation that removes a portion of edges with minimal gradient values and adds a portion of edges with maximal gradient values during model training. ADGCL [57] designs a learnable edge dropping by building a random graph model, in which each edge will be associated with a random mask variable drawn from a parametric Bernoulli distribution. MH-Aug [43] utilizes Metropolis-Hastings algorithm to sample the parameters of edge perturbation from target distribution, and then generates accepted augmented graphs via a designed acceptance ratio.

Lastly, edge removing is more commonly used than edge addition in practice. The former can be regarded as a process of graph sparsification, which can 1) denoise or prune graphs by removing misleading or uninformative links; 2) enable multiple views for random subset aggregation. The latter can restore missing links to a certain extent, but may also introduce noisy connections. In addition, when the target graph contains edge weights or attributes, edge addition operation needs to account for the generation of additional edge information inevitably [66].

4.4 Subgraph-level Augmentation

Subgraph-level augmentation is generally a hybrid method because its manipulation object, the subgraph, consists of multiple graph elements. Existing methods mainly include subgraph sampling and subgraph substitution.

4.4.1 Subgraph Sampling. This one is a commonly used technique to extract substructure from a graph. Analogous to image cropping, subgraph sampling can be viewed as performing cropping on a graph, and thus can also serve for augmenting data. Here we unify existing methods, such as subgraph sampling and graph cropping, and present a generalized definition of data augmentation based on subgraph sampling:

**Definition 4.6. Subgraph Sampling.** For a given graph $G = (A, X_v, X_e)$, subgraph sampling strategically extract node subset $\hat{V} \subseteq V$ and edge subset $\hat{E} \subseteq E$ from $G$ to derive an augmented subgraph $g = (\hat{V}, \hat{E}, \hat{X}_v, \hat{X}_e)$, where

$$\hat{X}_v, \hat{X}_e = X_v[\hat{V}, :], X_e[\hat{E}, :]$$

In general, subgraph sampling first determines the subset of nodes to be sampled from the graph and then determines the edge subset. This process can be guided by different sampling strategies, as summarized in Table 5 and illustrated in Fig. 6.
Table 5. Summary of different subgraph sampling augmentations.

| Reference | Type (custom) | Subgraph Sampling Setting | how to get $\hat{\mathcal{V}}$ | how to get $\hat{\mathcal{E}}$ and $g$ |
|-----------|---------------|---------------------------|-----------------------------|-----------------------------------|
| [14, 21]  | uniform sampling | nodes randomly sampled from graph | $\mathcal{A}[\hat{\mathcal{V}}, \hat{\mathcal{V}}]$ |                                  |
| [52, 61, 98] | ego-net sampling | $\{v_i \mid sp(v_j, v_i) \leq k\}$ | $\mathcal{A}[\hat{\mathcal{V}}, \hat{\mathcal{V}}]$ |                                  |
| [56, 80]  | search sampling | nodes visited by BFS/DFS starting from a node | $\mathcal{A}[\hat{\mathcal{V}}, \hat{\mathcal{V}}]$ |                                  |
| [46, 47, 79, 80] | random-walk sampling | nodes visited by a random walk starting from a node | $\mathcal{A}[\hat{\mathcal{V}}, \hat{\mathcal{V}}]$ |                                  |
| [19, 20, 67, 94] | importance sampling | select top-$k$ most important neighbors for a node | $\mathcal{A}[\hat{\mathcal{V}}, \hat{\mathcal{V}}]$ |                                  |
| [35]      | learnable sampling | nodes selected by a learned node mask vector | $\mathcal{A}[\hat{\mathcal{V}}, \hat{\mathcal{V}}]$ |                                  |
| [91]      | learnable sampling | sample no more than $k$ edges for each node | $\mathcal{A}[\hat{\mathcal{V}}, \hat{\mathcal{V}}]$ |                                  |

Uniform sampling [14, 21] uniformly selects a portion of nodes $\hat{\mathcal{V}}$ from $\mathcal{V}$ and then induces the subgraph topology by $\hat{\mathcal{A}} = \mathcal{A}[\hat{\mathcal{V}}, \hat{\mathcal{V}}]$, which is similar to node dropping defined in Eq. (3).

Ego-net sampling is based on the strong correlation between central nodes and their local neighborhood, and is generally used to provide patch (local) views during contrastive learning, such as in DGI [61] and InfoGraph [52]. Given a node-level encoder with $l$ layers, the computation of patch representation for node $v_i$ only depends on its $l$-hop neighborhood, aka $l$-hop ego-net. A $l$-hop ego-net sampling for a central node $v_i$ is essentially to obtain its receptive field subgraph with node set $\hat{\mathcal{V}} = \{v_j \mid d(v_j, v_i) \leq l\}$, where $d(v_j, v_i)$ represents the shortest path distance between $v_j$ and $v_i$ in the graph $G$. Ego-net sampling can be regarded as a special version of Breadth-first search (BFS) sampling, which can also be used for subgraph augmentation. For example, SUGAR [56] first selects the top-$k$ most important nodes according to degree ranking, and then extracts subgraph for each selected node by BFS sampling. GraphCL [80] compares the performance of contrastive learning with three kinds of subgraphs, which are extracted via BFS sampling, Depth-first search (DFS) sampling and random-walk sampling, respectively. And it finds that the subgraphs extracted by DFS sampling preserve less structure information but help contrastive learning achieve better performance.

Random-walk sampling [46, 47, 79, 80] is a popular strategy for extracting informative subgraphs. A random-walk sampling starting from a given node iteratively collects node subset $\hat{\mathcal{V}}$. At
each iteration, the walk travels to its neighborhood with the probability proportional to the edge weight. For the random walk with restart (RWR) applied in GCC [47], the walk has a probability of returning to the starting node.

**Importance sampling** [19, 67, 91, 94] is proposed to extract contextual subgraphs with more structure information and less noise for given nodes. For a given node, importance sampling first measures the importance scores of its neighbor nodes by several importance metrics or graph information, and then chooses the top- \( k \) important neighbors to construct a subgraph. For example, SUBG-CON [19] and GraphCrop [67] utilize the Personalized PageRank centrality [42] to measure the node importance, while Ethident [94] evaluates the importance of neighbors according to different edge attributes.

In addition to the above model-agnostic augmentations, several studies have proposed **learnable sampling** strategies to automatically extract task-relevant subgraphs. NeuralSparse [91] trains a sparsification network to sample no more than \( k \) edges for each node from a learned distribution, yielding a sparsified \( k \)-neighbors subgraph that preserves task-relevant edges. GREA [35] trains a separator that maps the node representations to a mask vector, and then uses the learned node mask to extract the rationale subgraph.

### 4.4.2 Subgraph Substitution

Analogous to CutMix [83] that replaces the removed region with a patch from another image, subgraph substitution replaces a subgraph of the given graph with another. Here we present a generalized definition of subgraph substitution as follows:

**Definition 4.7. Subgraph Substitution.** For a pair of graphs \( G = (\mathcal{V}, \mathcal{E}, Y) \) and \( G' = (\mathcal{V'}, \mathcal{E'}, Y') \), subgraph substitution first drops a subgraph \( g = (\mathcal{V}_g, \mathcal{E}_g) \) from \( G \), and then merges the remaining part with another subgraph \( g' = (\mathcal{V}_{g'}, \mathcal{E}_{g'}) \) sampled from \( G' \), finally yielding an augmented graph \( \hat{G} = (\mathcal{V}, \hat{\mathcal{E}}, \hat{Y}) \), i.e.,

\[
\mathcal{V} = (\mathcal{V} \setminus \mathcal{V}_g) \cup \mathcal{V}_{g'}, \quad \hat{\mathcal{E}} = (\mathcal{E} \setminus \mathcal{E}_g) \cup \mathcal{E}_{g'} \cup \mathcal{E}_{connect}, \quad \hat{Y} = (1 - \lambda) \cdot Y + \lambda \cdot Y'
\]

where \( \mathcal{E}_{break} \) is the set of edges that break when dropping \( g \) from \( G \), \( \mathcal{E}_{connect} \) is the set of edges that performs merging operation to guarantee connectivity, and \( \lambda \) is the adaptive label interpolation ratio.

Note that subgraph substitution is a hybrid augmentation that incorporates multiple operations like subgraph sampling, subgraph merging, and label interpolation to generate new graphs, as summarized in Table 6 and illustrated in Fig. 7. During subgraph sampling for the graph pair \((G, G')\), the two extracted substructures \((g, g')\) for substitution are generally of similar importance to their respective graphs, i.e., \( g \) and \( g' \) play similar roles in \( G \) and \( G' \), respectively. For example, MoCL [55] replaces a valid substructure in a molecule with a bioisostere [40] that shares similar chemical properties. SubMix [78] uses the importance sampling (as described in Sec. 4.4.1) to extract connected and clustered subgraphs from the given graph pair. GREA [35] replaces the environment subgraph that can be regarded as natural noises in \( G \) with another environment subgraph sampled from \( G' \).

Furthermore, it is also essential to guarantee the connectivity of augmented graphs. SubMix [78] inserts a subgraph \( g' \) of the same size as \( g \) into \( G \) without breaking the edges that connect \( \mathcal{V}_g \) with \( \mathcal{V} \setminus \mathcal{V}_g \), having \( \mathcal{E}_{connect} = \mathcal{E}_{break} \). Similarly, MoCL [55] retains the chemical bonds (edges in molecular graphs) connected to \( g \) before augmentation, and uses them to connect \( g' \) during subgraph substitution. Graph Transplant [44] proposes two strategies for merging subgraphs. One is uniform edge sampling to connect nodes whose degree values change during augmentation, and the other is differentiable edge prediction that considers the feature similarity of node pairs for connectivity. As an exception, GREA [35] performs subgraph substitution by swapping the
Table 6. Summary of different subgraph substitution strategies.

| Reference            | Subgraph Substitution Setting | Subgraph Sampling | Subgraph Merging       | Label Generation |
|----------------------|------------------------------|-------------------|------------------------|------------------|
| MoCL [55]            | valid molecular substructure  | bioisostere       | \( E_{\text{connect}} = E_{\text{break}} \) | \( \lambda = 0 \) |
| SubMix [78]          | connected and clustered subgraph | connected and clustered subgraph | \( E_{\text{connect}} = E_{\text{break}} \) | \( \lambda = \frac{|E_{\text{g}}|}{|E|} \) |
| GREA [35]            | environment subgraph         | environment subgraph | \( E_{\text{connect}} = 0 \) | \( \lambda = 0 \) |
| Graph Transplant [44]| partial \( l \)-hop ego-net | partial \( l \)-hop ego net | edge sampling or prediction | subgraph saliency |

Fig. 7. Illustration of subgraph substitution augmentation.

node representations of subgraphs in the embedding space, which is free from edge generation (\( E_{\text{connect}} = \emptyset \)).

Lastly, subgraph substitution generally serves for graph-level tasks, especially for graph classification, so it is necessary to assign appropriate labels for augmented graphs. Since \( g \) and \( g' \) play similar roles in their respective graphs, the adaptive label interpolation ratio \( \lambda \) can be derived according to the contribution of \( g' \) to the augmented graph \( \hat{G} \). For example, SubMix [78] assumes that edges are crucial factors in determining graph labels, and hence defines \( \lambda \) as the ratio of contained edges in \( g' \), i.e., \( \lambda = \frac{|E_{\text{g}}'|}{|E'|} \). Graph Transplant [44] quantifies the contribution of \( g' \) using the total saliency of contained nodes. In addition, both MoCL [55] and GREA [35] replace non-critical structures in the original graphs, so the augmented graph \( \hat{G} \) and the original graph \( G \) are considered to have consistent labels, i.e., \( g' \) is now a non-critical subgraph and assigned a low label weight (\( \lambda = 0 \)).

4.5 Graph-level Augmentation

Graph-level augmentation mainly manipulates the graph from a global level to generate data diversity, and existing methods concentrate on graph propagation and graph interpolation.

4.5.1 Graph Propagation. This augmentation can learn global topological information from graphs through a generalized graph propagation process and generate high-order augmented views. Without loss of generality, we define it as follows:

\[ \hat{Y} = (1 - \lambda) \cdot Y + \lambda \cdot Y' \]
Table 7. Summary of different graph propagation augmentation.

| Algorithm                  | Propagation Setting | Propagation equation |
|---------------------------|---------------------|----------------------|
| PageRank [42]             | $\alpha (1-\alpha)^k$ | $AD^{-1} \cdot \frac{\alpha}{\sum_{k=0}^{\infty}} \cdot \left(I - (1-\alpha)AD^{-1}\right)^{-1} \cdot \frac{1}{|V|}$ |
| Personalized PageRank [42]| $\alpha (1-\alpha)^k$ | $AD^{-1}$ personalized $P_t$ | $\sum_{k=0}^{\infty} \alpha (1-\alpha)^k \cdot \left(I - (1-\alpha)AD^{-1}\right)^{-1} \cdot P_t$ |
| Heat Kernel [5]           | $e^t \cdot \frac{\alpha}{\sum_{k=0}^{\infty}}$ | $AD^{-1}$ identity matrix $I$ | $\sum_{k=0}^{\infty} e^t \cdot \frac{1}{\sum_{k=0}^{\infty}} \cdot \left(I - (1-\alpha)AD^{-1}\right)^{-1} \cdot \frac{1}{|V|}$ |
| Katz-index [26]           | $\beta^k$           | $A$ identity matrix $I$ | $\sum_{k=0}^{\infty} \beta^k A^k = (I - \beta A)^{-1} \cdot \beta A$ |

**Definition 4.8. Graph Propagation.** For a given graph $G = (A, X)$, graph propagation measures the proximity between any two nodes from the perspective of global probabilistic transition, and injects high-order topological information into the graph adjacency, yielding an augmented global view $\hat{G} = (\hat{\Pi}, \hat{X})$, i.e.,

$$\hat{\Pi} = \sum_{k=0}^{\infty} \theta_k \cdot T^k \cdot P^T$$

(11)

where $\hat{\Pi}$ is the generated propagation matrix, $\text{Sparsification}(\cdot)$ is a sparsification function, $\theta_k$ is the weighting coefficient that controls the ratio of global-local information, $T \in \mathbb{R}^{|V| \times |V|}$ is the generalized transition matrix, $P \in \mathbb{R}^{|V| \times |V|}$ is formed by stacking the teleport location probability distribution vectors of all nodes and satisfies $\|P\|_2 = 1$ for all $i \in V$.

Here we summarize several graph propagation instantiations specified by different parameter settings, as listed in Table 7 and illustrated in Fig. 8. An earlier study has shown that employing higher-order message propagation mechanisms can significantly improve the performance of graph learning [29], which inspired the use of generalized graph diffusion methods such as **Personalized PageRank (PPR)** [42] and **Heat Kernel (HK)** [5] to generate higher-order augmented views [14, 21, 27, 82]. The graph diffusion powered by Personalized PageRank (PPR) is defined by setting $T = AD^{-1}$ and $\theta_k = \alpha (1-\alpha)^k$, and Heat Kernel (HK) corresponds to choosing $T = AD^{-1}$ and $\theta_k = e^{-t} \cdot \frac{t^k}{k!}$, formulated as follows:

$$\Pi^{PPR} = \sum_{k=0}^{\infty} \alpha (1-\alpha)^k \cdot \left(I - (1-\alpha)AD^{-1}\right)^{-1} \cdot P^T$$

$$\Pi^{HK} = \sum_{k=0}^{\infty} e^{-t} \cdot \frac{t^k}{k!} \cdot \left(I - (1-\alpha)AD^{-1}\right)^{-1} \cdot \frac{1}{|V|}$$

(12)

where $\alpha \in (0, 1)$ is the tunable teleport probability in random walk, and $t$ denotes the diffusion time. Notably, compared to teleport operation with equal probability in PageRank ($P = \frac{1}{|V|} \cdot 1$), PPR is special in that each node has a user-defined (personalized) teleport location probability distribution $P_t$. In addition, SelfGNN [27] also uses the **Katz-index** [26] to capture high-order topological information and generates augmented views. The Katz-index characterizes the relative importance of nodes from a global perspective by weighting and integrating the reachable paths of different lengths between nodes. We unify it into the generalized graph propagation formula by setting $T = A$ and $\theta_k = \beta^k$, formulated as follows:

$$\Pi^{Katz} = \sum_{k=1}^{\infty} \beta^k A^k = (I - \beta A)^{-1} \cdot \beta A$$

(13)

where $\beta$ is the attenuation factor that controls the path weights.
Finally, it is worth noting that the graph propagation augmentation will yield a dense propagation matrix $\tilde{\Pi}$ [29], in which the elements represent the influence between all pairs of nodes. To recover the sparsity of propagation matrix, there are two tricks in practice: 1) threshold-$\epsilon$, which sets elements below $\epsilon$ to zero; 2) top-$k$, which keeps the $k$ elements with the largest values per column. Both of two sparsification tricks help to truncate small values in $\Pi$, yielding a sparse propagation matrix $\hat{\Pi}$ that can provide a global view during contrastive learning.

4.5.2 Graph Interpolation. This one aims to create synthetic graphs by combining the existing graphs via linear interpolation. Compared with node interpolation, graph interpolation can be more intuitively analogous to Mixup [85] in CV. Existing work [62, 85, 87] has demonstrated that Mixup can work well on regular, well-aligned and Euclidean data such as images. However, the success of Mixup on image augmentation is difficult to reproduce in the graph domain due to the irregular structure of graph data. Currently, graph-level interpolation is relatively less explored. Here we just present a rough definition of graph interpolation:

**Definition 4.9.** Graph Interpolation. For a pair of graphs $G_i = (A_i, X_i, Y_i)$ and $G_j = (A_j, X_j, Y_j)$, graph interpolation first aligns them in feature space $\mathcal{F}$ and then performs linear interpolation to yield an augmented graph $\hat{G}$ with label $\hat{Y}$, i.e.,

$$\begin{align*}
(G_i, G_j) &= \mathcal{T}(G_i, G_j) \\
\hat{G} &= (1 - \lambda) \cdot G_i + \lambda \cdot G_j \\
\hat{Y} &= (1 - \lambda) \cdot Y_i + \lambda \cdot Y_j
\end{align*}$$

where $\mathcal{T}$ is a generalized transformation to align the two graphs.

We review several existing related work and illustrates the generalized graph interpolation augmentation in Fig. 9. For example, ifMixup [11] aligns the sizes of two graphs by introducing isolated virtual nodes whose features are set to all-zero vector, and then interpolates nodes, edges...
4.6 Label-level Augmentation

Most of the above-mentioned GDAug strategies mainly manipulate the features and structure of existing graphs to achieve augmentation, without specific constraints on labels. While label-level augmentation is another important technique used to augment the limited labeled data using the unlabeled data. We divide the existing label-level augmentations into pseudo-labeling and sharpening-labeling.

4.6.1 Pseudo-Labeling. This strategy is generally regarded as a semi-supervised method to augment the limited labeled data by generating pseudo-labels for unlabeled data. It is commonly used in conjunction with self-training [73, 77] and co-training [2]. Here we present the following generalized definition of pseudo-labeling:

**Definition 4.10. Pseudo-Labeling.** For a given partially labeled dataset \( \mathcal{D} = \mathcal{D}_l \cup \mathcal{D}_u \) that can be split into a labeled set \( \mathcal{D}_l = \{ (x_i, y_i^l) \}_{i=1}^{\lvert \mathcal{D}_l \rvert} \) and an unlabeled set \( \mathcal{D}_u = \{ x_i^u \}_{i=1}^{\lvert \mathcal{D}_u \rvert} \), pseudo-labeling first trains a predictor using the partially labeled set, then generates pseudo labels for the unlabeled set, and finally filters out the pseudo labels with high confidence as the augmented labeled set, i.e.,

\[
\begin{align*}
    f &: \mathcal{D} \rightarrow \mathbb{R}^c, \quad \mathcal{Y}_u = f(\mathcal{D}_u) \\
    \mathcal{D}_p &= \text{LabelFilter}(\mathcal{D}_u, \mathcal{Y}_u) = \{ (x_i^p, y_i^u) \mid x_i^u \in \mathcal{D}_u, y_i^u \in \mathcal{Y}_u \}_{i=1}^{K} \\
    \hat{\mathcal{D}}_l &= \mathcal{D}_l \cup \mathcal{D}_p
\end{align*}
\]

where \( f \) is the pre-trained label predictor, \( \mathcal{Y}_u \) is the predictive labels of unlabeled set, LabelFilter is a process of filtering the pseudo labels with high confidence, \( \mathcal{D}_p \) is the retained pseudo-labeled set of size \( K \) and \( 1 \leq K \leq \lvert \mathcal{D}_u \rvert \).

After pseudo-labeling, the augmented data \( \hat{\mathcal{D}}_l \) can be used to retrain the predictor or train a new model. And the process of pseudo-labeling and model training can go through multiple rounds. We summarize several graph related works using pseudo-labeling techniques and divide them into two categories, as listed in Table 8 and illustrated in Fig. 10. The threshold-based methods mainly construct pseudo-labels via model predictions and determine whether a pseudo-labeled sample has high confidence by comparing the model prediction probability with a threshold. M-Evolve [96] first generates the virtual graphs via edge rewiring and assigns them the labels of the original graphs as
### Table 8. Summary of different label-level augmentations.

| Reference     | Type (custom) | Label-level Augmentation Setting                                                                 |
|---------------|---------------|-------------------------------------------------------------------------------------------------|
| M-Evolve [96] | threshold-based | same as the original graph                                                                     |
| AutoGRL [53]  | threshold-based | label propagation algorithm (LPA) [92]                                                          |
| NRGNN [6]     | threshold-based | semi-supervised prediction                                                                     |
| CGCN [18]     | clustering-based | pass the label of the labeled node to it in the same cluster                                    |
| M3S [54]      | clustering-based | assign the label of the nearest cluster of labeled nodes to the cluster it locates              |
| GraphMix [63] | sharpening     | apply sharpening to the average predictions across multiple perturbations of it /                |
| GRAND [8]     | sharpening     | apply sharpening to the average predictions across multiple augmentations of it /               |
| NASA [3]      | sharpening     | apply sharpening to the average of its neighbors’ predictions /                                |

**Fig. 10.** Illustration of pseudo-labeling augmentation. The general workflow proceeds as follows: 1) pre-train predictor using the partially labeled dataset; 2) predict the pseudo labels for unlabeled data using predictor; 3) filter the pseudo labels with high confidence; 4) retrain the predictor using the augmented set.

pseudo-labels. Then a concept of label reliability is introduced based on the intuition that pseudo-labels generally have higher reliability when matched to predictions. M-Evolve finally uses the label reliability threshold to filter out the virtual graphs with high label reliability as the augmented data. NRGNN [6] first inserts the missing edges between labeled and unlabeled nodes through edge prediction, then trains a GNN model on the rewired graph and uses the predictions of unlabeled nodes as their pseudo-labels, and finally retains the unlabeled nodes with their pseudo-labels whose predicted probability is greater than a threshold as augmented data. The **clustering-based** methods mainly use cluster assignments as pseudo-labels by introducing unsupervised clustering tasks, and then filter pseudo-labeled samples with high confidence by matching the consistency of supervised predictions and cluster assignments. M3S [54] first runs K-means clustering on the node embeddings, then aligns labeled and unlabeled clusters by comparing the distance of centroids between clusters, and finally passes the label of the labeled cluster to the nearest unlabeled cluster. CGCN [18] first learns clusters by GMM-VGAE model, then select the highest confidence (softmax prediction score) labeled sample of each class, and finally passes their labels to the unlabeled nodes in the clustering network.
4.6.2 Sharpening-Labeling. Pseudo-labeling techniques are obsessed with generating high-confidence pseudo-labels for unlabeled data, which usually fail when unlabeled data has low-confidence predictions. While sharpening-labeling does not rely on high-confidence predictions and is suitable for more unlabeled scenarios. Here we present the definition of sharpening-labeling as follows:

**Definition 4.11. Sharpening-Labeling.** Given predicted probability distributions \(\{p_i\}_{i=1}^{N}\) across \(N\) augmentations of \(x^u\), sharpening-labeling first computes the average prediction distribution, followed by a sharpening function to generate the sharpened label of \(x^u\), yielding augmented data \((x^u, y^u)\), i.e.,

\[
\hat{p} = \frac{1}{N} \sum_{i=1}^{N} p_i = [\hat{p}_1, \hat{p}_2, \cdots, \hat{p}_C]
\]

\[
y_k^u = \frac{\hat{p}_k^T}{\sum_{j=1}^{C} \hat{p}_j^T}, \quad 1 \leq k, j \leq C
\]

\[
y^u = [y_1^u, y_2^u, \cdots, y_C^u]
\]

where \(\hat{p}\) is the average prediction distribution, \(C\) is the number of classes, and \(T\) is the temperature hyperparameter.

The process of sharpening-labeling is illustrated in Fig. 11. Note that in practice, we usually choose temperature sharpening [31] as the sharpening function to reduce the entropy of the prediction distribution. It is commonly used in conjunction with consistency regularization [3, 8, 63]. Related work of sharpening-labeling is summarized in Table 8. GraphMix [63] applies the average prediction on multiple random perturbations of an input unlabeled sample along with sharpening trick, further augments training data and improve prediction accuracy. GRAND [8] utilizes sharpening-labeling to construct labels for unlabeled nodes based on the average prediction over multiple data augmentation, and further assists the implementation of consistency regularization. NASA [3] proposes a neighbor-constrained regularization to enforce the predictions of neighbors to be
consistent with each other, in which the sharpening trick is used to generate label for the center node based on the average predictions of its neighbors.

5 EVALUATION METRICS AND DESIGN GUIDELINES

In this section, we summarize existing metrics and guidelines for evaluating or designing graph data augmentation. We first introduce several evaluation metrics that are commonly used in graph analysis tasks, and then introduce some new metrics and guidelines specifically designed for graph data augmentation.

5.1 Common Metrics

Since graph data augmentation is an auxiliary technique, existing studies usually indirectly reflect the effectiveness of GDAug by evaluating the performance of downstream tasks. For classification tasks like node classification [66, 69] and graph classification [94, 95], it is common to use accuracy-based metrics such as Accuracy, Precision, F1 score, Area Under Curve (AUC) and Average Precision (AP) for reflecting the classification performance from different perspectives. For graph representation learning [14, 19, 52, 101], the learned embeddings will be fed into the downstream classifiers or clustering algorithms, and evaluated via accuracy-based metrics as mentioned above, or clustering-based metrics such as Normalized Mutual Information (MNI) and Adjusted Rand Index (ARI). Additionally, several works apply GDAug in pre-training task [47] or recommender system [70], followed evaluation with ranking-based metrics like HITS@k.

5.2 Specific Metrics and Design Guidelines

Besides the common metrics above, several special metrics and guidelines have been proposed to evaluate the performance of GDAug or guide the design of GDAug. Here we present the detailed definitions and descriptions of them.

5.2.1 Change Ratio. This metric is mainly used to measure the degree of modification of graph structure and features during manipulation-based augmentation (as mentioned in Sec. 3.4). Formally, we have the following generalized definition of change ratio:

**Definition 5.1. Change Ratio.** Given a graph $G = (V, E, X)$ and its augmentation $\hat{G} = (\hat{V}, \hat{E}, \hat{X})$, the change ratio of $G$ to $\hat{G}$ is measured by the number of modified nodes (or edges, features) divided by the number of original nodes (or edges, features), i.e.,

\[
M_{\Delta V} = \frac{|V - \hat{V}| + |\hat{V} - V|}{|V|} \\
M_{\Delta E} = \frac{|E - \hat{E}| + |\hat{E} - E|}{|E|} \\
M_{\Delta X} = \frac{\|\hat{x} - x\|_0}{F}
\]

where $F$ is the dimension of feature vector, and $\| \cdot \|_0$ is the zero norm.

It describes the modification ratio of nodes, edges, or features before and after augmentations like node dropping [43], edge rewiring [43, 96] and feature masking [100], and can also be regarded as a probability hyperparameter to guide augmentations. For example, in global uniform feature masking, the probability $p^m_{ij}$ of masking an attribute is equivalent to $M_{\Delta X}$. Furthermore, this metric can also be used as a constraint when designing augmentation strategies. For example, M-Evolve [96] follows the structure-preserving principle, which requires that the augmentation strategy does not change the number of edges in the target graph, i.e., setting $M_{\Delta E} = 0$. SubMix [78] proposes five desired properties for effective graph augmentations, including size preservation, which states that augmentation should satisfy an unbiased change of graph size, i.e., equivalent to $M_{\Delta V} = 0$ and $M_{\Delta E} = 0$. 

J. ACM, Vol. 37, No. 4, Article 111. Publication date: August 2018.
5.2.2 Tradeoff in GDAug via Consistency and Diversity. NASA [3] proposes two metrics, i.e., consistency and diversity, to measure the correctness and generalization of GDAug, respectively. We present the definition of them as follows:

**Definition 5.2. Consistency vs. Diversity.** For two models \( f_\theta \) and \( \hat{f}_\theta \), which are trained from the training set \( D_{\text{train}} \) and its augmentation \( \hat{D}_{\text{train}} \) respectively, the consistency can be represented by the accuracy of augmented model \( \hat{f}_\theta \) on validation set \( D_{\text{val}} \), i.e.,

\[
M_c = \text{Acc}(\hat{f}_\theta(D_{\text{val}}), Y_{\text{val}})
\]

where \( Y_{\text{val}} \) is the labels of validation set. And the diversity can be represented by the prediction difference between augmented model \( \hat{f}_\theta \) and original model \( f_\theta \) on validation set, i.e.,

\[
M_d = \| \hat{f}_\theta(D_{\text{val}}) - f_\theta(D_{\text{val}}) \|_2^2
\]

where \( \| \cdot \|_2 \) is the Frobenius norm.

Specifically, a lower consistency indicates that the augmentation hurts the original data distribution, but a higher consistency may not contribute well to the generalization of the model while maintaining correctness. On the other hand, a lower diversity indicates that the augmentation contributes little to the generalization of the model, while a higher diversity cannot ensure the correctness of the augmentation. Neither metric alone can fully evaluate the quality of augmentation. Therefore, NASA combines these two metrics to trade off the design of GDAug, expecting to achieve augmentation with better correctness and generalization, improve the performance of augmented models, and build generalized decision boundaries.

5.2.3 Tradeoff in GDAug via Affinity and Diversity. Trivedi et al. [60] states that augmentation should generate samples that are close enough to the original data to share task-relevant semantics, while being sufficiently different to prevent trivially similar samples. They utilize two metrics to quantify the above tradeoff, affinity and diversity, as proposed in [9]. We present the definition of them as follows:

**Definition 5.3. Affinity vs. Diversity.** For a model \( f_\theta \) trained from the training set \( D_{\text{train}} \), the affinity can be measured by the accuracy on augmented validation set \( \hat{D}_{\text{val}} \) divided by the accuracy on the original validation set \( D_{\text{val}} \), i.e.,

\[
M_A = \frac{\text{Acc}(f_\theta(\hat{D}_{\text{val}}), Y_{\text{val}})}{\text{Acc}(f_\theta(D_{\text{val}}), Y_{\text{val}})}
\]

where \( Y_{\text{val}} \) is the labels of validation set. And the diversity can be measured by the ratio of the final training loss on the augmented training set \( \hat{D}_{\text{train}} \), relative to the final training loss on the original training set \( D_{\text{train}} \), i.e.,

\[
M_D = \mathbb{E}[\hat{L}_{\text{train}}] / \mathbb{E}[L_{\text{train}}]
\]

Specifically, the affinity metric is used to quantify the distribution shift of the augmented data compared to the original data, with a lower affinity indicating that the augmented data is out-of-distribution for the model. On the other hand, the diversity metric quantifies how difficult it is for a model to learn from augmented data rather than original data.

5.2.4 Preserving Connectivity. Several works [78, 96] state that the connectivity information of a graph before and after augmentation should not be changed, as defined below.

**Definition 5.4. Preserving Connectivity.** For a graph \( G \) and its augmentation \( \hat{G} \), \( \hat{G} \) should follow the connectivity information of \( G \), i.e., \( \hat{G} \) should be connected if and only if \( G \) is connected.
Table 9. Summary of representative graph data augmentation works for graph learning. GDAug categories: FS: Feature Shuffling; FM: Feature Masking; ND: Node Dropping; NI: Node Interpolation; ER: Edge Rewiring; SSa: Subgraph Sampling; SSu: Subgraph Substitution; GP: Graph Propagation; GI: Graph Interpolation; PL: Pseudo-Labeling; SL: Sharpening-Labeling.

| Ref | Model | Publication | Year | GDAug | Code |
|-----|-------|-------------|------|-------|------|
| [61] | DGI | ICLR | 2019 | FS, ER | https://github.com/PotarV-DGI |
| [41] | STSGI | ICLR-workshop | 2019 | FS | — |
| [39] | STARE | KDD | 2022 | FS, ER | — |
| [2] | HDMM | WWW | 2021 | FS, ER | https://github.com/bayinge/hdmm |
| [80] | HDGI | AAAI-workshop | 2020 | FS | https://github.com/linxiangren/Heterogeneous-Deep-Graph-Informax |
| [6] | HGC | Arxiv | 2021 | FS | — |
| [38] | ContrastReg | Arxiv | 2021 | FS | — |
| [10] | FLAG | CVPR | 2022 | FM | https://github.com/devnong/FLAG |
| [9] | Ethdust | ICLR-TIFS | 2022 | FM, ER, SSa | https://github.com/JulianGottschall/Ethdust |
| [62] | SDCL | JCSS | 2022 | FM, ER, SSa | https://github.com/CIDAG/SDCL |
| [50] | GraphCL | NeurIPS | 2020 | FM, ER, SSa | — |
| [39] | MOA | ICML | 2021 | FM, ER, SSa | — |
| [23] | HDMI | WWW | 2021 | FS | https://github.com/baoyujing/HDMI |
| [48] | HDGI | AAAI-workshop | 2020 | FS | https://github.com/YuxiangRen/Heterogeneous-Deep-Graph-Infomax |
| [64] | HTC | Arxiv | 2021 | FS | — |
| [38] | ContrastReg | Arxiv | 2021 | FS | — |
| [48] | GTC | Arxiv | 2021 | FS | — |
| [69] | NodeAug | KDD | 2020 | FM, ER | — |
| [66] | MeTA | NeurIPS | 2021 | FM, ER | — |
| [21] | MERIT | IJCAI | 2021 | FS, ER, GP | https://github.com/GRAND-Lab/MERIT |
| [5] | HeCo | KDD | 2021 | ND | https://github.com/aamann/HeCo |
| [3] | GRAND | NeurIPS | 2021 | NI, ER | https://github.com/THUDAM/GRAND |
| [54] | MH-Aug | NeurIPS | 2021 | NI, ER | https://github.com/iyinjie/mh-aug |
| [45] | C openid | AAAI | 2021 | FM, ER, SSa | https://github.com/CIDAG/SMICLR |
| [89] | two-branch Mixup | WWW | 2021 | NI, GI | https://github.com/vaswani232/MirgForGraph |
| [47] | GraphMix | WWW | 2021 | NI | https://github.com/vikasverma1077/GraphMix |
| [8] | GraphMOT | WWW | 2021 | NI | https://github.com/TanxuanZhou/GraphMOT |
| [75] | GraphIES | AAAI | 2022 | NI | https://github.com/jasonlyang-Park/GraphIES |
| [50] | NodeAug-INS | CDS | 2021 | NI | — |
| [72] | GraphMixup | EUSILF | 2021 | NI | https://github.com/Lazeng99a/GraphMixup |
| [4] | AugGAN | Arxiv | 2022 | NI | — |
| [19] | DropEdge | ICLR | 2020 | FS, ER | https://github.com/DeepEdge/DeepEdge |
| [6] | GAUG | AAAI | 2021 | ER | https://github.com/zhao-tong/GAUG |
| [10] | RobustEC | IEEE-TDK | 2021 | ER | https://github.com/zhao-tong/RobustEC |
| [36] | FastDrop | IEEE TAI | 2021 | ER | https://github.com/xuqin/FastDrop |
| [9] | AD-GCL | NeurIPS | 2021 | ER | https://github.com/mosheal/adgcl |
| [11] | PTDNet | WSMM | 2021 | ER | https://github.com/zyhongpeng/PTDNet |
| [9] | MetaEdge | IEEE-TNM | 2020 | ER, PL | — |
| [5] | SUGAR | WWW | 2021 | SSa | https://github.com/RingBDStack/SUGAR |
| [47] | GCC | KDD | 2020 | SSa | https://github.com/THUDAM/GCC |
| [79] | SUB-G-Graph | KDD | 2020 | SSa | https://github.com/yijiaojia/Sub-G-Graph |
| [7] | GraphCrop | Arxiv | 2020 | SSa | — |
| [32] | InfoGraph | ICLR | 2020 | SSa | https://github.com/1f7opp/InfoGraph |
| [46] | ELE | NeurIPS | 2020 | SSa | https://github.com/Geordzi23/EGI |
| [8] | NeuralParse | ICM | 2020 | SSa | https://github.com/hungdinh07/NeuralParse |
| [14] | MCGRL | ICM | 2020 | SSa, GP | https://github.com/koushiboan/mcg |
| [9] | SubMix | WWW | 2022 | SSa | https://github.com/moonaata/GraphAug |
| [46] | GraphTransplant | AAAI | 2022 | SSa | — |
| [5] | McGRL | KDD | 2021 | SSa | https://github.com/islamislab/McGRL |
| [3] | GREA | KDD | 2022 | SSa | https://github.com/Lingjiao-COE/GREA |
| [21] | Sactison | WWW | 2021 | GP | https://github.com/azmari-sam/3actionol |
| [29] | MV-GCN | CBM | 2021 | GP | — |
| [29] | GDC | NeurIPS | 2019 | GP | https://github.com/gaoting/eo/gdcv |
| [11] | G-mixup | Arxiv | 2021 | GI | — |
| [10] | NASA | AAAI | 2021 | SL | https://github.com/BUPT-GAMMA/nasa |
| [10] | CCGN | AAAI | 2021 | PL | — |
| [46] | M3S | AAAI | 2020 | PL | — |
| [5] | NRGNN | KDD | 2021 | PL | https://github.com/EnyanDai/NRGNN |
| [6] | GCC | KDD | 2020 | GP | https://github.com/THUDAM/GCC |
| [9] | GraphENS | AAAI | 2022 | NI | — |
| [14] | M-Evolve | IEEE-TNM | 2020 | ER, PL | — |
| [7] | GraphCrop | Arxiv | 2020 | SSa | — |
| [32] | InfoGraph | ICLR | 2020 | SSa | https://github.com/1f7opp/InfoGraph |
| [46] | ELE | NeurIPS | 2020 | SSa | https://github.com/Geordzi23/EGI |
| [8] | NeuralParse | ICM | 2020 | SSa | https://github.com/hungdinh07/NeuralParse |
| [14] | MCGRL | ICM | 2020 | SSa, GP | https://github.com/koushiboan/mcg |
| [9] | SubMix | WWW | 2022 | SSa | https://github.com/moonaata/GraphAug |
| [4] | GraphTransplant | AAAI | 2022 | SSa | — |
| [5] | McGRL | KDD | 2021 | SSa | https://github.com/islamislab/McGRL |
| [3] | GREA | KDD | 2022 | SSa | https://github.com/Lingjiao-COE/GREA |
| [21] | Sactison | WWW | 2021 | GP | https://github.com/azmari-sam/3actionol |
| [29] | MV-GCN | CBM | 2021 | GP | — |
| [29] | GDC | NeurIPS | 2019 | GP | https://github.com/gaoting/eo/gdcv |
| [11] | G-mixup | Arxiv | 2021 | GI | — |
| [10] | NASA | AAAI | 2021 | SL | https://github.com/BUPT-GAMMA/nasa |
| [10] | CCGN | AAAI | 2021 | PL | — |
| [46] | M3S | AAAI | 2020 | PL | — |
| [5] | NRGNN | KDD | 2021 | PL | https://github.com/EnyanDai/NRGNN |
6 APPLICATIONS OF GRAPH DATA AUGMENTATION

In this section, we review and discuss how GDAug improves graph learning from two application levels, i.e., data and model.

6.1 Data-level Application

Collecting and constructing graph-structured data on real systems usually inevitably suffers from several dilemmas, such as label scarcity, class imbalance, information redundancy, disturbing noise, etc., which directly lead to low-quality graph data and indirectly lead to poor graph learning results. GDAug technology has been proposed to alleviate the problems of over-fitting, weak generalization, and low fairness caused by low-quality graph data at the data level.

6.1.1 Label Scarcity. In practical scenarios, obtaining data labels requires human labor and is time-consuming and laborious, leading to the label scarcity problem. For example, labeling account types in financial transaction networks is subject to privacy restrictions due to sensitive identity information; Toxicity labeling of molecular graphs requires extensive toxicology detection experiments; Labeling documents in citation networks requires summarizing their topics in terms of their content. Graph learning methods tend to fall into over-fitting and weak generalization when working on small and sparsely labeled graph datasets. To alleviate the issue, data augmentation is a prevalent remedy that can expand data distribution and increase data diversity, achieving an improvement in the generalization power of machine learning models trained on augmented data.

Among the aforementioned GDAug techniques, label-level augmentation combined with graph self-training works well as a general solution to improve semi-supervised graph learning when training data is limited. Specifically, graph self-training can generate high confidence pseudo labels for unlabeled data as supervision via pre-trained models trained with limited labeled data, and the augmented data with pseudo labels can be used to retrain pre-trained models or train new models. Representative works include M3S [54], CGCN [18], NRGNN [6] and M-Evolve [96], as discussed in Sec. 4.6.1. Moreover, GDAug has also been applied in graph self-supervised learning (GSSL) [71]. For contrastive GSSL, GDAug is generally used to generate augmented views for each instance. And two views generated from the same instance are generally regarded as a positive pair, while those generated from different instances are generally regarded as a negative pair. For example, GraphCL [80] proposes four GDAug strategies, including feature masking, node dropping, edge rewiring and subgraph sampling, to generate augmented views for graphs. Other representative works include GCA [101], MVGRL [14], MERIT [21], CSSL [84], GBT [1], etc. For generative GSSL, it first uses GDAug to mask partial features or structures of graph data, and then uses pretext tasks such as reconstruction to take the masked features or structures as self-supervised signals. For example, Hu et al. [17] first masked node and edge attributes, and then used the pretext task of attribute prediction to capture the domain knowledge of molecular graphs.

6.1.2 Class Imbalance. Class imbalance is another form of label scarcity when there is an unequal distribution of classes in the training data. In other words, the labeled minority classes may have significantly fewer samples than the majority classes. This problem is extremely common in practice and can be observed in various research fields such as anomaly detection and fraud detection [24]. For example, in the financial transaction network, most accounts belong to normal users, while the number of abnormal or fraudulent accounts labeled is far less than normal accounts. Since most existing graph learning methods are mainly based on the class-balance assumption, directly training graph models on the class-imbalanced data cannot learn the features of the minority class samples well, resulting in sub-optimal performance and low fairness. To alleviate the issue in graph data, GDAug can be used to balance the class distribution. Existing works mainly
Data Augmentation on Graphs: A Survey

Utilize node interpolation augmentation to generate synthetic nodes for minority classes, such as GraphMixup [72], GraphENS [45], and GraphSMOTE [90], as described in Sec. 4.2.2.

6.1.3 Structural Noise. Real-world graphs generally contain noisy and task-irrelevant edges, which will interfere with message propagation and aggregation in graph learning, resulting in sub-optimal performance. For example, automatic following of bot accounts in social networks affects the characterization of user preferences by graph algorithms; The key structures that determine a certain property of a molecule often only occupy a small part of the entire molecular graph. In this regard, edge-level augmentations are used in graph structure learning to optimize the noisy graph structure and learn more robust graph representation. For example, Luo [37] et al. proposed a learnable topological denoising network to remove task irrelevant edges, further improving the robustness and generalization of GNNs. Other representative works include NeuralSparse [91], TO-GNN [76], RobustECD [93].

6.2 Model-level Application

Despite the excellent performance of graph representation learning methods in characterizing the features of graph data, they still expose many weaknesses and limitations, such as over-smoothing on deep GNNs, vulnerability to adversarial attacks, and transferability of graph models. In this regard, the combination of GDAug techniques and existing graph learning paradigms can alleviate these model limitations to some extent.

6.2.1 Over-smoothing. When the over-smoothing problem exists, all node representations will gradually become indistinguishable with the increase of network depth, and finally no longer relevant to the input features, resulting in vanishing gradients. Many works [16, 32, 34, 49] have discussed the over-smoothing phenomenon, some of them combined with GDAug to perturb the graph topology or features, thereby alleviating the over-smoothing problem. For example, DropEdge [49] utilizes edge removing augmentation to randomly perturb the message propagation process, thereby alleviating over-smoothing. AdaEdge [16] utilizes adaptive edge rewiring to iteratively optimize graph topology, i.e., removing inter-class edges and adding intra-class edges based on model predictions, further relieving the over-smoothing issue. GRAND [8] randomly perturb the message propagation process via node feature dropping, that is, to augment the node’s receptive field during representation learning, thereby reducing the risk of over-smoothing.

6.2.2 Vulnerability. Graph neural networks have been shown to inherit the vulnerability of deep neural networks [22], i.e., they are susceptible to being fooled by small input perturbations known as adversarial attacks. To address this problem, some works combine graph adversarial learning and GDAug to learn robust graph representations. For example, FLAG [30] iteratively optimizes node features by using gradient-based feature masking during training, making graph models invariant to small perturbations in the input, and further improving the robustness and generalization of graph models. GROC [25] uses gradient-based edge rewiring as adversarial transformation during graph contrastive learning to generate augmented views, further improving the robustness of GNNs against adversarial attacks. GraphCL [80] also performs adversarial experiments to show that graph contrastive learning with GDAug can boost the robustness of GNNs under multiple evasion attacks.

6.2.3 Transferability. Existing graph representation learning methods usually train dedicated models for domain-specific data and have weak transferability to out-of-distribution data. In this regard, several existing works utilize subgraph sampling augmentations for graph pre-training and transfer learning. For example, GCC [47] performs random-walk sampling to augment the

J. ACM, Vol. 37, No. 4, Article 111. Publication date: August 2018.
ego-net subgraphs, and EGI [98] utilizes ego-net sampling and information maximization for training transferable GNNs.

7 OPEN ISSUES AND FUTURE DIRECTIONS
Although GDAug technology has attracted considerable attention and has been widely used, there are still some shortcomings and challenges in the existing research. In this section, we summarize some open issues and discuss future research directions to address them.

7.1 Comprehensive Evaluation System
Most related works mainly use some common performance metrics to evaluate the effectiveness of GDAug. However, they only measure the quality of GDAug according to the performance of downstream tasks, lacking the interpretability of augmentation mechanisms. Although a small number of existing works [3, 9, 60] propose consistency and diversity metrics to measure the correctness and generalization of GDAug, these metrics are still some combination of predictive metrics with limited interpretability. Besides, these works also utilize multiple metrics to trade-off different properties of GDAug, lacking flexibility and generalization. Therefore, it is necessary to establish a comprehensive evaluation system for GDAug techniques.

7.2 Complex Graph Types
Most of the existing GDAug methods are designed for plain or homogeneous attributed graphs. However, due to the complexity of real-world systems, they are usually constructed as complex graphs to maximally retain related information. For example, financial transaction scenarios can be modeled as heterogeneous graphs, transportation systems can be modeled as spatio-temporal dynamic graphs, and wikipedia data can be modeled as knowledge graphs. GDAug techniques on these complex graphs are less studied, and the existing studies are only generalizations of the augmentation techniques on simple graphs. Therefore, designing effective graph augmentation strategies for complex graphs is worth exploring.

8 CONCLUSION
In this paper, we present a comprehensive survey of graph data augmentation (GDAug). Specifically, we classify GDAug methods into six categories according to the fine-grained graph elements, i.e., feature-level, node-level, edge-level, subgraph-level, graph-level, and label-level augmentations. We then summarize several common performance metrics and specific design metrics for evaluating GDAug. Furthermore, we review and discuss the data-level and model-level applications of GDAug. Finally, we outline existing open issues as well as future directions in this field.

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Data Augmentation on Graphs: A Survey

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