Generated Graph Detection

Yihan Ma [1] **Zhikun Zhang** [1 2] **Ning Yu** [3] **Xinlei He** [1] **Michael Backes** [1] **Yun Shen** [4] **Yang Zhang** [1]

Abstract

Graph generative models become increasingly effective for data distribution approximation and data augmentation. While they have aroused public concerns about their malicious misuses or misinformation broadcasts, just as what *Deepfake* visual and auditory media has been delivering to society. Hence it is essential to regulate the prevalence of generated graphs. To tackle this problem, we pioneer the formulation of the generated graph detection problem to distinguish generated graphs from real ones. We propose the first framework to systematically investigate a set of sophisticated models and their performance in four classification scenarios. Each scenario switches between seen and unseen datasets/generators during testing to get closer to real-world settings and progressively challenge the classifiers. Extensive experiments evidence that all the models are qualified for generated graph detection, with specific models having advantages in specific scenarios. Resulting from the validated generality and oblivion of the classifiers to unseen datasets/generators, we draw a safe conclusion that our solution can sustain for a decent while to curb generated graph misuses.[1]

1. Introduction

Graph generative models aim to learn the distributions of real graphs and generate synthetic ones (Xie et al., 2022; Liu et al., 2021; Wu et al., 2021b). Generated graphs have found applications in numerous domains, such as social networks (Qiu et al., 2018), e-commerce (Li et al., 2020), chemoinformatics (Kearnes et al., 2016), etc. In particular, with the development of deep learning, graph generative models have witnessed significant advancement in the past 5 years (Stoyanovich et al., 2020; Liao et al., 2019; Kipf & Welling, 2016; You et al., 2018a).

However, a coin has two sides. There is a concern that synthetic graphs can be misused. For example, molecular graphs are used to design new drugs (Simonovsky & Komodakis, 2018; You et al., 2018a). The generated graphs can be misused in this process (e.g., leading to unresolved protein-ligand binding (Walters & Murcko, 2020; Bian & Xie, 2021; Zeng et al., 2022)), hence it is essential for the pharmaceutical factory to vet the authenticity of the molecular graphs. Also, synthetic graphs make deep graph learning models more vulnerable to well-designed attacks. Existing graph-level backdoor attacks (Xi et al., 2021) and membership inference attacks (Wu et al., 2021a) require the attackers to train their local models using the same or similar distribution data as those for the target models. Adversarial graph generation enables attackers to generate graphs that are close to the real graphs. It facilitates the attackers to build better attack models locally hence keeping those attacks more stealthy (since the attackers can minimize the interaction with the target models). This advantage also applies to the latest graph attacks such as the property inference attack (Zhang et al., 2022) and GNN model stealing attack (Shen et al., 2022).

As a result, it is essential to regulate the prevalence of generated graphs. In this paper, we propose to target the generated graph detection problem, i.e., *to study whether generated graphs can be differentiated from real graphs with machine learning classifiers*.

To detect generated graphs, we train graph neural network (GNN)-based classifiers and show their effectiveness in encoding and classifying graphs (Zhang et al., 2020; Kipf & Welling, 2017; Hamilton et al., 2017). Figure 2 (in Appendix A) illustrates the general pipeline of the generated graph detection. To evaluate their accuracy and generalizability, we test graphs from varying datasets and/or varying generators that are progressively extended toward the unseen during training. The *seen* concept in dataset or generator means that the graphs used in the training and testing stage are from the same dataset or generated by the same generator, respectively. That is to say, they share the same or similar distribution. And the *unseen* concept represents the

[1]CISPA Helmholtz Center for Information Security [2]Stanford University [3]Salesforce Research [4]NetApp. Correspondence to: Yihan Ma <yihan.ma@cispa.de>.

Proceedings of the 40th International Conference on Machine Learning, Honolulu, Hawaii, USA. PMLR 202, 2023. Copyright 2023 by the author(s).

[1]Our code is available at https://github.com/Yvonnemamama/GGD

opposite, which is that compared with the training stage, the graphs used in the testing stage may come from different datasets or are generated by different generators.

To sophisticate our solution space, we study three representative classification models. The first model is a direct application of GNN-based end-to-end classifiers (Kipf & Welling, 2017; Hamilton et al., 2017; Chen et al., 2018; Xu et al., 2019b). The second model shares the spirit of contrastive learning for images (Chen et al., 2020; Wu et al., 2018; Hénaff, 2020) and graphs (Zhu et al., 2021a; You et al., 2020; Hassani & Ahmadi, 2020; Zhu et al., 2021b), which, as one of the cutting-edge self-supervised representation learning models, learns similar representations for the same data under different augmentations. The third model is based on deep metric learning (Xing et al., 2002; Schroff et al., 2015; Song et al., 2016), which learns close/distant representations for the data from the same/different classes. *Note that in this paper, our goal is not proposing a new algorithm, but solving a novel real-world problem using existing methods to identify practical solutions.* Thus the 3 proposed models are all based on previous work.

We systematically conduct experiments under different settings for all the classification models to demonstrate the effectiveness of our framework. Moreover, we conduct the dataset-oblivious study which mixes various datasets in order to evaluate the influence along the dataset dimension. The evidenced dataset-oblivious property makes them independent of a specific dataset and practical in real-world situations.

2. Preliminaries

Notations. We define an undirected and unweighted homogeneous graph as $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{A})$, where $\mathcal{V} = \{v_1, v_2, ..., v_n\}$ represents the set of nodes, $\mathcal{E} \subseteq \{(v, u) \mid v, u \in \mathcal{V}\}$ is the set of edges and $\mathbf{A} \in \{0, 1\}^{n \times n}$ denotes $\mathcal{G}$'s adjacency matrix. We denote the embedding of a node $u \in \mathcal{V}$ as $\mathbf{h}_u$ and the embedding of the whole graph $\mathcal{G}$ as $\mathbf{h}_{\mathcal{G}}$.

Graph Neural Networks. Graph neural networks (GNNs) have shown great effectiveness in fusing information from both the graph topology and node features (Zhang et al., 2020; Hamilton et al., 2017; Kipf & Welling, 2017). In recent years, they become the state-of-the-art technique serving as essential building blocks in graph generators and graph classification algorithms. A GNN normally takes the graph structure as the input for message passing, during which the neighborhood information of each node u is aggregated to get a more comprehensive representation $\mathbf{h}_u$. The detailed information of GNN is described in Appendix A.1.

Graph Generators. Graph generators aim to produce graph-structured data of observed graphs regardless of the domains, which is fundamental in graph generative models. The study of graph generators dated back at least to the work by Erdös-Rényi (Erdös & Rényi, 1959) in the 1960s. These traditional graph generators focus on various random models (Erdös & Rényi, 1959; Albert & Barabási, 2002), which typically use simple stochastic generation methods such as a random or preferential attachment mechanism. However, the traditional models require prior knowledge to obtain/tune the parameters and tie them specifically to certain properties (e.g., probability of connecting to other nodes, etc.), hence their limited capacity of handling the complex dependencies of properties. Recently, graph generators using GNN as the foundation has attracted huge attention (Liao et al., 2019; You et al., 2018b; Grover et al., 2019; Simonovsky & Komodakis, 2018). The GNN-based graph generators can be further grouped into two categories: autoencoder-based generators and autoregressive-based generators. Autoencoder-based generator (Kipf & Welling, 2016; Grover et al., 2019; Mehta et al., 2019; Simonovsky & Komodakis, 2018) is a type of neural network which is used to learn the representations of unlabeled data and reconstruct the input graphs based on the representations. Autoregressive-based generator (Liao et al., 2019; You et al., 2018b) uses sophisticated models to capture the properties of observed graphs better. By generating graphs sequentially, the models can leverage the complex dependencies between generated graphs. In this paper, we selectively focus on eight graph generators that span the space of commonly used architectures, including ER (Erdös & Rényi, 1959), BA (Albert & Barabási, 2002), GRAN (Liao et al., 2019), VGAE (Kipf & Welling, 2016), Graphite (Grover et al., 2019), GraphRNN (You et al., 2018b), SBMGNN (Mehta et al., 2019), and GraphVAE (Simonovsky & Komodakis, 2018) (see more detailed information about graph generators in Appendix A.2).

3. Generated Graph Detection

3.1. Problem Statement

The generated graph detection problem studied in this paper can be formulated as follows. Suppose we have a set of *real* graphs $\mathbf{RG} = \{\mathbf{rg}_1, \ldots, \mathbf{rg}_\ell\}$, m *seen* graph generators $\varphi_{seen} = \{\phi_1, \ldots, \phi_m\}$, k *unseen* graph generators $\varphi_{unseen} = \{\phi_{m+1}, \ldots, \phi_{m+k}\}$, and a collection of *generated graphs* by seen and unseen generators $\mathbf{GG} = \{\mathbf{GG}_1, \ldots, \mathbf{GG}_{m+k}\}$. Here each $\mathbf{GG}_i$ is a set of graphs generated by a graph generator ϕ_i. To be specific, let $D = \{(x_1, y_1), (x_2, y_2), \ldots, (x_z, y_z)\}$, where $x_i \in \mathbf{RG} \bigcup \mathbf{GG}$, y_i represents the label of each graph (i.e., real or generated) and $z = \sum_{i=1}^{m+k} |\mathbf{GG}_i|$ is the total number of samples. A generated graph detector $f(\cdot)$ is later trained on D. Once trained, it classifies each testing graph as real or generated. However, it is normal to see the arrival of graphs from un-

known generators that have never been seen in training, and the graphs may not bear similar properties as the training data in the real world. The existing solutions usually leverage model retraining to cope with the problem. Yet, it is impractical to retrain a model from scratch every time a new graph generator is added or unseen data is encountered. Ideally, $f(\cdot)$ *should be built in a way that it can be generalized to previously unseen data/generator in the real world*.

3.2. A General Framework for Generated Graph Detection and Analysis

In this paper, we propose a general framework to detect generated graphs. Specifically, this framework consists of four scenarios depending on whether the dataset or graph generator has been used to train the model. These scenarios comprehensively cover from the simplest close-world scenario to the most challenging full open-world detection scenario. We discuss how we choose different ML models to implement this framework in Section 3.3.

Closed World. In this scenario, the training and testing graphs are sampled from *seen dataset* and generated by *seen generators*. The goal is to predict whether a graph is real or generated by seen generators. Under this setting, to train the generated graph detector $f(\cdot)$, we sample real graphs from $\mathbf{RG}$ as positive samples and sample graphs generated by seen generators φ_{seen} as negative samples. The graphs used to test $f(\cdot)$ share the same distribution with the training set, i.e., they consist of real graphs sampled from $\mathbf{RG}$ and generated graphs generated by seen generators φ_{seen}.

Open Generator. In this scenario, the negative samples of the testing graphs are generated by unseen generators but are in the same or similar distribution of training data (i.e., seen dataset). The training data of $f(\cdot)$ does not contain any graphs generated by unseen generators φ_{unseen}. Since only the graph generators used in the testing dataset are not seen at the time of training, we thus name it the "Open Generator" scenario. Under this setting, the detector $f(\cdot)$ is trained with the graphs sampled from $\mathbf{RG}$ (positive samples) and graphs generated by seen generators φ_{seen} (negative samples). The positive samples used to test $f(\cdot)$ are also from $\mathbf{RG}$ while the negative samples are generated by unseen generators φ_{unseen}. The goal is to predict whether a graph is real or generated by unseen generators.

Open Set. In this scenario, the testing graphs are from seen generators that are trained on unseen datasets. Concretely, the graph generators that the system sees in training are what it will see in testing (i.e., seen generators). However, the testing graphs are of different distributions of training data (i.e., unseen datasets). For instance, $f(\cdot)$ was trained using both real and generated graphs from chemical graphs, yet, the testing graphs (either real or generated) are social network graphs that are inherently different. As such, we name this scenario the "Open Set" scenario. Similar to the "Open Generator" scenario, the detector $f(\cdot)$ is trained with the graphs sampled from $\mathbf{RG}$ (as positive samples) and the graphs generated by seen generators φ_{seen} (as negative samples). Unlike the previous experiments, the graphs used to test $f(\cdot)$ are from different datasets. The testing graphs of $f(\cdot)$ consist of real graphs sampled from other datasets and graphs generated by seen generators φ_{seen} based on other datasets. The goal is to predict whether a graph from the unseen dataset is real or generated.

Open World. In this scenario, the testing graphs are from unseen generators that are trained on unseen datasets. This setting is the most challenging yet common in the real world. It is normal to see the arrival of graphs from unknown generators that have never been seen at the training time, and the graphs may not bear with similar properties as of the training data. To be specific, certain generators that the classifier sees at the testing time are not included in its training stage (i.e., unseen generators), and the testing graphs are of the different distribution of training data (i.e., unseen datasets). Similar to "Open Generator" and "Open Set" scenarios, the generated graph detector $f(\cdot)$ is trained with the graphs sampled from $\mathbf{RG}$ (as positive samples) and the graphs generated by seen generators φ_{seen} (as negative samples). The testing graphs consist of real graphs sampled from other datasets and graphs generated by unseen generators φ_{unseen}. The goal is to predict whether a graph from the unseen dataset is real or generated by unseen generators.

3.3. Detection Methodologies

As discussed in Section 3.2, we need an ML model $f(\cdot)$ to cope with the four generated graph detection scenarios. In this section, we introduce three ML models – end-to-end classifier (Kipf & Welling, 2017; Hamilton et al., 2017; Chen et al., 2018; Xu et al., 2019b), contrastive learning-based model (Zhu et al., 2021a; You et al., 2020; Hassani & Ahmadi, 2020; Zhu et al., 2021b), and metric learning-based model (Xing et al., 2002; Schroff et al., 2015; Song et al., 2016) – to implement the aforementioned detection framework. All the models can work as the $f(\cdot)$ to do the final detection in all scenarios. For each scenario, $f(\cdot)$ has the same structure, while trained or tested by different samples. The pros and cons of each model are evaluated and discussed in Section 4.

End-To-End Classifier. The most straightforward approach to distinguishing between real and generated graphs is to train a binary classifier in an end-to-end manner. As aforementioned, among all the research, graph classification methods based on graph convolutional networks (GCNs) are commonly recognized as the state-of-the-art technique in deep learning-based graph classification (Kipf & Welling, 2017; Hamilton et al., 2017; Chen et al., 2018; Xu et al.,

2019b). Also, we can also see the results from Appendix A.5 also shows that GCN performs better most of the time compared with other GNN networks. Therefore we choose the GCN model (Kipf & Welling, 2017) as our end-to-end classifier. The end-to-end classifier consists of four GCN layers and a fully connected layer. We use a four-layer GCN network to embed the graph data into a 128-dimensional vector, and use a fully connected layer to compute the final classification result.

Contrastive Learning-Based Model. Previous studies have shown that contrastive learning helps to improve the graph encoding performance (Zhu et al., 2021a; You et al., 2020; Hassani & Ahmadi, 2020; Zhu et al., 2021b). Different from the traditional binary classifier that trains the GNN model in an end-to-end manner, the contrastive learning-based model first learns a powerful graph encoder in a self-supervision manner, then uses the graph encoder to transform the graphs into graph embeddings, and employs a binary classifier to predict the results. Figure 3 (in Appendix A.3) illustrates the general workflow of our contrastive learning-based model. We use support vector machines (SVM) as the final classifier following the previous work (Sun et al., 2020a; You et al., 2020). The implementation details of the contrastive learning-based model are introduced in Appendix A.3.

Metric Learning-Based Model. In the past few years, deep metric learning has consistently achieved state-of-the-art model performance (Xing et al., 2002; Schroff et al., 2015; Song et al., 2016). As one of the cutting-edge unsupervised representation learning models, deep metric learning aims to map input data into a metric space, where data from the same class get close while data from different classes fall apart from each other. However, unlike other tasks such as classification or face recognition in which only one training sample is needed to get the output, in metric learning, at least two training samples are needed at one time, as the output of metric learning is whether the two input samples are from the same category (Guo et al., 2017; He et al., 2018). Based on the core concept of metric learning, siamese network (Guo et al., 2017; He et al., 2018) is proposed, which takes paired samples as inputs and outputs whether the paired samples are from the same category. The implementation details of the metric learning-based model are introduced in Appendix A.4. Since the metric learning-based model takes paired samples as input and only predicts whether the two input samples are from the same label, to evaluate the performance of the metric learning-based model in the perspective of getting prediction results of each graph, we still need to predict the exact label for each testing sample by querying the model using paired samples consists of one testing sample needs to be predicted and one sample with the known label.

In order to get the final classification results, for each testing sample, we randomly select N_k samples of each label from the training set and generate $N_k * N_{class}$ paired samples. Here N_{class} equals 2 (i.e., real and generated). After feeding the paired samples into the siamese network, we will get N_k posteriors for each label. Each posterior represents the probability of the paired samples from the same label. After calculating the mean value of the N_k posteriors for each label, we can find the maximum mean value and take the corresponding label as the predicted result of the testing sample. For example, if the maximum mean value of the posteriors is from label *real*, then we consider using *real* as the final classification result.

Table 1: Dataset statistics.

Dataset	# of graphs	Avg. Nodes	Avg. Edges
AIDS	2,000	15.69	16.20
Alchemy	202,579	10.10	10.44
Deezer	9,629	23.49	65.25
DBLP	19,456	10.48	19.65
GitHub	12,725	113.79	234.64
COLLAB	5,000	74.49	2,457.78
Twitch	127,094	29.67	86.59

4. Experiments

We first introduce the datasets and implementation details of our experiments. Then following the application scenarios described in Section 3, the experiments are conducted based on each scenario.

4.1. Experimental Setup

Datasets. We use 7 benchmark datasets from TU-Dataset (Morris et al., 2020) to evaluate the performance, including AIDS (Riesen & Bunke, 2008), Alchemy (Chen et al., 2019), Deezer ego nets (abbreviated as Deezer) (Rozemberczki et al., 2020), DBLP (DBL), GitHub StarGazer (abbreviated as GitHub) (Rozemberczki et al., 2020), COLLAB (Yanardag & Vishwanathan, 2015) and Twitch ego nets (abbreviated as Twitch) (Rozemberczki et al., 2020). Among them, Deezer, GitHub, and Twitch are social networks with nodes representing users and edges indicating friendships. DBLP and COLLAB are collaboration networks with nodes representing papers/researchers and edges indicating citations/collaborations. AIDS and Alchemy are molecular graphs with nodes representing atoms of the compound and edges corresponding to chemical bonds. These graphs form our *real* datasets for the rest of the evaluation. The statistics of all the datasets are summarized in Table 1.

Sampling High-Quality Generated Graphs. Although the graph generators are capable to generate graphs with similar distribution as real graphs, some of the generated

Table 2: The accuracy/F1-score of generated graph detection in "Closed World" scenario and "Open Generator" scenario.

	Closed World					Open Generator				
Dataset	FC(MLP)	FC(XGBoost)	End-To-End	Contrastive	Metric	FC(MLP)	FC(XGBoost)	End-To-End	Contrastive	Metric
AIDS	0.75/0.73	0.74/0.74	0.89/0.85	0.87/0.84	**0.91/0.90**	0.73/0.70	0.72/0.71	0.82/0.81	0.84/0.82	**0.87/0.84**
Alchemy	0.78/0.78	0.79/0.78	0.87/0.87	0.85/0.80	**0.90/0.89**	0.74/0.73	0.76/0.76	0.80/0.77	0.82/0.79	**0.84/0.82**
Deezer	0.78/0.78	0.80/0.80	0.97/0.95	0.95/0.94	**0.98/0.97**	0.74/0.74	0.77/0.75	0.90/0.88	**0.92/0.92**	0.91/0.91
DBLP	0.70/0.68	0.72/0.71	**0.84/0.83**	0.82/0.82	0.82/0.82	0.75/0.74	0.75/0.75	0.79/0.79	**0.82/0.82**	0.80/0.79
Github	0.81/0.81	0.84/0.82	0.95/0.94	0.92/0.92	**0.96/0.96**	0.80/0.82	0.81/0.80	0.94/0.94	0.91/0.91	**0.96/0.92**
COLLAB	0.56/0.55	0.60/0.60	0.85/0.84	0.84/0.82	**0.89/0.89**	0.50/0.49	0.51/0.50	0.78/0.76	0.80/0.79	**0.84/0.82**
Twitch	0.56/0.55	0.61/0.60	0.92/0.89	0.90/0.88	**0.95/0.93**	0.51/0.49	0.53/0.51	0.85/0.85	**0.90/0.89**	0.86/0.86
Mixed	0.64/0.62	0.65/0.64	**0.84/0.83**	0.80/0.80	0.82/0.81	0.60/0.59	0.62/0.62	0.78/0.76	**0.82/0.80**	0.79/0.78

graphs may still contain obvious artifacts in some cases. There is a concern that the classification may be biased by such artifacts. Thus we compute the number of nodes, the number of edges, density, diameter, average clustering, and transitivity as the statistical features of each graph and use Euclidean Distance to measure the 1-nearest-neighbor similarity between each generated graph and real graph sets (Yu et al., 2019). We select 20% generated graphs with the highest similarity for the following experiments.

To evaluate the quality of generated graphs, we use maximum mean discrepancy (MMD) over these graph features to measure the similarity between real graphs and graphs generated by different generators. The MMD results show that the graphs generated by different generators and real graphs are very similar at the statistical level. The MMD results are shown in Table 6 in Appendix A.6.

Implementation Details. We use the GCN to embed the graphs in the end-to-end classifier and metric learning-based model. The GCN is implemented in PyTorch (PyT). The optimizer we used is Adam optimizer (Kingma & Ba, 2015). Each model is trained for 200 epochs. The learning rate is set to 0.001 and we adopt Cross-Entropy Loss as the loss function. The ratio of the training set and testing set is 8:2. The contrastive learning-based model is trained following the implementation details in GraphCL (You et al., 2020). As mentioned in Section 3.3, we generate $N_{ps} * 2$ paired samples to train the siamese network in the metric learning-based model and use N_k samples from each label to predict the final results. $N_{ps}*2$ is the number of paired samples used to train the siamese network. Here we conduct experiments to fine-tune the metric learning-based model and find the best $N_{ps} = 200,000$ and $N_k = 10$ which makes the model perform the best. The corresponding results are displayed in Appendix A.5 (Figure 5 and Figure 6).

Baseline. To better evaluate the performance of our proposed models, We incorporate a new model named Feature Classification (FC) as the baseline. FC model leverages the graph's statistical features as input and uses state-of-the-art machine learning models to do the final classification. Here we use Multilayer perceptron (MLP) and XGBoost (Chen & Guestrin, 2016) as the classifier since they are both powerful but effective models. The statistical features we used are the number of nodes, the number of edges, density, diameter, average clustering, and transitivity, which are the same as the features we used to sample high-quality graphs.

4.2. Experiments for the "Closed World" Scenario

In this scenario, we want to explore whether real graphs and generated graphs can be distinguished when the distribution of all testing graphs is known. As introduced before, we propose three methods to classify graphs. The evaluation metrics we used in this paper are accuracy and F1-score.

Overall Results. The accuracy and F1-score of all the binary classifiers are summarized in Table 2. In general, our proposed models outperform the 2 FC models in all datasets, demonstrating that the GNN-based models can better capture the characteristics of graphs compared to using machine learning models with only statistical features. Also, we observe that among the three methods, the metric learning-based model performs the best in most cases, while the contrastive learning-based model performs the least satisfactorily. Moreover, the results show that in general, the performance of Deezer, Github, and Twitch is better than other datasets. Compared to other datasets, the graphs in Twitch, Github, and Deezer are bigger and the three datasets also have a richer amount of graphs. This implies that the binary classifiers can distinguish between real graphs and generated graphs with higher accuracy for larger datasets with bigger graphs.

Although the contrastive learning-based model and metric learning-based model have a similar goal, i.e. training an encoder that can map graphs to a latent space where graphs with the same label get close while graphs with different labels fall apart from each other, the metric learning-based model performs better than the contrastive learning-based model in this scenario. Thus we can draw the conclusion that the embeddings produced by metric learning tend to be distinguished easily in the "Closed World" scenario.

Dataset Oblivious Study. Besides the evaluation from the

perspective of a single dataset, we also conduct the dataset oblivious study. In this experiment, we first randomly sample 1,000 real graphs from each dataset. Then we randomly select 1,000 generated graphs which are evenly generated by all the generators based on each dataset. Finally, we obtain a *mixed* dataset consisting of 7,000 real graphs and 7,000 generated graphs to train and test the binary classifier. The ratio of the training set and testing set is 8:2.

Surprisingly, a persuasive performance can be noticed even when we don't take the dimension of the dataset into consideration. The performance indicates that the models can still distinguish real graphs from generated graphs even when the graphs used to train the model don't belong to any specific dataset. This is more meaningful in the real-world scenario as we may not know which dataset the graphs come from. In the mixed dataset, the end-to-end classifier performs the best, which means when the graphs which need to be classified do not belong to one specific dataset, the end-to-end classifier can better capture the complex dependencies of graphs and detect generated graphs with higher accuracy.

4.3. Experiments for the "Open Generator" Scenario

The experiments above have proved that the real graphs and generated graphs can be distinguished in the close-world scenario. In order to further evaluate if our models can still detect generated graphs when given unseen generators, we choose three different generators - GraphRNN (You et al., 2018b), SBMGNN (Mehta et al., 2019), and GraphVAE (Simonovsky & Komodakis, 2018) - as unseen generators to test the utility of the proposed models. For all datasets, we use real graphs as the positive samples and graphs generated by unseen generators as the negative samples to test the models.

Overall Results. The final classification results are shown in Table 2, from which we can see that the binary classification results of all the datasets are over 0.75, which indicates that even when the graphs are generated by unseen algorithms, the models can still have a relatively good performance. This indicates that all the models can be generalized to other graph generators. Also, compared with the "Closed World" scenario, the contrastive learning-based model starts to show some advantages when new generators arrive. We can see a comparable performance with the metric learning-based model, which exemplifies that the contrastive learning-based model suits the "Open Generator" scenario more. Similar to the previous scenario, the accuracies and F1-score of all the models in Deezer, Github, and Twitch are better than other datasets, which indicates that the models can be generalized to other datasets better for larger datasets with bigger graphs.

Dataset Oblivious Study. Moreover, we also conduct experiments for the mixed dataset. It can be noticed that the model performance in the mixed dataset is in line with those of other datasets. The experimental results suggest that our models can still generalize to previously unseen generators even when we don't take the dimension of the dataset into consideration.

Table 3: Distinguishing graphs generated by unseen generators.

	Accuracy	F1-score
AIDS	0.78	0.78
Alchemy	0.82	0.82
Deezer	0.93	0.93
DBLP	0.75	0.74
GitHub	0.95	0.95
COLLAB	0.83	0.83
Twitch	0.89	0.89
MIXED	0.64	0.64

The accuracy of the contrastive learning-based model for the mixed dataset is even better for COLLAB and is the best among all three models. This suggests that the contrastive learning-based model can better generalize to other generators in datasets with a wide range of node numbers and graph densities, i.e. mixed dataset.

Distinguishing Graphs Generated by Unseen Generators. Apart from classifying real graphs and graphs generated by unseen generators, we use metric learning to predict whether two graphs generated by unseen generators are generated by the same generator. To evaluate the performance of predicting whether any two graphs generated by unseen generators are generated by the same generator, we randomly generate 50,000 positive graph pairs and 50,000 negative graph pairs and use metric learning to take the graph pairs as input (the performance is shown in Table 3). It can be noticed that the metric learning-based model can predict whether two graphs generated by unseen generators are generated by the same generator to some extent. Moreover, we can see that the performance of Deezer, Github, and TWITCH is better than other datasets, which is consistent with the results of the "Open Generator" scenario.

However, when we use the mixed dataset to train and test the metric learning-based model, the performance is much worse than in other datasets. It is reasonable since we can see from Table 2 that the metric learning-based model with a mixed dataset performs the worst among all the datasets. The visualization of graphs generated by the unseen generators shown in Figure 7 also supports our results, the embeddings of the mixed dataset can not be separated explicitly compared to other datasets.

4.4. Experiments for the "Open Set" Scenario

Apart from distinguishing between real graphs and graphs generated by unseen algorithms, we also conduct experiments to evaluate whether graphs generated by unseen datasets can still be distinguished from real graphs. In this experiment, we use graphs from AIDS, Alchemy, Deezer, DBLP, and Github as the seen datasets to train all the models, and use COLLAB and Twitch as unseen datasets to test the models.

For each seen dataset, we randomly select 1,000 real graphs and 1,000 generated graphs which are evenly generated by the seen generators. In the end, we use the final dataset with 5,000 real graphs and 5,000 generated graphs to train all the models.

In this scenario, we want to evaluate whether the fake graphs generated by seen generators based on unseen datasets can be distinguished from the real graphs. Thus to test the model, for each unseen dataset, we randomly select real graphs and the same amount of generated graphs that are evenly generated by the seen generators. The final testing set contains 2,000 real graphs and 2,000 generated graphs. The performance of all the models is summarized in Table 4.

We can see from the table that, in general, the real graphs and generated graphs can be distinguished with an accuracy higher than 0.78. This implies that our models have the ability to generalize to unseen datasets. Moreover, the accuracy of the contrastive learning-based model is higher than 0.85 and the best among the three models, which suggests that the contrastive learning-based model can generalize to the unseen datasets better.

After comparing the performance with the "Closed World" scenario in Section 4.2, we find that the performance drops. It is reasonable because the graphs used to test the models come from new datasets which are not seen in the training set, which makes the task harder than in the previous experiment.

4.5. Experiments for the "Open World" Scenario

The fourth scenario is to evaluate whether the fake graphs generated by unseen algorithms in unseen datasets can be distinguished from the real graphs. To test the model, for each unseen dataset, we randomly select real graphs and the same amount of generated graphs that are evenly generated by the unseen generators. The final testing set contains 2,000 real graphs and 2,000 generated graphs. The performance of all the models is summarized in Table 4.

The scenario is called the "Open World" scenario as described before since the datasets and generators are both unseen in the training phase. It is the hardest task among the four scenarios. We can see from Table 4 that the performance, as expected, is lower than those in Section 4.4 and Section 4.5.

Table 4: Generated graph detection in "Open Set" scenario and "Open World" scenario.

	Open Set	Open World
FC(MLP)	0.57/0.54	0.64/0.62
FC(XGBoost)	0.60/0.62	0.65/0.64
End-To-End	0.82/0.82	0.76/0.75
Contrastive	**0.85**/0.84	**0.83**/0.83
Metric	0.78/0.76	0.74/0.74

Although the performance is not as competent, the accuracies of all models are still higher than 0.74. This suggests that the models can still distinguish real graphs and graphs generated by unseen generators in unseen datasets to some extent. Apart from that, the contrastive learning-based model performs the best among all the models, which is in line with the previous experiments.

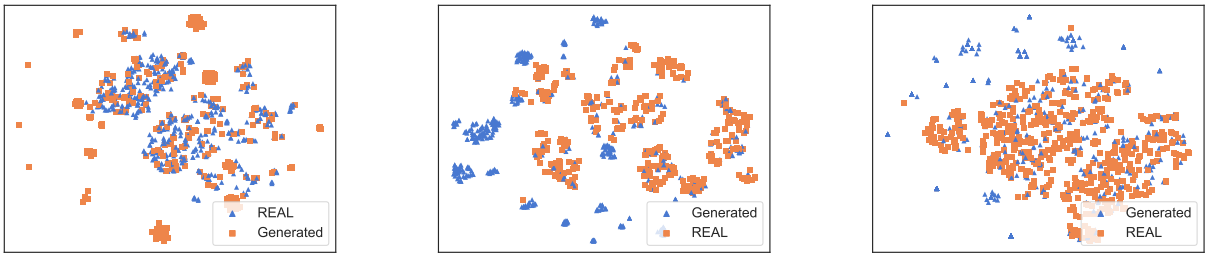
Throughout all the experiments, we can draw a conclusion that the metric learning-based model tends to perform better in the "Closed World" scenario while the contrastive learning-based model shows advantages in "Open Generator", "Open Set" and "Open World" scenarios. The results give us an insight that metric learning can learn better representations of graphs with known graph distributions. On the contrary, as a representative self-supervised method, the contrastive learning-based model can learn representations that are more general and can be transferred to different graph distributions.

4.6. Visualization Analysis

From the previous experiment, we can draw the conclusion that contrastive learning-based models tend to perform better in "Open Generator", "Open Set" and "Open World" scenarios with the mixed dataset, we further explore the reason behind it. To this end, we use t-Distributed Stochastic Neighbor Embedding (t-SNE) (van der Maaten & Hinton, 2008) to visualize the graphs embedded by different models. Figure 1 shows the t-SNE results of the testing samples used in the fourth scenario. It can be easily noticed that the embeddings produced by the contrastive encoder can be divided better, which may be the major reason why the contrastive learning-based model outperforms other models in the "Open World" Scenario.

5. Related Work

We have already covered several highly-related works (e.g., graph generative models and graph neural networks) in Section 2. We discuss additional related work in a broader



(a) End-to-end (b) Contrastive (c) Metric

Figure 1: The visualization results of different models in "Open World" scenario.

scope below.

Generated Data Detection. Although it remains an unexplored area in generated graph detection, there has been some research about generated image detection in the past few years. Rössler et al. showed that simple classifiers can detect images created by a single category of networks (Rössler et al., 2019). Wang et al. demonstrated that a simple image classifier trained on one specific CNN generator (ProGAN (Karras et al., 2018)) is able to generalize well to unseen architectures (Wang et al., 2020). Ning et al. learned the GAN fingerprints towards image attribution and showed that even a small difference in GAN training (e.g., the difference in initialization) can leave a distinct fingerprint that can be detected (Yu et al., 2019). Most of the previous studies focus on image data; as far as we know, we are the first to investigate the generated graph detection.

Privacy and Security Issues in GNN. Rising concerns about the privacy and security of GNNs have led to a surge of research on graph adversarial attacks. Broadly speaking, they can be grouped into two categories — causative attacks and exploratory attacks. Causative attacks on GNNs add unnoticeable adversarial perturbations to node features and graph structures to reduce the accuracy of or intentionally change the outcome of node classification (Bojchevski & Günnemann, 2019; Caverlee et al., 2020; Ma et al., 2020; Sun et al., 2020b; Wu et al., 2019; Xu et al., 2019a), link prediction (Bojchevski & Günnemann, 2019; Lin et al., 2020), graph classification (Dai et al., 2018; Xi et al., 2021), etc. To conduct causative attacks, attackers must be able to tamper with the training process of GNNs or influence the fine-tuning process of pre-trained GNNs. Exploratory attacks on GNNs send (carefully crafted) query data to the target GNNs and observe their decisions on these input data. Attackers then leverage the responses to build shadow models to achieve different attack goals, such as link re-identification (He et al., 2021), property inference (Zhang et al., 2022), membership inference (Wu et al., 2020), model stealing (Duddu et al., 2020), etc. To launch exploratory attacks, attackers must be able to interact with the GNNs (e.g., via publicly accessible API) at the runtime.

6. Conclusion and Future Work

In this paper, we propose a general framework for generated graph detection. In this framework, we introduce four application scenarios based on different training data and testing data and design three kinds of models to accomplish experiments in each scenario. The experimental results show that all models can distinguish real graphs from generated graphs successfully in all scenarios, which means that although the generative models show great advantage and success in many domains, the generated graphs can still be detected by GNN-based models. Also, we notice that the metric learning-based model tends to perform the best in the close world scenario while the contrastive learning-based model always shows advantages in "Open Generator", "Open Set" and "Open World" scenarios, which suggests that the contrastive learning-based model can generalize to new datasets and generators better. Our experiment about dataset oblivious study shows that the proposed models can still work with a persuasive performance when we use the mixed dataset to train and test the models. This is an interesting finding since the graphs in different datasets vary a lot, hence the mixed dataset tends to have a wide range of node numbers and densities. The results imply that the proposed models can handle datasets with many disparate graphs. The finding also fits more to the real-world situation, where the graphs that need to be detected may not be from a specific dataset. Moreover, although we only discuss the detection of generated graphs in this paper, the framework can also be extended to other research areas, such as images, text, or audio.

References

https://github.com/GRAND-Lab/graph_datasets.

https://pytorch.org/.

Albert, R. and Barabási, A. Statistical mechanics of complex networks. *Reviews of modern physics*, 2002.

Bian, Y. and Xie, X.-Q. Generative Chemistry: Drug Discovery with Deep Learning Generative Models. *Journal of Molecular Modeling*, 2021.

Bojchevski, A. and Günnemann, S. Adversarial Attacks on Node Embeddings via Graph Poisoning. In *International Conference on Machine Learning (ICML)*, pp. 695–704. PMLR, 2019.

Caverlee, J., Hu, X. B., Lalmas, M., and Wang, W. All You Need Is Low (Rank): Defending Against Adversarial Attacks on Graphs. In *ACM International Conference on Web Search and Data Mining (WSDM)*, pp. 169–177. ACM, 2020.

Chen, G., Chen, P., Hsieh, C., Lee, C., Liao, B., Liao, R., Liu, W., Qiu, J., Sun, Q., Tang, J., Zemel, R. S., and Zhang, S. Alchemy: A Quantum Chemistry Dataset for Benchmarking AI Models. *CoRR abs/1906.09427*, 2019.

Chen, J., Ma, T., and Xiao, C. FastGCN: Fast Learning with Graph Convolutional Networks via Importance Sampling. In *International Conference on Learning Representations (ICLR)*, 2018.

Chen, T. and Guestrin, C. XGBoost: A Scalable Tree Boosting System. In *ACM Conference on Knowledge Discovery and Data Mining (KDD)*, pp. 785–794. ACM, 2016.

Chen, T., Kornblith, S., Norouzi, M., and Hinton, G. E. A Simple Framework for Contrastive Learning of Visual Representations. In *International Conference on Machine Learning (ICML)*, pp. 1597–1607. PMLR, 2020.

Dai, H., Li, H., Tian, T., Huang, X., Wang, L., Zhu, J., and Song, L. Adversarial Attack on Graph Structured Data. In *International Conference on Machine Learning (ICML)*, pp. 1123–1132. PMLR, 2018.

Duddu, V., Boutet, A., and Shejwalkar, V. Quantifying Privacy Leakage in Graph Embedding. *CoRR abs/2010.00906*, 2020.

Erdös, P. and Rényi, A. On Random Graphs I. *Publicationes Mathematicae Debrecen*, 1959.

Grover, A., Zweig, A., and Ermon, S. Graphite: Iterative Generative Modeling of Graphs. In *International Conference on Machine Learning (ICML)*, pp. 2434–2444. PMLR, 2019.

Guo, Q., Feng, W., Zhou, C., Huang, R., Wan, L., and Wang, S. Learning Dynamic Siamese Network for Visual Object Tracking. In *IEEE International Conference on Computer Vision (ICCV)*, pp. 1781–1789. IEEE Computer Society, 2017.

Hamilton, W. L., Ying, Z., and Leskovec, J. Inductive Representation Learning on Large Graphs. In *Annual Conference on Neural Information Processing Systems (NIPS)*, pp. 1025–1035. NIPS, 2017.

Hassani, K. and Ahmadi, A. H. K. Contrastive Multi-View Representation Learning on Graphs. In *International Conference on Machine Learning (ICML)*, pp. 4116–4126. PMLR, 2020.

He, A., Luo, C., Tian, X., and Zeng, W. A Twofold Siamese Network for Real-Time Object Tracking. In *IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 4834–4843. IEEE Computer Society, 2018.

He, X., Jia, J., Backes, M., Gong, N. Z., and Zhang, Y. Stealing Links from Graph Neural Networks. In *USENIX Security Symposium (USENIX Security)*, pp. 2669–2686. USENIX, 2021.

Hénaff, O. J. Data-Efficient Image Recognition with Contrastive Predictive Coding. In *International Conference on Machine Learning (ICML)*, pp. 4182–4192. PMLR, 2020.

Karras, T., Aila, T., Laine, S., and Lehtinen, J. Progressive Growing of GANs for Improved Quality, Stability, and Variation. In *International Conference on Learning Representations (ICLR)*, 2018.

Kearnes, S., McCloskey, K., Berndl, M., Pande, V., and Riley, P. Molecular Graph Convolutions: Moving Beyond Fingerprints. *Journal of Computer-Aided Molecular Design*, 2016.

Kingma, D. P. and Ba, J. Adam: A Method for Stochastic Optimization. In *International Conference on Learning Representations (ICLR)*, 2015.

Kingma, D. P. and Welling, M. Auto-Encoding Variational Bayes. In *International Conference on Learning Representations (ICLR)*, 2014.

Kipf, T. N. and Welling, M. Variational Graph Auto-Encoders. In *NeurIPS Workshop on Bayesian Deep Learning (NeurIPS-16 BDL)*, 2016.

Kipf, T. N. and Welling, M. Semi-Supervised Classification with Graph Convolutional Networks. In *International Conference on Learning Representations (ICLR)*, 2017.

Li, X., Saúde, J., Reddy, P., and Veloso, M. Classifying and Understanding Financial Data Using Graph Neural Network. In *The AAAI Workshop on Knowledge Discovery from Unstructured Data in Financial Services (KDF)*. AAAI, 2020.

Liao, R., Li, Y., Song, Y., Wang, S., Hamilton, W. L., Duvenaud, D., Urtasun, R., and Zemel, R. S. Efficient Graph Generation with Graph Recurrent Attention Networks. In *Conference on Neural Information Processing Systems (NeurIPS)*, pp. 4257–4267, 2019.

Lin, W., Ji, S., and Li, B. Adversarial Attacks on Link Prediction Algorithms Based on Graph Neural Networks. In *ACM Asia Conference on Computer and Communications Security (ASIACCS)*, pp. 370–380. ACM, 2020.

Liu, Y., Pan, S., Jin, M., Zhou, C., Xia, F., and Yu, P. S. Graph Self-Supervised Learning: A Survey. *CoRR abs/2103.00111*, 2021.

Ma, J., Ding, S., and Mei, Q. Towards More Practical Adversarial Attacks on Graph Neural Networks. In *Annual Conference on Neural Information Processing Systems (NeurIPS)*. NeurIPS, 2020.

Mehta, N., Carin, L., and Rai, P. Stochastic Blockmodels meet Graph Neural Networks. In *International Conference on Machine Learning (ICML)*, pp. 4466–4474. PMLR, 2019.

Morris, C., Kriege, N. M., Bause, F., Kersting, K., Mutzel, P., and Neumann, M. TUDataset: A collection of benchmark datasets for learning with graphs. In *The ICML Workshop on Graph Representation Learning and Beyond (GRL)*. ICML, 2020.

Qiu, J., Tang, J., Ma, H., Dong, Y., Wang, K., and Tang, J. DeepInf: Social Influence Prediction with Deep Learning. In *ACM Conference on Knowledge Discovery and Data Mining (KDD)*, pp. 2110–2119. ACM, 2018.

Riesen, K. and Bunke, H. IAM Graph Database Repository for Graph Based Pattern Recognition and Machine Learning. In *Structural, Syntactic, and Statistical Pattern Recognition, Joint IAPR International Workshop (SSPR)*, pp. 287–297. Springer, 2008.

Rössler, A., Cozzolino, D., Verdoliva, L., Riess, C., Thies, J., and Nießner, M. FaceForensics++: Learning to Detect Manipulated Facial Images. In *IEEE International Conference on Computer Vision (ICCV)*, pp. 1–11. IEEE, 2019.

Rozemberczki, B., Kiss, O., and Sarkar, R. Karate Club: An API Oriented Open-Source Python Framework for Unsupervised Learning on Graphs. In *ACM International Conference on Information and Knowledge Management (CIKM)*, pp. 3125–3132. ACM, 2020.

Schroff, F., Kalenichenko, D., and Philbin, J. FaceNet: A Unified Embedding for Face Recognition and Clustering. In *IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 815–823. IEEE, 2015.

Shen, Y., He, X., Han, Y., and Zhang, Y. Model stealing attacks against inductive graph neural networks. pp. 1175–1192. IEEE, 2022.

Simonovsky, M. and Komodakis, N. Dynamic Edge-Conditioned Filters in Convolutional Neural Networks on Graphs. In *IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 29–38. IEEE Computer Society, 2017.

Simonovsky, M. and Komodakis, N. GraphVAE: Towards Generation of Small Graphs Using Variational Autoencoders. In *International Conference on Artificial Neural Networks (ICANN)*, pp. 412–422. Springer, 2018.

Sohn, K. Improved Deep Metric Learning with Multi-class N-pair Loss Objective. In *Annual Conference on Neural Information Processing Systems (NIPS)*, pp. 1849–1857, 2016.

Song, H. O., Xiang, Y., Jegelka, S., and Savarese, S. Deep Metric Learning via Lifted Structured Feature Embedding. In *IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 4004–4012. IEEE Computer Society, 2016.

Stoyanovich, J., Howe, B., and Jagadish, H. V. Responsible Data Management. *Proceedings of the VLDB Endowment*, 2020.

Sun, F., Hoffmann, J., Verma, V., and Tang, J. InfoGraph: Unsupervised and Semi-supervised Graph-Level Representation Learning via Mutual Information Maximization. In *International Conference on Learning Representations (ICLR)*, 2020a.

Sun, Y., Wang, S., Tang, X., Hsieh, T.-Y., and Honavar, V. Non-target-specific Node Injection Attacks on Graph Neural Networks: A Hierarchical Reinforcement Learning Approach. In *The Web Conference (WWW)*, pp. 673–683. ACM, 2020b.

van der Maaten, L. and Hinton, G. Visualizing Data using t-SNE. *Journal of Machine Learning Research*, 2008.

Velickovic, P., Cucurull, G., Casanova, A., Romero, A., Liò, P., and Bengio, Y. Graph attention networks. In *6th International Conference on Learning Representations (ICLR)*, 2018.

Walters, W. P. and Murcko, M. Assessing the impact of generative AI on medicinal chemistry. *Nature Biotechnology*, 2020.

Wang, S., Wang, O., Zhang, R., Owens, A., and Efros, A. A. CNN-Generated Images Are Surprisingly Easy to Spot... for Now. In *IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 8692–8701. Computer Vision Foundation / IEEE, 2020.

Wu, B., Yang, X., Pan, S., and Yuan, X. Model Extraction Attacks on Graph Neural Networks: Taxonomy and Realization. *CoRR abs/2010.12751*, 2020.

Wu, B., Yang, X., Pan, S., and Yuan, X. Adapting membership inference attacks to GNN for graph classification: Approaches and implications. In *IEEE International Conference on Data Mining, ICDM 2021, Auckland, New Zealand, December 7-10, 2021*, pp. 1421–1426. IEEE, 2021a.

Wu, H., Wang, C., Tyshetskiy, Y., Docherty, A., Lu, K., and Zhu, L. Adversarial Examples for Graph Data: Deep Insights into Attack and Defense. In *International Joint Conferences on Artifical Intelligence (IJCAI)*, pp. 4816–4823. IJCAI, 2019.

Wu, L., Lin, H., Tan, C., Gao, Z., and Stan.Z.Li. Self-supervised Learning on Graphs: Contrastive, Generative,or Predictive. *IEEE Transactions on Knowledge and Data Engineering*, 2021b.

Wu, Z., Xiong, Y., Yu, S. X., and Lin, D. Unsupervised Feature Learning via Non-Parametric Instance Discrimination. In *IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 3733–3742. IEEE, 2018.

Xi, Z., Pang, R., Ji, S., and Wang, T. Graph Backdoor. In *USENIX Security Symposium (USENIX Security)*. USENIX, 2021.

Xie, Y., Xu, Z., Wang, Z., and Ji, S. Self-Supervised Learning of Graph Neural Networks: A Unified Review. *IEEE Transactions on Knowledge and Data Engineering*, 2022.

Xing, E. P., Ng, A. Y., Jordan, M. I., and Russell, S. J. Distance Metric Learning with Application to Clustering with Side-Information. In *Annual Conference on Neural Information Processing Systems (NIPS)*, pp. 505–512. MIT Press, 2002.

Xu, K., Chen, H., Liu, S., Chen, P., Weng, T., Hong, M., and Lin, X. Topology Attack and Defense for Graph Neural Networks: An Optimization Perspective. In *International Joint Conferences on Artifical Intelligence (IJCAI)*, pp. 3961–3967. IJCAI, 2019a.

Xu, K., Hu, W., Leskovec, J., and Jegelka, S. How Powerful are Graph Neural Networks? In *International Conference on Learning Representations (ICLR)*, 2019b.

Yanardag, P. and Vishwanathan, S. V. N. Deep Graph Kernels. In *ACM SIGKDD International Conference on Knowledge Discovery and Data (SIGKDD)*, pp. 1365–1374. ACM, 2015.

You, J., Liu, B., Ying, Z., Pande, V. S., and Leskovec, J. Graph Convolutional Policy Network for Goal-Directed Molecular Graph Generation. In *Conference on Neural Information Processing Systems (NeurIPS)*, pp. 6412–6422, 2018a.

You, J., Ying, R., Ren, X., Hamilton, W. L., and Leskovec, J. GraphRNN: Generating Realistic Graphs with Deep Auto-regressive Models. In *International Conference on Machine Learning (ICML)*, pp. 5694–5703. PMLR, 2018b.

You, Y., Chen, T., Sui, Y., Chen, T., Wang, Z., and Shen, Y. Graph Contrastive Learning with Augmentations. In *Annual Conference on Neural Information Processing Systems (NeurIPS)*. NeurIPS, 2020.

Yu, N., Davis, L., and Fritz, M. Attributing Fake Images to GANs: Learning and Analyzing GAN Fingerprints. In *IEEE International Conference on Computer Vision (ICCV)*, pp. 7555–7565. IEEE, 2019.

Zeng, X., Wang, F., Luo, Y., gu Kang, S., Tang, J., C.Lightstone, F., F.Fang, E., Cornell, W., Nussinov, R., and Cheng, F. Deep Generative Molecular Design Reshapes Drug Discovery. *Cell Reports Medicine*, 2022.

Zhang, Z., Cui, P., and Zhu, W. Deep Learning on Graphs: A Survey. *IEEE Transactions on Knowledge and Data Engineering*, 2020.

Zhang, Z., Chen, M., Backes, M., Shen, Y., and Zhang, Y. Inference Attacks Against Graph Neural Networks. In *USENIX Security Symposium (USENIX Security)*. USENIX, 2022.

Zhu, Y., Xu, Y., Liu, Q., and Wu, S. An Empirical Study of Graph Contrastive Learning. *CoRR abs/2109.01116*, 2021a.

Zhu, Y., Xu, Y., Yu, F., Liu, Q., Wu, S., and Wang, L. Graph Contrastive Learning with Adaptive Augmentation. In *The Web Conference (WWW)*, pp. 2069–2080. ACM, 2021b.

A. Appendix

A.1. The Detailed Information of Graph Neural Networks

Graph Neural Networks (GNNs) have shown great effectiveness in fusing information from both the graph topology and node features (Zhang et al., 2020; Hamilton et al., 2017; Kipf & Welling, 2017). In recent years, they become the start-of-the-art technique as essential building blocks in graph generators and graph classification algorithms.

General Definition. Most of the GNNs learn the node representations for graph-structured data by a neighborhood aggregation strategy, where a model iteratively updates the representation of a node through message passing and aggregating representations of its neighbors. After k iterations of aggregation, we can get the node's representation h_v which stores the structural information within its k-hop neighborhood. Typically, the GNN contains multiple graph convolutional layers. The definition of each layer is as follows:

$$\mathbf{h}_v^k = \phi\left(\mathbf{h}_v^{k-1}, \psi\left(\mathbf{h}_v^{k-1}, \mathbf{h}_u^{k-1}\right)\right), \forall u \in \mathcal{N}(v), \quad (1)$$

where $\mathcal{N}(v)$ is a set of nodes adjacent to node v. $\mathbf{h}_v^{k-1}$ is the node embedding of node u after k iterations, $\psi\left(\mathbf{h}_v^{k-1}, \mathbf{h}_u^{k-1}\right)$ represents the message received from the neighbours, and $\phi(\cdot)$ is an aggregation operation.

Aggregator.. Recently, researchers have proposed different kinds of practical implementations of aggregation operations (Kipf & Welling, 2017; Hamilton et al., 2017; Chen et al., 2018; Xu et al., 2019b), among which the Graph Convolutional Networks (GCN) is the most representative method which uses the symmetric normalization method to aggregate all the information from the neighbors and shows great success (Kipf & Welling, 2017). The aggregation process of GCN can be defined as follows:

$$\mathbf{h}_v^k = \phi\left(\mathbf{h}_u^{k-1}, u \in \mathcal{N}(v) \cup v\right) = \sum_{u \in \mathcal{N}(v) \cup v} \mathbf{h}_j^{(k-1)} / \sqrt{d_u d_v} \quad (2)$$

where d_u and d_v are the node degrees of node u and v, respectively. Here $\phi(\cdot)$ is a mean aggregation operator.

Graph Pooling. After obtaining the embeddings of all nodes, we use a graph pooling operation to integrate the embeddings of all nodes in the graph to get the embedding of the whole graph. In our graph classification model, we use a straightforward but efficient approach called *mean pooling* that averages all the node embeddings to obtain the graph embedding, i.e., $\mathbf{h}_{\mathcal{G}} = \frac{1}{|\mathcal{V}|} \sum_{u \in \mathcal{V}} \mathbf{h}_u$.

A.2. The Detailed Information of Graph Generators

Traditional Graph Generator. Erdös-Rényi (ER) model (Erdös & Rényi, 1959) and Barabási-Albert (BA) model (Albert & Barabási, 2002) are two commonly used traditional graph generators. Given a few parameters, these generators can be explicitly expressed by formulas. ER model generates random graphs with a fixed number of nodes and edges. BA model is often used to generate scale-free graphs using a preferential attachment mechanism. That is, a new node will be added each time, and the edges will be randomly added to connect the new node and the existing nodes.

Autoencoder-based Generator. The autoencoder-based generator is a type of neural network which is used to learn the representations of unlabeled data and reconstruct the input graphs based on the representations. We consider VGAE (Kipf & Welling, 2016), Graphite (Grover et al., 2019), SBMGNN (Mehta et al., 2019), and GraphVAE (Simonovsky & Komodakis, 2018) in this paper. VGAE uses a graph convolutional network (GCN) as the encoder and the inner product as the decoder. The model can obtain the node features and capture the overall distribution of input graphs. Based on VGAE, Grover et al. proposed Graphite, a latent variable generative model which also utilizes GCN as the encoder. Unlike VGAE, Graphite adds a multi-layer iterative neural network before the inner product to construct the decoder. SBMGNN produces graphs by modeling sparse latent variables, which makes it competitive in preserving the community structure. It uses a sparse variational autoencoder (VAE) (Kingma & Welling, 2014) to model graphs. The decoder consists of a fast recognition model which models the probability of an edge exists between two nodes by a nonlinear function. GraphVAE is also an autoencoder based-model. It uses a feed-forward network with edge-conditioned graph convolutions (ECC) (Simonovsky & Komodakis, 2017) to encode the graphs into continuous representations. The main idea of the decoder is to output the probabilistic fully-connected graph and at last use a standard graph matching algorithm to align it to the original graph.

Autoregressive-based Generator. To capture the complex dependencies of all nodes and edges, autoregressive-based generators are proposed. An autoregressive-based generator adds nodes and edges sequentially. In this paper, we include GRAN (Liao et al., 2019) and GraphRNN (You et al., 2018b) as the Autoregressive-based model. GRAN generates a block of nodes and associated edges at each step. It uses GNN with attention to utilizing the topology of the generated part of the graph, which makes the GRAN model the dependencies between the already generated part and the newly generated part more effectively. GraphRNN uses two recurrent neural networks (RNN), which are called *graph-*

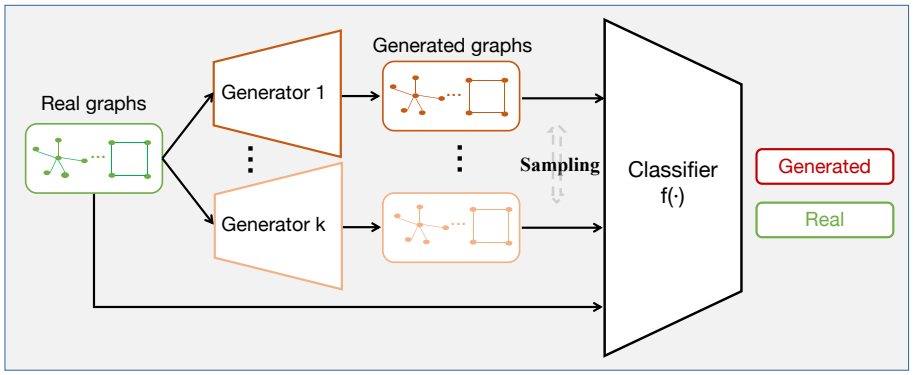


Figure 2: **The pipeline of generated graph detection.** The real graphs are from real-world datasets, and the generated graphs are generated by different graph generators based on real graphs. The GNN-based classifier is built to classify real graphs and generated graphs.

level RNN and *edge-level* RNN. The *graph-level* RNN is used to maintain the state of a generated graph and generate new nodes. The *edge-level* RNN is used to generate the edges between new nodes and the already existing graph.

A.3. The Implementation Details of Contrastive Learning-based Model

Training Contrastive Encoder. As one of the cutting-edge unsupervised representation learning models, contrastive learning aims at learning similar representations of the same data under different augmentations. It is widely used in visual representation learning (Chen et al., 2020; Wu et al., 2018; Hénaff, 2020) and graph embedding (Zhu et al., 2021a; You et al., 2020; Hassani & Ahmadi, 2020; Zhu et al., 2021b). In this paper, we use GraphCL (You et al., 2020) as the graph contrastive encoder.[2]

In the graph contrastive encoder, we first use the graph augmentation method to get two correlated augmented views $\hat{\mathcal{G}}_i$ and $\hat{\mathcal{G}}_j$ as a positive pair. We use node dropping as the first augmentation, and randomly select one augmentation from the augmentation pool as the second one. The augmentation pool consists of node dropping, edge perturbation, and subgraph. Then the $\hat{\mathcal{G}}_i$ and $\hat{\mathcal{G}}_j$ will be embedded by a GNN-based encoder f_θ. After that, a projection head $g(\cdot)$ is used to map the embeddings to a different latent space to calculate the contrastive loss. The projection head $g(\cdot)$ used in contrastive learning is a multi-layer perceptron (MLP). Then the contrastive loss function is used to maximize the agreement between the positive pairs. Here the loss function is the normalized temperature-scaled cross-entropy loss (NT-Xent) (Sohn, 2016; Wu et al., 2018).

When training the contrastive encoder, a mini-batch of N graphs will be randomly sampled and processed, which means that $2 * N$ augmented graphs and the corresponding loss need to be optimized each time. We denote the augmented nth graph in the mini-batch as $z_{n,i}$, $z_{n,j}$ and use them as the positive pairs. The negative pairs are generated by $z_{n,i}$, $z_{n,j}$ and other augmented graphs within the same mini-batch except for $z_{n,i}$, $z_{n,j}$. Finally, the NT-Xent for the nth graph is defined as follows:

$$\text{sim}\left(\boldsymbol{z}_{n,i}, \boldsymbol{z}_{n,j}\right) = \frac{\boldsymbol{z}_{n,i}^{\top} \boldsymbol{z}_{n,j}}{\|\boldsymbol{z}_{n,i}\| \, \|\boldsymbol{z}_{n,j}\|} \tag{3}$$

$$\text{Loss} = -\log \frac{\exp\left(\text{sim}\left(\boldsymbol{z}_{n,i}, \boldsymbol{z}_{n,j}\right)/\tau\right)}{\sum_{n'=1, n' \neq n}^{N} \exp\left(\text{sim}\left(\boldsymbol{z}_{n,i}, \boldsymbol{z}_{n',j}\right)/\tau\right)} \tag{4}$$

where $\text{sim}\left(\boldsymbol{z}_{n,i}, \boldsymbol{z}_{n,j}\right)$ means the cosine similarity of $z_{n,i}$, $z_{n,j}$. τ denotes the temperature parameter. After generating the loss for each graph in the mini-batch, the overall loss is computed across all the positive pairs in the mini-batch.

A.4. The Implementation Details of Metric Learning-based Model

Training Siamese Network. Figure 4 shows the workflow of the siamese network. Two graphs G_i and G_j are fed into the encoder f_θ one by one to get the embeddings h_i and h_j. In the siamese network, the paired samples are fed into the same encoder and the weights of them are shared. Then the L1 distance d between the two embeddings is calculated by the following equation.

$$d = abs(||h_i - h_j|\,|) \tag{5}$$

d is used to feed into the loss function and tune the network to get a better embedding. The loss function we used in this paper is called binary cross-entropy loss, which is commonly used in classification tasks. The equation of binary

[2]The source code of GraphCL is in https://github.com/Shen-Lab/GraphCL.

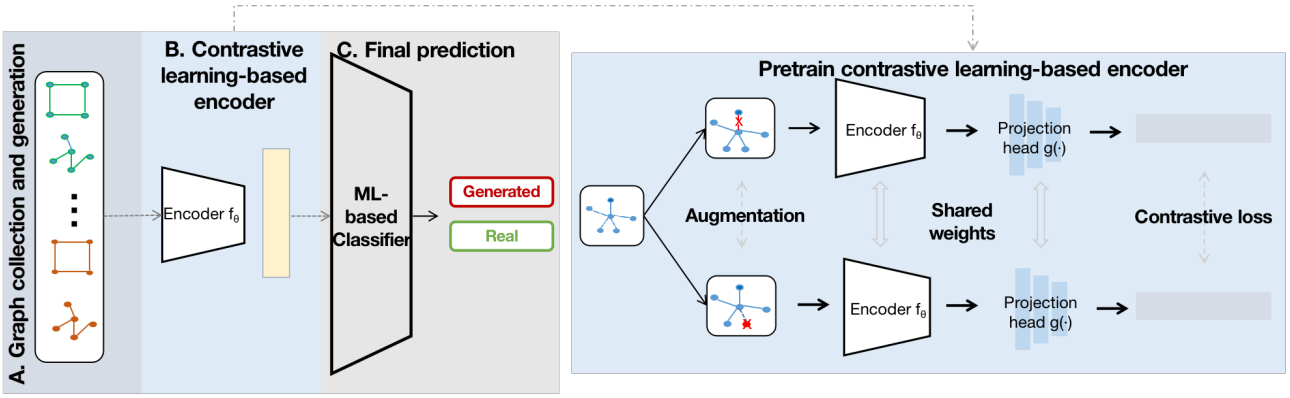


Figure 3: **The workflow of the contrastive learning-based model.** The model trains a contrastive encoder to embed the graphs and uses a machine learning-based classifier to do the final classification. The contrastive encoder is based on GraphCL (You et al., 2020), which uses the graph augmentation method to get two correlated augmented views as a positive pair and embed them with a GNN-based encoder $f(\cdot)$ and projection head $g(\cdot)$. Then the contrastive loss function is used to maximize the agreement between the positive pairs. After embedding all the graphs, we use support vector machines (SVM) to do the final prediction.

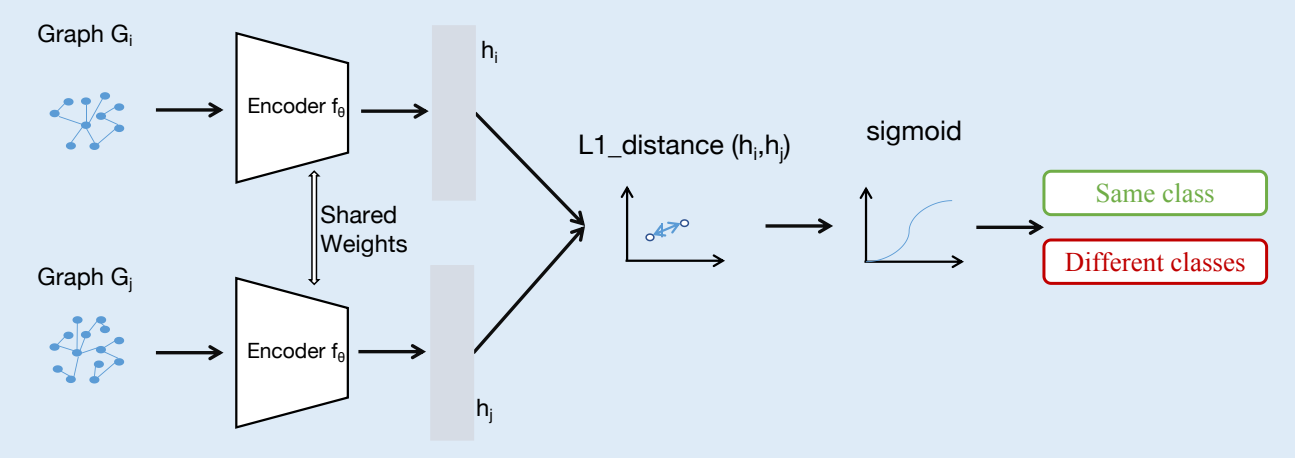


Figure 4: The workflow of the metric learning-based model. In this model, two graphs G_i and G_j are fed into the encoder f_θ one by one to get the embeddings h_i and h_j. The L1 distance between h_i and h_j are calculated and used to do the final prediction.

cross-equation loss is as follows:

$$\text{Loss} = -(y\log(p) + (1-y)\log(1-p)) \tag{6}$$

d is used to feed into the loss function and tune the network to get a better embedding. The loss function we used in this paper is called binary cross-entropy loss, which is commonly used in classification tasks.

To train the siamese network, we sample a training set that consists of Num_{ps} paired samples with the same label and Num_{ps} paired samples with different labels for each dataset.

A.5. Ablation Study

Different GNN Networks. Our end-to-end model uses GCN as the backbone. We replace it with GIN (Xu et al., 2019b) and GAT (Velickovic et al., 2018), and compare the performance of different backbones. We can see from Table 5 that in most of the time, GCN performs better than the others, thus we choose GCN as the final backbone of the end-to-end model in our experiment.

Metric Learning-based Model.. To achieve the best classification results of the metric learning-based model, we evaluate the impact of different N_{ps} and N_k on model performance. Here N_{ps} represents the number of paired sam-

Table 5: The accuracy of different backbones in end-to-end model.

Dataset	GAT	GIN	GCN
AIDS	0.89	0.88	0.89
Alchemy	0.88	0.86	0.87
Deezer	0.96	0.96	0.97
DBLP	0.86	0.82	0.84
Github	0.93	0.94	0.95
COLLAB	0.84	0.82	0.85
Twitch	0.91	0.91	0.92
Mixed	0.82	0.83	0.84

ples used to train the siamese network. N_k denotes the reference samples used to obtain the final prediction results.

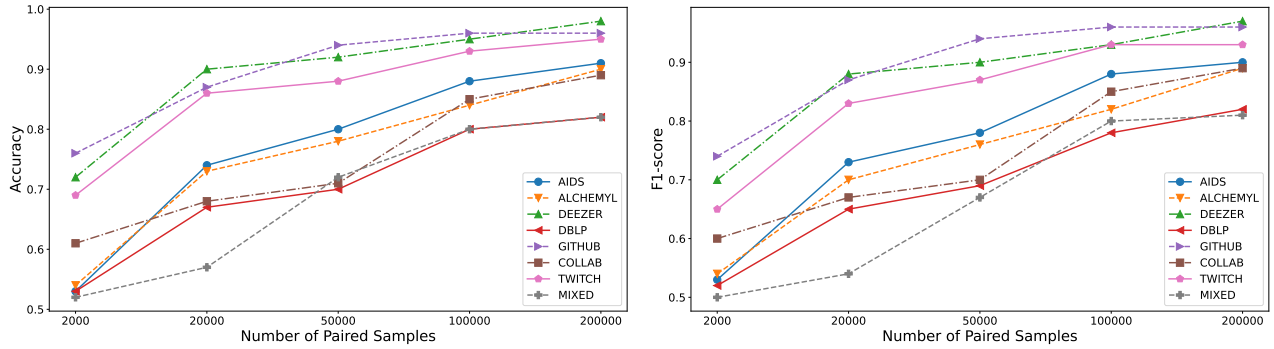
We can see from Figure 5 that if we use more paired samples to train the siamese network, the metric learning-based model tends to perform better. Due to time and resource limitations, we finally choose to use 20,000 paired samples to train the siamese network. Figure 6 shows that in general, the metric learning-based model shows the best performance when $N_k = 10$. Thus we use $N_k = 10$ in the following experiments.

A.6. Additional Results

In the appendix, plots are illustrated for additional information and experimental results as mentioned throughout the paper.

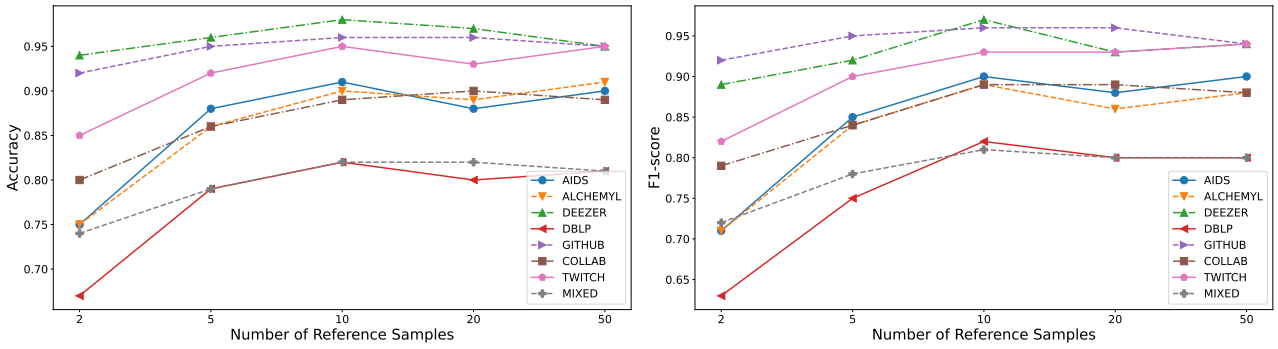
MMD Results. Table 6 shows the MMD results of real graphs and graphs generated by different generators.

The Visualization Results of Graphs Generated by Unseen Generators. Figure 7 shows the visualization results of three unseen generators (GraphRNN, GRAPHVAE, and SBMGNN) produced by the metric learning-based model.



(a) Accuracy (b) F1-score

Figure 5: **Different N_{ps}.** The impact of different numbers of paired samples on the metric learning-based model.

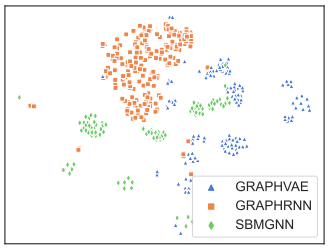


(a) Accuracy (b) F1-score

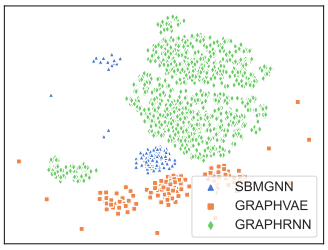
Figure 6: **Different N_k.** The impact of different numbers of reference samples on the metric learning-based model.

Table 6: The MMD results of real graphs and graphs generated by different generators.

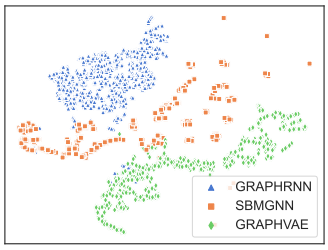
	ER	BA	graphite	VGAE	GRAN	GraghRNN	GraghVAE	sbmgnn
AIDS	0.0863	0.1070	0.0547	0.0324	0.0534	0.1016	0.0526	0.1884
Alchemy	0.0139	0.1167	0.0205	0.0088	0.0641	0.1493	0.0284	0.2844
Deezer	0.0356	0.1161	0.1869	0.2565	0.1168	0.0755	0.1167	0.1363
DBLP	0.0601	0.3117	0.0759	0.1168	0.4496	0.3835	0.1808	0.0238
Github	0.0249	0.2513	0.0398	0.0452	0.0315	0.1635	0.0314	0.0294
COLLAB	0.0270	0.0362	0.0092	0.0118	0.0024	0.0099	0.0021	0.0175
Twitch	0.0148	0.0336	0.0728	0.0589	0.0182	0.0663	0.0218	0.0681



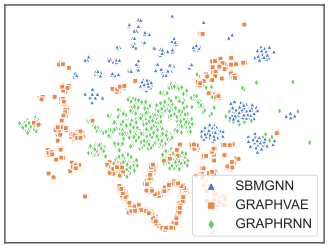
(a) AIDS



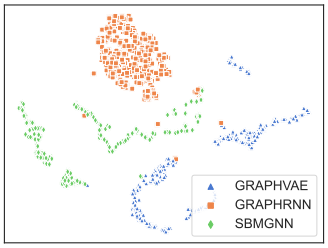
(b) Alchemy



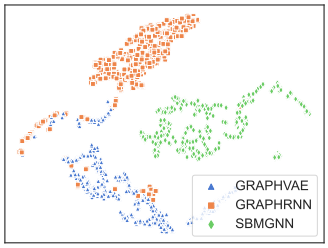
(c) Deezer



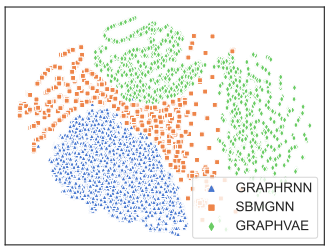
(d) DBLP



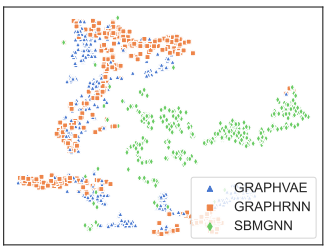
(e) Github



(f) COLLAB



(g) Twitch



(h) Mixed

Figure 7: The visualization results of graphs generated by unseen generators.