# ANOMALY DETECTION THROUGH CONDITIONAL DIF-FUSION PROBABILITY MODELING ON GRAPHS

Anonymous authors

004

010 011

012

013

014

015

016

017

018

019

021

023

025

026

027 028 029

030 031 Paper under double-blind review

### ABSTRACT

Existing Graph Neural Network-based anomaly detection methods suffer from over-smoothing issues during feature aggregation. Moreover, most existing methods are discriminative models that learn the boundaries between anomalous and normal data points, allowing malicious nodes in a dynamic adversarial environment to bypass detection boundaries. We propose an advanced Conditional Graph Anomaly Diffusion Model (CGADM) to model and capture the joint distribution of anomalies on the whole graph, thereby enabling generative graph anomaly detection. By iteratively refining node anomaly distributions during the denoising process, CGADM effectively mitigates over-smoothing and reconstructs obfuscated features by leveraging contextual neighborhood information. To avoid starting the diffusion process from a random state, CGADM introduces a priorguided denoising diffusion probability model. To circumvent the need for iterative denoising samplings for each node on large-scale graphs, we adopt a prior confidence-aware mechanism to dynamically adjust the reverse sampling steps for each node, significantly reducing the computationagl burden on large-scale graphs. We conducted experiments on CGADM using standard benchmarks, and the results demonstrated excellent performance in graph anomaly detection tasks. Ablation studies confirmed our framework's computational advantages.<sup>1</sup>

## 1 INTRODUCTION

Anomaly detection is aimed at identifying objects that deviate significantly from the majority within a vast array of objects. With the massive flow of information on Internet, it is inherently suitable to use the non-Euclidean graphs for modeling. Examples include social networks formed by users on social media, transaction networks formed by mobile payments, and bipartite graphs formed by users and contents. Consequently, graph anomaly detection (GAD) has emerged as a crucial research field, achieving successful applications, such as financial fraud detection (Huang et al., 2022; Dou et al., 2020), and telecommunication fraud detection (Yang et al., 2021), among others.

Among the methods employed for GAD, Graph Neural Networks (GNNs) have ascended to prominence, chiefly due to their exceptional capability to model topological structures. GNNs excel in 040 their iterative refinement of node representations, operating by focusing on a particular node and 041 aggregating attributes from neighboring nodes via the Message Passing (MP) paradigm (Kipf & 042 Welling, 2017; Hamilton et al., 2017; Velickovic et al., 2018; Xu et al., 2019). Subsequent to this 043 feature aggregation, node representations, now enriched with information from their neighboring 044 nodes, are fed into a classifier to determine whether they are outliers or anomalies. This process effectively leverages the power of GNNs in capturing high-order information within the graph, pro-046 viding a common paradigm for anomaly detection (Li et al., 2019; Wang et al., 2021; Liu et al., 2021b; Zhu et al., 2020; He et al., 2021). 047

However, discriminative models based on feature aggregation exhibit inherent shortcomings. From
 a topology-level perspective, vanilla GNNs suffer from the over-smoothing problem. As a low pass filter, GNNs with feature aggregation tend to average the representations of anomalies, making
 them less distinguishable. As illustrated in the left part of Figure 1, some fraudulent nodes can ma nipulate their representations by intentionally connecting with a large number of carefully selected

<sup>&</sup>lt;sup>1</sup>The code is available on https://github.com/CGADManonymous/CGADM

neighbors. For instance, in money laundering transactions, fraudsters can distribute transactions or
 create numerous interactions with bot accounts to blend in with the crowd. From a feature-level
 perspective, discriminative models perform anomaly detection by learning the boundaries between
 anomalous and normal data points. This approach may lead to a lack of generalization, as fraudulent
 nodes always co-evolve with the detection system. By continuously obfuscating their node features,
 these deceptive entities can cross the classifier's boundary and masquerade as normal nodes.

060 To address these issues, contemporary research can be summarized along two lines. The first line of 061 work focuses on enhancing the generalizability of GNN models, such as applying attention mech-062 anisms (Wang et al., 2019a; Liu et al., 2021a), designing auxiliary losses (Zhao et al., 2022), and 063 utilizing contrastive learning (Chen et al., 2023a). The second line of work involves leveraging gen-064 erative models, such as Generative Adversarial Networks (GANs), to perform data augmentation, thereby enriching the diversity of training samples (Chen et al., 2020b). However, these methods 065 primarily focus on enhancing the discriminative boundary for each individual node, rather than con-066 sidering the interdependencies of node anomalies from a holistic graph perspective. Inspired by 067 the recent powerful capabilities of diffusion models (DMs) in generating high-dimensional data, 068 such as high-resolution images (Dhariwal & Nichol, 2021), we propose the use of diffusion models 069 to model the joint distribution of anomaly on the whole graph, capturing the the interdependencies of node anomalies. To address topology-level flaw, we leverage the iterative refinement of 071 diffusion models. Instead of increasing GNN depth to aggregate distant information, which risks 072 over-smoothing, our approach applies GNN-based denoiser within each denoising iteration to refine 073 anomaly modeling. Each iterative refinement step incorporates neighborhood information while pre-074 serving node-specific high-frequency anomaly information via a residual propagation mechanism, 075 thereby preventing oversmoothing and effectively capturing long-range dependencies. To address feature-level flaw, we leverage the denoising reconstruction of diffusion models. This reconstruc-076 tion process ensures that even when malicious nodes disguise their features to blend in with normal 077 nodes, their underlying anomaly patterns can be recovered.

To achieve these goal, we need to address two notable challenges, as shown in right part of Figure 1:

Effectiveness. Traditional denoising models have primarily focused on unconditional generative modeling (Song & Ermon, 2019; Song et al., 2021b; Ramesh et al., 2022). While many tasks in the image or video domain have introduced guided-diffusion models to generate high-resolution photo-realistic images that match the semantic meanings or content of the label, text, or corrupted images, most work in the graph domain has started generating from white noise or empty or fully connected graphs. However, for anomaly detection on graphs, due to various deceptive and obfuscating tactics employed by anomalous nodes, directly recovering the underlying true distribution from a random noise distribution may not yield satisfactory results.

- Efficiency. The reverse process of DMs requires numerous iterative denoising samplings (Yi et al., 2023; Chen et al., 2023b). Existing graph diffusion models utilize a GNN-based encoder to update all nodes at time step t during each iterative refinement to obtain the nodes at time step t - 1. While this approach is feasible for standard graph generation tasks, it becomes computationally prohibitive for anomaly detection tasks on extremely large graphs. Performing such iterative operations generation across potentially millions of nodes in the entire graph can significantly increase computational overhead, thereby affecting the practical applicability of the algorithm.
- In this paper, we propose a novel <u>Conditional Graph Anomaly Diffusion Model</u> (CGADM) for graph anomaly detection to address the aforementioned challenges synergistically.

To tackle the effectiveness issue, we propose a prior-guided diffusion process, which injects a pretrained conditional anomaly estimator into both the forward and reverse diffusion chains. This approach constructs a denoising diffusion probabilistic model for more accurate anomaly detection. Specifically, we introduce a lightweight model to estimate an anomaly prior for each node, serving as the endpoint for our forward noise addition process and the starting point for our reverse denoising process. Based on this new probabilistic model, we redesign the probability model and optimization objective of our CGADM.

To tackle the efficiency issue, we build on the intuition that normal nodes are generally farther
 from the decision boundary compared to anomalous nodes that have narrowly evaded detection.
 Therefore, in the reverse process, we introduce a prior confidence-aware mechanism to adaptively
 determine the reverse time step for each node. Nodes with high confidence in their anomaly prior

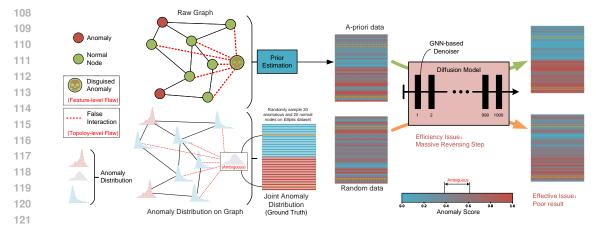


Figure 1: An illustration of Generative Graph Anomaly Detection.

require fewer time steps, while those with lower confidence require more sampling time steps. To facilitate inference over arbitrary numbers of steps, we propose a conditional non-Markovian reverse process, and derive its closed-form expression within the framework of the CGADM. This approach not only accurately estimates the anomaly probability for each node but also reduces the number of predictions in the reverse process, thereby decreasing computational time.

Our main contributions can be summarized as follows:

- We innovatively propose CGADM, which employs a prior-guided denoising diffusion probabilistic model to capture the joint distribution of anomalies on the whole graph, thereby enabling generative graph anomaly detection.
- We propose a prior confidence-aware mechanism to dynamically allocate disparate sampling time steps during the inference process. In support of this mechanism, we derive a conditional non-Markovian reverse process within the framework of the CGADM. This approach significantly mitigates the computational burden associated with anomaly detection in large-scale graphs.
- Through experiments on benchmarks for graph anomaly detection, CGADM achieves state-ofthe-art results. Additional studies confirm the computational advantages of our framework.
- 139 140 141

142 143

144

122

123

129

130

131

132

133 134

135

136

137 138

2 RELATED WORK

## 2.1 GRAPH ANOMALY DETECTION

145 Graph anomaly detection (Duan et al., 2023) aims to identify nodes that deviate significantly from 146 most other nodes. FdGars (Wang et al., 2019b) utilized a predefined tagging system to classify 147 users according to their content and behavioral characteristics, and employed a multi-layered GNN to identify fraudulent users. CARE-GNN (Dou et al., 2020) proposed to adjust the threshold in 148 the process of aggregating neighbors through reinforcement learning, thereby addressing the incon-149 sistency issue. FRAUDRE (Zhang et al., 2021) aggregates different relational neighbors of nodes 150 by applying an imbalanced loss function, addressing the class imbalance problem. PC-GNN (Liu 151 et al., 2021b) resolves the class imbalance issue by selecting training nodes using a label-balanced 152 sampler. AMNet (Chai et al., 2022) captures features of normal and abnormal frequency bands 153 using a dual filter based on Bernstein polynomials and aggregates them through an attention mech-154 anism. BWGNN (Tang et al., 2022) adopts a Beta-kernel-based GNN model, effectively dealing 155 with abnormal high-frequency features by applying multiple filters to various frequency bands. 156 GHRN (Gao et al., 2023b) eliminates harmful heterogeneous connections on any qualified fraud 157 detection model through approximating pre-training labels. Recent advancements in graph anomaly 158 detection have tackled various challenges. Gao et al. (2023a) addressed structural distribution shifts 159 through feature-specific constraints in Graph Decomposition Networks (GDN), while Xu et al. (2024) proposed SEC-GFD to handle heterophily and label imbalance via spectral filtering. Qiao 160 et al. (2024) introduced a semi-supervised generative framework (GGAD) that leverages labeled 161 normal nodes to generate pseudo-anomalies, and He et al. (2024) developed ADA-GAD to mitigate anomaly overfitting through anomaly-denoised graph augmentation. Unlike these methods, our CGADM adopts a novel generative diffusion approach to model the joint anomaly distribution over the graph, enabling holistic and scalable anomaly detection without reliance on augmentation strategies.

However, the aforementioned methods predominantly rely on discriminative models based on feature aggregation, which are susceptible to the over-smoothing problem inherent in GNNs and the camouflage deception of fraudulent nodes. We departs from this traditional perspective and proposes a novel generative model to jointly model the anomaly distribution of each node on the graph.

170 171 172

## 2.2 DIFFUSION MODEL

173 Denoising diffusion probabilistic models (DDPMs) (Ho et al., 2020; Song et al., 2021a), or simply 174 diffusion models, are a class of probabilistic generative models that transform noise into data sam-175 ples, hence primarily used for generative tasks (Dhariwal & Nichol, 2021; Rombach et al., 2022). 176 Diffusion-based generative models have demonstrated strong capabilities in generating high-quality graphs (Niu et al., 2020; Liu et al., 2019; Jo et al., 2022; Haefeli et al., 2022; Chen et al., 2022; 177 Vignac et al., 2023; Kong et al., 2023). Haefeli et al. (2022) designed a model limited to graphs 178 without attributes and similarly observed the benefits of discrete diffusion for graph generation. Pre-179 vious graph diffusion models were based on Gaussian noise. Niu et al. (2020) generated adjacency matrices indicating the presence of edges by thresholding continuous values, while Jo et al. (2022) 181 extended this model to handle node and edge attributes. Digress (Vignac et al., 2023) was the first 182 to propose a discrete diffusion model for graphs. Regarding the severe label imbalance problem 183 in anomaly detection, many existing anomaly detection methods improve datasets by generating 184 synthetic anomalies (Chen et al., 2020b; Ding et al., 2020), creating a more balanced environment.

We approaches from a different angle, using diffusion models to model the distribution of anomalies on large-scale graphs for more precise and robust anomaly detection. To the best of our knowledge, there is currently no work on modeling the distribution of anomalies based on diffusion models.

#### 189 190 3 PRELIMINARIES

191

**Attributed Graph** We typically characterize an attributed graph as  $\mathcal{G} = \{\mathcal{V}, \mathcal{E}, \mathbf{X}\}$ , where  $\mathcal{V} = \{v_1, v_2, \ldots, v_N\}$  represents the set of all N nodes on graph  $\mathcal{G}$ , and  $\mathcal{E} = \{e_{ij} | v_i, v_j \in \mathcal{V}\}$  signifies the set of edges, indicating the existence of an edge between nodes  $v_i$  and  $v_j$ . For each node  $v_i$ , there exists a *d*-dimensional feature vector,  $x_i \in \mathbb{R}^d$ . The feature vectors of all nodes together form the feature matrix of the graph, denoted as  $\mathbf{X} = [x_1, x_2, \ldots, x_N] \in \mathbb{R}^{N \times d}$ . For convenience, An adjacency matrix  $\mathbf{A}$  records the relationships between nodes on graph  $\mathcal{G}$ . Each entry  $\mathbf{A}_{ij} = 1$  if there exists  $e_{ij} \in \mathcal{E}$ , otherwise,  $\mathbf{A}_{ij} = 0$ . Additionally, the degree matrix  $\mathbf{D} \in \mathbb{N}^{N \times N}$  is a diagonal matrix, in which each entry  $\mathbf{D}_{ii}$  denotes the number of nonzero entries in the *i*-th row of  $\mathbf{A}$ .

Anomaly Detection on Graph Consider two disjoint subsets of  $\mathcal{V}$ , namely  $\mathcal{V}_a$  and  $\mathcal{V}_n$ , such that  $\mathcal{V}_a \cap \mathcal{V}_n = \emptyset$ .  $\mathcal{V}_a$  contains all nodes labeled as anomalous, and  $\mathcal{V}_n$  comprises all normal nodes. The goal of graph anomaly detection (GAD) is to compute anomaly probability  $p(\mathbf{y}|\mathcal{E}, \mathbf{X})$  of the unlabeled nodes with partial node labels. Please refer Appendix E for challenges of GAD.

**Diffusion Probabilistic Model** To construct an efficient diffusion model, it must satisfy three key properties: (1) The conditional distribution  $q(z_t|x)$  should possess a closed-form equation to circumvent the recursive application of noise during training. (2) The posterior  $q(z_{t-1}|z_t, x)$  should also have a closed-form solution to serve as the neural network's target. (3) The limiting distribution  $q_{\infty} = \lim_{T \to \infty} q(z_T|x)$  should be independent of x, enabling its use as a prior distribution for inference. These properties are all met when the noise follows a Gaussian distribution. The common steps in the diffusion model are shown in Appendix A.

211

## 4 Methodology

212 213

214 We formulate the GAD problem as a task of modeling the joint conditional distribution of anoma-215 lies on the graph. Given an attributed graph, a lightweight mean estimator is used to compute a 216 prior distribution of the anomaly. This prior distribution serves as the endpoint for adding noise and the starting point for inference. CGADM gradually transforms the ground truth anomaly dis tribution into the prior distribution instead of the conventional Guassian distribution. By utilizing
 a topological-guided denoising network, CGADM is capable of simultaneously modeling the topo logical information and features of nodes to iteratively recover the ground truth. To expedite the
 inference process, we introduce a prior-aware strided sampling strategy. To enable inference over
 arbitrary numbers of steps, we propose a conditional non-Markovian reverse process.

### 4.1 DIFFUSE GROUND TRUTH TO PRIOR

In light of Section 3, we propose to cast the graph anomaly detection problem as a generative task. We set  $\mathbf{y}_0$  as the anomaly ground truth and  $\mathbf{y}_{1:T}$  as the intermediate predictions generated in the forward process of the diffusion model. The objective of graph anomaly detection then becomes the maximization of the log-likelihood  $p(\mathbf{y}_0|\mathcal{E}, \mathbf{X})$ . Consequently, Equation 2 can be restructured as the following Conditional Evidence Lower Bound (CELBO) to serve as our new optimization target:

$$\log p_{\theta}(\mathbf{y}_{0}|\mathcal{E}, \mathbf{X}) = \log \int p_{\theta}(\mathbf{y}_{0:T}|\mathcal{E}, \mathbf{X}) d\mathbf{y}_{1:T} \ge \mathbb{E}_{q(\mathbf{y}_{1:T}|\mathbf{y}_{0}, \mathcal{E}, \mathbf{X})} \left[ \log \frac{p_{\theta}(\mathbf{y}_{0:T}|\mathcal{E}, \mathbf{X})}{q(\mathbf{y}_{1:T}|\mathbf{y}_{0}, \mathcal{E}, \mathbf{X})} \right],$$
(1)

where  $p_{\theta}(\mathbf{y}_{0:T}|\mathcal{E}, \mathbf{X})$  is the joint distribution of the target and the predictions under the denoising model parameters  $\theta$ , and  $q(\mathbf{y}_{1:T}|\mathbf{y}_0, \mathcal{E}, \mathbf{X})$  is the conditional distribution of forward or diffusion process given the ground truth and the input data.

By substituting Equation 1 into Equation 16, we can express our optimization objective as follows:

$$\mathcal{L} = \mathbb{E}_{q} \left[ -\log p_{\theta}(\mathbf{y}_{0} | \mathbf{y}_{1}, \mathcal{E}, \mathbf{X}) \right] + \mathbb{E}_{q} \left[ \mathbb{D}_{KL} \left( q(\mathbf{y}_{T} | \mathbf{y}_{0}, \mathcal{E}, \mathbf{X}) \| p(\mathbf{y}_{T} | \mathcal{E}, \mathbf{X}) \right] \right.$$

$$+ \sum_{t=2}^{T} \mathbb{E}_{q} \left[ \mathbb{D}_{KL} \left( q(\mathbf{y}_{t-1} | \mathbf{y}_{t}, \mathbf{y}_{0}, \mathcal{E}, \mathbf{X}) \| p_{\theta}(\mathbf{y}_{t-1} | \mathbf{y}_{t}, \mathcal{E}, \mathbf{X}) \right].$$

$$(2)$$

237 238 239

253

256 257

259

260

261

264 265

267

268 269

222

223 224

230

234

235 236

Following the conventions of Denoising Diffusion Probabilistic Models (DDPM) (Ho et al., 2020), we respectively name the first, second, and third terms of the above objective function as the reconstruction term  $\mathcal{L}_{recon}$ , the prior matching term  $\mathcal{L}_{prior}$ , and the consistency term  $\mathcal{L}_{con}$ .

To avoid our CGADM recovering the joint anomaly distribution starting from random noise (Han et al., 2022b), we modify the endpoint of the diffusion process from the conventional Guassian distribution N(0, I) to:

$$p(\mathbf{y}_T | \mathcal{E}, \mathbf{X}) = N(g_\phi(\mathcal{E}, \mathbf{X}), I), \tag{3}$$

where  $g_{\phi}(\mathcal{E}, \mathbf{X})$  is a parameterized network pretrained on training set D to estimate the mean value of the final normal distribution. By doing so, we effectively utilize the condition  $\mathcal{E}, \mathbf{X}$  in the distribution  $p(\mathbf{y}_T | \mathcal{E}, \mathbf{X})$  to help us establish a prior understanding of the joint anomaly distribution.

The prior matching term  $\mathcal{L}_{prior}$  is a parameter-free term. In order to make it close to zero, we need to adjust the forward process in combination with the calculation of the prior  $g_{\phi}(\mathcal{E}, \mathbf{X})$ . Following the practice of Pandey et al. (2022), we define the noise-adding process at each step as follows:

$$q(\mathbf{y}_t|\mathbf{y}_{t-1}, g_{\phi}(\mathcal{E}, \mathbf{X})) = \mathcal{N}(\mathbf{y}_t; \sqrt{1 - \beta_t} \mathbf{y}_{t-1} + (1 - \sqrt{1 - \beta_t}) g_{\phi}(\mathcal{E}, \mathbf{X}), \beta_t I),$$
(4)

where  $\mathcal{N}$  represents the Gaussian Distribution, and  $\beta_t \in (0,1)$  regulates the noise scales added at step t. This noise-adding step allows for a closed-form sampling distribution at any arbitrary timestep t, according to the additivity of the Gaussian distribution:

$$q(\mathbf{y}_t|\mathbf{y}_0, \mathcal{E}, \mathbf{X}) = q(\mathbf{y}_t|\mathbf{y}_0, g_\phi(\mathcal{E}, \mathbf{X})) = \mathcal{N}(\mathbf{y}_t; \sqrt{\bar{\alpha}_t}\mathbf{y}_0 + (1 - \sqrt{\bar{\alpha}_t})g_\phi(\mathcal{E}, \mathbf{X}), (1 - \bar{\alpha}_t)I),$$
(5)

where  $\alpha_t := 1 - \beta_t$  and  $\bar{\alpha}_t := \prod_t \alpha_t$ . This sampling distribution enables  $\mathcal{L}_{prior}$  to be close to zero when t = T. Intuitively, the noise-adding process defined by Equation 5 can be interpreted as an interpolation between the true data  $\mathbf{y}_0$  and the estimated prior  $g_{\phi}(\mathcal{E}, \mathbf{X})$ , which exhibits a gradual transition from the true data towards the estimated prior over the course of the forward process.

With the above formulation, we can derive a tractable posterior that serves as the target for our denoising network. It can be expressed as follows:

$$q(\mathbf{y}_{t-1}|\mathbf{y}_t, \mathbf{y}_0, \mathcal{E}, \mathbf{X}) = q(\mathbf{y}_{t-1}|\mathbf{y}_t, \mathbf{y}_0, g_{\phi}(\mathcal{E}, \mathbf{X})) = \mathcal{N}\left(\mathbf{y}_{t-1}; \tilde{\mu}(\mathbf{y}_t, \mathbf{y}_0, g_{\phi}(\mathcal{E}, \mathbf{X})), \tilde{\beta}_t \mathbf{I}\right),$$
(6)

where  $\tilde{\mu} := \gamma_0 \mathbf{y}_0 + \gamma_1 \mathbf{y}_t + \gamma_2 g_\phi(\mathcal{E}, \mathbf{X})$  and  $\tilde{\beta}_t := \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t} \beta_t$ , with:

$$\gamma_0 = \sqrt{\beta_t \bar{\alpha}_{t-1}}, \quad \gamma_1 = \frac{(1 - \bar{\alpha}_{t-1})\sqrt{\alpha_t}}{(\alpha_t - 1)(\sqrt{\alpha_t} + \sqrt{\bar{\alpha}_{t-1}})}, \quad \gamma_2 = \frac{1}{1 - \bar{\alpha}_t}.$$
(7)

For detailed derivation, please refer to Appendix B.

#### 270 4.2 TOPOLOGICAL-GUIDED DENOISING NETWORK 271

275 276

286 287

288

298

302 303

304

317 318

321 322

272 According to Equation 4, we define  $p_{\theta}(\mathbf{y}_{t-1}|\mathbf{y}_t, \mathcal{E}, \mathbf{X})$  as  $N(\mathbf{y}_{t-1}; \mu_{\theta}(\mathbf{y}_t, t, \mathcal{E}, \mathbf{X}), \Sigma_{\theta}(\mathbf{y}_t, t, \mathcal{E}, \mathbf{X}))$ for  $1 < t \leq T$ . Following the setup of DDPM, we set  $\Sigma_{\theta}(\mathbf{y}_t, t, \mathcal{E}, \mathbf{X}) = \sigma_t^2 \mathbf{I}$  to untrained time-273 dependent constants and set  $\sigma_t^2 = \tilde{\beta}_t$ . For the parameterization, we may select: 274

$$\mu_{\theta}(\mathbf{y}_{t}, t, \mathcal{E}, \mathbf{X}) = \frac{1}{\sqrt{\alpha_{t}}} (\mathbf{y}_{t} - \frac{\beta_{t}}{\sqrt{1 - \bar{\alpha}_{t}}} \epsilon_{\theta}(\mathbf{y}_{t}, t, \mathcal{E}, \mathbf{X})),$$
(8)

277 where  $\epsilon_{\theta}$  is a parameterized network intended to predicts the forward diffusion noise  $\epsilon$  sampled for 278 anomaly scores  $\mathbf{y}_t$ . 279

An anomalous node is typically strongly correlated not only with its node features but also with the 280 its local topological structure. The bias brought about by a few anomalous nodes is high-frequency 281 information in the frequency domain. Most existing GNNs act as low-pass filters and cannot ef-282 fectively capture the high-frequency signals carried by anomalous nodes. Borrowing the idea from 283 GCNII (Chen et al., 2020a), we adopt a residual propagation mechanism that prevents the high-284 frequency information of nodes from being overlooked due to over-smoothing in the multi-layer graph convolution process: 285

$$\mathbf{h}_{v}^{l} = \sigma \left( \mathbf{W}^{l-1} \left( \mathbf{h}_{v}^{l-1} - \frac{1}{|\mathcal{N}(v)|} \sum_{u \in \mathcal{N}(v)} \mathbf{h}_{u}^{l-1} \right) \right), \quad \mathbf{h}^{final} = AGG(\mathbf{h}_{v}^{0}, \mathbf{h}_{v}^{1}, \dots, \mathbf{h}_{v}^{L}), \tag{9}$$

289 where L is the number of graph convolution layers and  $AGG(\cdot)$  can be a simple aggregation function such as summation or concatenation. With this message-passing mechanism, we define our 290 topological-aware denoising network as  $\epsilon_{\theta}(\mathbf{y}_t, t, \mathcal{E}, \mathbf{X}) = \epsilon_{\theta}(\mathbf{y}_t, t, \mathbf{H}^{final})$ . For more details about 291 the denoising network, please refer to Appendix G. 292

293 To execute our training, we sample  $y_t$  according to Equation 5. Through the reparameterization 294 trick, we can derive: 295

$$\mathbf{y}_t = \sqrt{\bar{\alpha}_t} \mathbf{y}_0 + (1 - \sqrt{\bar{\alpha}_t}) g_\phi(\mathcal{E}, \mathbf{X}) + \sqrt{1 - \bar{\alpha}_t} \epsilon.$$
(10)

296 We simplify  $\mathcal{L}_{recon}$  and  $\mathcal{L}_{con}$  to obtain the final loss  $\mathcal{L}$  as follows: 297

$$\mathcal{L}_{\epsilon} = ||\epsilon - \epsilon_{\theta}(\sqrt{\bar{\alpha}_{t}}\mathbf{y}_{0} + (1 - \sqrt{\bar{\alpha}_{t}})g_{\phi}(\mathcal{E}, \mathbf{X}) + \sqrt{1 - \bar{\alpha}_{t}}\epsilon, t, \mathcal{E}, \mathbf{X})||^{2}$$
(11)

299 Where elements in t is uniformly distributed between 1 and T. The case of t = 1 corresponds to 300  $\mathcal{L}_{recon}$ . Similar to DDPM, the cases where t > 1 correspond to an unweighted version of  $\mathcal{L}_{con}$ . The 301 whole process of training is shown in Appendix H.

#### 4.3 INFERENCE FOR ANOMALY DETECTION

In image synthesis tasks, DMs draw random Gaussian noises for reverse generation, and the gener-305 ation results are guided by a pre-trained classifier or other signals such as textual queries. However, 306 for generating anomaly scores on graphs, due to various deceptive and obfuscating tactics employed 307 by anomalous nodes, generating directly from pure noise may not yield accurate anomaly detection 308 results. Therefore, we propose a simple inference strategy that aligns with the CGADM training for 309 anomaly inference, which is shown in Algorithm 1. 310

#### 4.4 PRIOR-AWARE STRIDED SAMPLING 311

312 As can be seen from Equation 11, our training actually results in a topological-aware denoising 313 network capable of denoising the predicted prior score at arbitrary time step t. Inspired by Song et al. (2021a), we can use this denoising network to perform time-step skipping sampling, greatly 314 reducing the number of sampling steps. By discarding the Markov constraint brought by Equation 4, 315 we can obtain the conditional non-Markovian reverse process different from Equation 6 as follows: 316

$$\mathbf{y}_{t-1} = \sqrt{\bar{\alpha}_{t-1}} \hat{\mathbf{y}}_0 + (1 - \sqrt{\bar{\alpha}_{t-1}}) g_{\phi}(\mathcal{E}, \mathbf{X}) + \sqrt{1 - \bar{\alpha}_{t-1} - \sigma_t^2 \epsilon_{\theta}(\mathbf{y}_t, t, \mathcal{E}, \mathbf{X})} + \sigma_t \epsilon_t$$
(13)

where  $\hat{\mathbf{y}}_0$  is the denoised score in Equation 12. For detailed derivation, please refer to Appendix C. 319 By substituting Equation 12 into Equation 13, we can obtain: 320

$$\mathbf{y}_{t-1} = \sqrt{\frac{\bar{\alpha}_{t-1}}{\bar{\alpha}_t}} \left( \mathbf{y}_t - (1 - \sqrt{\bar{\alpha}_t}) g_{\phi}(\mathcal{E}, \mathbf{X}) - \sqrt{1 - \bar{\alpha}_t} \epsilon_{\theta}(\mathbf{y}_t, t, \mathcal{E}, \mathbf{X}) \right) \\ + (1 - \sqrt{\bar{\alpha}_{t-1}}) g_{\phi}(\mathcal{E}, \mathbf{X}) + \sqrt{1 - \bar{\alpha}_{t-1} - \sigma_t^2} \epsilon_{\theta}(\mathbf{y}_t, t, \mathcal{E}, \mathbf{X}) + \sigma_t \epsilon_t, \tag{14}$$

	Initialize $\mathbf{y}_T \sim \mathcal{N}(g_{\phi}(\mathcal{E}, \mathbf{X}), I)$ for $t = T$ to 1 do	
2. 3:		
	$\hat{\mathbf{y}}_0 = rac{1}{\sqrt{ar{lpha}_t}} \left( \mathbf{y}_t - (1 - \sqrt{ar{lpha}_t}) g_{\phi}(\mathcal{E}, \mathbf{X}) - \sqrt{1 - ar{lpha}_t} \epsilon_{ heta}(\mathbf{y}_t, t, \mathcal{E}, \mathbf{X})  ight)$	(12)
	$\sqrt{\alpha_t}$	
4:	if $t > 1$ then	
5:	Draw $z \sim \mathcal{N}(0, I)$	
6:	$\mathbf{y}_{t-1} = \gamma_0 \hat{\mathbf{y}}_0 + \gamma_1 \mathbf{y}_t + \gamma_2 g_{\phi}(\mathcal{E}, \mathbf{X}) + \tilde{\beta}_t z$ , according to Equation 6.	
7:		
8:	Set $\mathbf{y}_{t-1} = \hat{\mathbf{y}}_0$	
9:	end if	
10:	end for	
11:	return $y_0$	

This allows the use of a forward process defined only on a subset of the latent variables  $\mathbf{y}_{\tau_1}, \dots, \mathbf{y}_{\tau_t}$ where  $\tau_1, \dots, \tau_t$  is an increasing subsequence of 1, ..., *T* with length *S*, where *S* could be much smaller than *T*. To reduce the number of sampling steps from *T* to *K*, we use *K* evenly spaced real numbers between 1 and *T* (inclusive), and then round each resulting number to the nearest integer, as follows:  $\{\tau_i\}_{i=1}^K = \left\{1 + \frac{(T-1)(i-1)}{K-1}\right\}_{i=1}^K$ .

Intuitively, when our prior is more confident, our model can use fewer sampling steps, or a smaller *K*, and vice versa. We propose a heuristic strategy to dynamically adjust the size of *K* according to the confidence of different prior scores of anomalies. We choose the inverse sigmoid function to simulate the decay of the ratio as the confidence  $|_{\phi}(\mathcal{E}, \mathbf{X}) - 0.5|$  increases:

$$K = \frac{r}{1 + \exp\left(\frac{|g_{\phi}(\mathcal{E}, \mathbf{X}) - 0.5|}{0.5}\right)} \times T \tag{15}$$

Typically, with r set to 2, our framework adjusts the sampling steps K to around 1000 for ambiguous priors near 0.5, and reduces it to about 500 for high-confidence priors close to 1. Notably, most nodes on the graph are associated with high prior confidence, which leads to a substantial decrease in computational demand. Conversely, for anomalous nodes that are adept at camouflage, the lower prior confidence necessitates a larger number of diffusion steps, facilitating their accurate detection. Our method thus strikes a balance between computational efficiency and thorough identification. We show the inference process with our prior-aware strided sampling in Appendix I.

5 EXPERIMENTS

338 339

350

351 352 353

354

355

356

357

358

359 360

361 362

364

#### 5.1 EXPERIMENTAL SETUP

Datasets We have extensively employed five diverse datasets from various domains to verify our method. They are the e-finance category dataset Elliptic (Weber et al., 2019), crowd-sourcing category datasets Tolokers (Platonov et al., 2023) and YelpChi (Rayana & Akoglu, 2015), and Social media datasets Question (Platonov et al., 2023) and Reddit (Kumar et al., 2019). For the detail of dataset statistics and processing, please refer to Appendix F.

Baselines We have compared our CGADM with two categories of methods in the context of graph
anomaly detection: (1) Standard GNNs, which include GCN (Kipf & Welling, 2017), GIN (Xu
et al., 2019), GraphSAGE (Hamilton et al., 2017), and GAT (Velickovic et al., 2018), and (2) GNNs
specifically designed for anomaly detection, such as GAS (Li et al., 2019), PCGNN (Liu et al., 2021b), BWGNN (Tang et al., 2022), and GHRN (Gao et al., 2023b). For detailed descriptions of
these methods, please refer to Appendix D.

376 Metrics Following the evaluation setup employed by most anomaly detection works (Han et al., 2022a), we have chosen the Area Under the Receiver Operating Characteristic Curve (AUROC) and the Area Under the Precision-Recall Curve (AUPRC) as our metrics for graph anomaly detection.

Both of these metrics range between 0 and 1, and we record them as percentages for convenience.
 For both metrics, a higher value indicates better performance.

**Implementation Details** For CGADM, the layer number of graph convolution is set to three, a value considered reasonable by most works (Liu et al., 2021b). For our diffusion process, the noise levels at the initial and final time steps,  $\beta_1$  and  $\beta_T$ , are set to 1e-4 and 0.02, respectively. Additionally, we employ linear interpolation to divide the time steps between them, which is consistent with DDPM (Ho et al., 2020). For other implementation details, please refer to Appendix J.

### 5.2 OVERALL COMPARISON

386

387 388 389

391 392 393

397

399

400

401

402

403

404

405

406

407

	El	lip	Ta	olo	Ye	elp	Qu	iest	Re	ddit
Model	AUPRC	AUROC	AUPRC	AUROC	AUPRC	AUROC	AUPRC	AUROC	AUPRC	AUROC
GCN	80.19	95.12	41.44	73.58	23.59	59.89	10.27	67.73	5.65	62.55
GIN	83.88	96.21	37.89	74.02	38.13	77.40	11.23	68.07	5.38	65.25
Graphsage	86.16	96.61	43.73	77.30	<u>50.23</u>	83.24	13.86	70.64	5.78	63.67
GAT	87.59	97.11	42.18	76.66	46.64	80.95	13.19	68.19	5.42	63.55
GAS	87.54	97.14	42.39	74.55	39.18	78.63	12.41	66.09	5.66	61.23
PCGNN	67.29	93.88	36.76	71.28	45.32	79.61	13.79	69.12	4.13	54.58
BWGNN	87.90	96.99	45.02	77.80	49.15	81.85	14.64	69.96	5.42	60.63
GHRN	88.13	97.04	45.25	77.98	49.78	82.36	14.61	69.32	<u>5.85</u>	63.51
CGADM	97.03	99.30	46.02	79.68	76.54	92.69	18.51	69.41	5.79	65.85

Boldface denotes the highest score, and underline indicates the best result of the baselines.

We summarize the performance of all algorithms in terms of AUROC and AUPRC across different datasets in Table 1. The results demonstrate that our CGADM outperforms most other baselines across all metrics. We conduct two-sample t-tests, and p – value < 0.05 indicates that the improvements are statistically significant. In addition to these findings, we make the following observations:

GAD methods such as GHRN and BWGNN represent state-of-the-art methods. This indicates
that GAD, with its unique challenges of data imbalance, data heterogeneity, and deliberate node
obfuscation, cannot be adequately addressed by general GNNs and requires specialized design.

No single baseline method consistently outperforms on all datasets. We believe this is because these discriminative models identify anomalous nodes through decision boundaries. Many anomalous nodes manage to cross these boundaries by obfuscating their features, making it difficult for these methods to adapt to various scenarios. In contrast, our CGADM consider the joint distribution of anomaly in a generative way, making it difficult for anomalous nodes to obfuscate.

Among standard GNN methods, GraphSage and GAT perform better than the other two methods, especially on the YelpChi dataset, which has significantly more edges. This aligns with our analysis in the introduction, where GNN, as a low-pass filter, blurs the distinctive features of anomalies in its inherent feature aggregation mechanism, a problem that worsens with an increased number of edges. GraphSage and GAT to some extent mitigate the over-smoothing issue by sampling neighbors or amplifying the weight of important neighbors, respectively.

• Our method performs exceptionally well on the edge-dense YelpChi dataset. This may be due to our topological-guided denoising network's use of a residual propagation mechanism. This mechanism effectively overcoming the over-smoothing problem during the generation process and ensuring that each node's anomaly distribution is influenced by its neighborhood distribution.

422 423 424

425

426

419

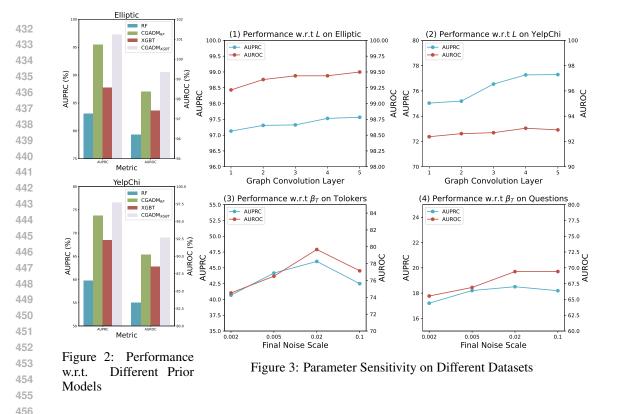
420

421

### 5.3 ABLATION STUDIES

#### 5.3.1 COMPARISON WITH DIFFERENT PRIOR MODEL

In generating the final anomaly value with CGADM, to ensure effectiveness, we do not start the reverse process from a random state. Instead, we opt for a conditional anomaly estimator to guide the reverse process of the model. For efficiency, we employ a lightweight ensemble trees model as the estimator. Here, we explore both Random Forest (RF) and Extreme Gradient Boosting Tree (XGBT) as estimator. We denote CGADM using RF and XGBT as conditional anomaly estimators as CGADM<sub>RF</sub> and CGADM<sub>XGBT</sub>, respectively. Figure 2 records the performance of these models



on the Elliptic and YelpChi datasets. Two observations can be made from figure 2. Firstly, both  $CGADM_{RF}$  and  $CGADM_{XGBT}$  outperform their corresponding initial priors. This proves that our CGADM's diffusion process can significantly enhance the performance of GAD. Secondly, the performance gap between  $CGADM_{RF}$  and  $CGADM_{XGBT}$  is significantly smaller than that between RF and XGBT. This indicates that our CGADM possesses strong robustness. Even in the face of initially inaccurate prior estimates, our CGADM can effectively correct the results under the iterative refinement of the topological-guided denoising network.

457

458

459

460

461

#### 5.3.2 PARAMETER SENSITIVITY

466 **Impact of Graph Convolution Laver** L In order to better capture the topological information sur-467 rounding nodes for joint distribution modeling, we employ a GNN-based encoder in our topological-468 guided denoising network. We explored the impact of the number of graph convolution layers on 469 the Elliptic and YelpChi datasets. The results are shown in Figures 3 (1) and (2). From the results, 470 we can observe a slowly gradual improvement in performance as the number of layers increases, 471 reaching farther topological structure information. Even at a depth of five layers, there is no perfor-472 mance degradation. This suggests that our CGADM can effectively overcome the over-smoothing problem commonly encountered in traditional discriminative methods based on GNNs. We attribute 473 this mainly to two factors. First, the paradigm shift to generating the joint distribution of anomaly 474 on the graph allows considering the influence of surrounding neighbor nodes. Second, our residual 475 propagation mechanism prevents the high-frequency information of nodes, thereby retaining more 476 valuable information for anomaly value generation. 477

478 **Impact of the Final Noise Scale**  $\beta_T$  We modify the endpoint of CGADM's diffusion process from 479 the conventional Gaussian distribution N(0, I) to  $N(g_{\phi}(\mathcal{E}, \mathbf{X}), I)$ . Intuitively,  $\beta_T$  represents the 480 maximum degree to which our noise-added  $y_t$  can deviate from the ground truth. It also represents 481 the maximum scale at which our denoising network can correct the prior. We studied the magnitude 482 of this degree on the Tolokers and Questions datasets, with the results shown in Figure 3 (3) and (4). 483 We can observe that as the maximum correction scale increases, the performance initially improves. This suggests that the bias of the prior can be better corrected at this point. However, when the 484 correction scale exceeds 0.02, the performance begins to decline as the maximum correction scale 485 continues to increase. This may because the maximum correction scale has already surpassed the

486 maximum bias produced by the prior. Overcorrection of the prior could prevent CGADM from 487 modeling the true distribution. Therefore, we recommend using  $\beta_T = 0.02$  in our cases, 488

#### 5.4 **EFFICIENCY ANALYSIS**

489

490 491

497

504

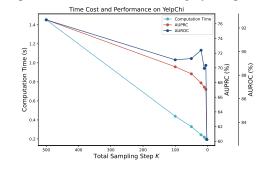
505 506 507

514 515

516 517 518

519

In Section 4.4, we designed a prior-aware strided sampling strategy to adaptively reduce the reverse 492 steps needed to generate anomaly values. To verify its efficiency, we designed the following two 493 ablation experiments. In the first experiment, we tested the computation time and corresponding 494 model performance of our CGADM with different sampling steps during generation. The results are shown in Figure 4. As can be seen, as our striding magnitude increases, i.e., the reverse steps of 495 sampling become fewer, both computation time and model performance decrease. However, the de-496 cline in computation time is much greater than the decline in graph anomaly detection performance. Even when the striding is not large at the beginning, the decline in performance is not significant. 498 This implies that sacrificing a little performance can result in substantial savings in computation 499 time. Therefore, we designed another ablation experiment. Here, we denote CGADM configured 500 with prior-aware strided sampling as CGADM<sub>s</sub> and present its model performance and average re-501 verse steps during inference in Table 2. Compared to the original 1000 sampling steps, our method 502 reduces the average sampling steps for all nodes to 583, while ensuring only a slight drop in model 503 performance, which remains highly competitive.



	CGADM	$\mathrm{CGADM}_S$
Average Reverse Step	1000	583.0256
AUPRC (%) AUROC (%)	76.5424 92.6930	73.6636 91.9423

Table 2: Performance Metrics

Figure 4: Time cost and Accuracy w.r.t. Sampling Steps K

#### CONCLUSIONS 6

520 Existing GNN-based graph anomaly detection methods are susceptible to fraudulent nodes in the 521 network due to their inherent feature aggregation and discriminative characteristics. Therefore, we 522 propose an advanced Conditional Graph Anomaly Diffusion Model (CGADM) that considers the 523 interdependencies of node anomalies from a holistic graph perspective, thereby generating a distribution of anomaly values across the entire graph. To address the issue of effectiveness, we propose 524 a prior-guided diffusion process, which injects a pre-trained conditional anomaly estimator to con-525 strain the entire diffusion process. Based on this, we redesign the forward and reverse processes. 526 To solve the efficiency issue, we introduce a prior confidence-aware mechanism to adaptively deter-527 mine the reverse time step for each node, thus significantly saving computational expenses. Through 528 experiments on standard benchmarks for graph anomaly detection, we demonstrate that CGADM 529 achieves state-of-the-art results.

530 531 532

537

# REFERENCES

533 Ziwei Chai, Siqi You, Yang Yang, Shiliang Pu, Jiarong Xu, Haoyang Cai, and Weihao Jiang. Can 534 abnormality be detected by graph neural networks? In Luc De Raedt (ed.), Proceedings of 535 the Thirty-First International Joint Conference on Artificial Intelligence, IJCAI 2022, Vienna, 536 Austria, 23-29 July 2022, pp. 1945–1951. ijcai.org, 2022.

Bo Chen, Jing Zhang, Xiaokang Zhang, Yuxiao Dong, Jian Song, Peng Zhang, Kaibo Xu, Evgeny 538 Kharlamov, and Jie Tang. GCCAD: graph contrastive coding for anomaly detection. *IEEE Trans.* Knowl. Data Eng., 35(8):8037-8051, 2023a.

554

- Ming Chen, Zhewei Wei, Zengfeng Huang, Bolin Ding, and Yaliang Li. Simple and deep graph convolutional networks. In *Proceedings of the 37th International Conference on Machine Learning*, *ICML 2020, 13-18 July 2020, Virtual Event*, volume 119 of *Proceedings of Machine Learning Research*, pp. 1725–1735. PMLR, 2020a.
- Nan Chen, Zemin Liu, Bryan Hooi, Bingsheng He, Rizal Fathony, Jun Hu, and Jia Chen. Consistency training with learnable data augmentation for graph anomaly detection with limited supervision. In *The Twelfth International Conference on Learning Representations, ICLR 2024, Vienna, Austria, May 7-11, 2024*. OpenReview.net, 2024.
- Tianqi Chen and Carlos Guestrin. Xgboost: A scalable tree boosting system. In Balaji Krishnapuram, Mohak Shah, Alexander J. Smola, Charu C. Aggarwal, Dou Shen, and Rajeev Rastogi (eds.), *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, San Francisco, CA, USA, August 13-17, 2016*, pp. 785–794. ACM, 2016.
  - Xiaohui Chen, Yukun Li, Aonan Zhang, and Li-Ping Liu. Nvdiff: Graph generation through the diffusion of node vectors. *CoRR*, abs/2211.10794, 2022.
- Xiaohui Chen, Jiaxing He, Xu Han, and Liping Liu. Efficient and degree-guided graph generation via discrete diffusion modeling. In Andreas Krause, Emma Brunskill, Kyunghyun Cho, Barbara Engelhardt, Sivan Sabato, and Jonathan Scarlett (eds.), *International Conference on Machine Learning, ICML 2023, 23-29 July 2023, Honolulu, Hawaii, USA*, volume 202 of *Proceedings of Machine Learning Research*, pp. 4585–4610. PMLR, 2023b.
- 561
  562
  563
  564
  564
  565
  565
  565
  566
  566
  566
  567
  568
  568
  568
  569
  569
  569
  560
  560
  560
  561
  561
  561
  562
  562
  563
  564
  565
  565
  565
  566
  566
- Prafulla Dhariwal and Alexander Quinn Nichol. Diffusion models beat gans on image synthesis. In Marc'Aurelio Ranzato, Alina Beygelzimer, Yann N. Dauphin, Percy Liang, and Jennifer Wortman Vaughan (eds.), Advances in Neural Information Processing Systems 34: Annual Conference on Neural Information Processing Systems 2021, NeurIPS 2021, December 6-14, 2021, virtual, pp. 8780–8794, 2021.
- Kaize Ding, Jundong Li, Nitin Agarwal, and Huan Liu. Inductive anomaly detection on attributed networks. In Christian Bessiere (ed.), *Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence, IJCAI 2020*, pp. 1288–1294. ijcai.org, 2020.
- Yingtong Dou, Zhiwei Liu, Li Sun, Yutong Deng, Hao Peng, and Philip S. Yu. Enhancing graph neural network-based fraud detectors against camouflaged fraudsters. In Mathieu d'Aquin, Stefan Dietze, Claudia Hauff, Edward Curry, and Philippe Cudré-Mauroux (eds.), *CIKM '20: The 29th ACM International Conference on Information and Knowledge Management, Virtual Event, Ireland, October 19-23, 2020*, pp. 315–324. ACM, 2020.
- Jingcan Duan, Siwei Wang, Pei Zhang, En Zhu, Jingtao Hu, Hu Jin, Yue Liu, and Zhibin Dong.
  Graph anomaly detection via multi-scale contrastive learning networks with augmented view.
  In Brian Williams, Yiling Chen, and Jennifer Neville (eds.), *Thirty-Seventh AAAI Conference on Artificial Intelligence, AAAI 2023, Thirty-Fifth Conference on Innovative Applications of Artificial Intelligence, IAAI 2023, Thirteenth Symposium on Educational Advances in Artificial Intelligence, EAAI 2023, Washington, DC, USA, February 7-14, 2023*, pp. 7459–7467. AAAI Press, 2023.
- Matthias Fey and Jan Eric Lenssen. Fast graph representation learning with pytorch geometric. *CoRR*, abs/1903.02428, 2019.
- Yuan Gao, Xiang Wang, Xiangnan He, Zhenguang Liu, Huamin Feng, and Yongdong Zhang. Alleviating structural distribution shift in graph anomaly detection. In Tat-Seng Chua, Hady W. Lauw, Luo Si, Evimaria Terzi, and Panayiotis Tsaparas (eds.), *Proceedings of the Sixteenth ACM International Conference on Web Search and Data Mining, WSDM 2023, Singapore, 27 February 2023 3 March 2023*, pp. 357–365. ACM, 2023a.

603

604

605

- Yuan Gao, Xiang Wang, Xiangnan He, Zhenguang Liu, Huamin Feng, and Yongdong Zhang. Addressing heterophily in graph anomaly detection: A perspective of graph spectrum. In Ying Ding, Jie Tang, Juan F. Sequeda, Lora Aroyo, Carlos Castillo, and Geert-Jan Houben (eds.), *Proceedings of the ACM Web Conference 2023, WWW 2023, Austin, TX, USA, 30 April 2023 4 May 2023*, pp. 1528–1538. ACM, 2023b.
- Kilian Konstantin Haefeli, Karolis Martinkus, Nathanaël Perraudin, and Roger Wattenhofer. Diffusion models for graphs benefit from discrete state spaces. *CoRR*, abs/2210.01549, 2022.
  - William L. Hamilton, Zhitao Ying, and Jure Leskovec. Inductive representation learning on large graphs. In Isabelle Guyon, Ulrike von Luxburg, Samy Bengio, Hanna M. Wallach, Rob Fergus, S. V. N. Vishwanathan, and Roman Garnett (eds.), Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, December 4-9, 2017, Long Beach, CA, USA, pp. 1024–1034, 2017.
- Songqiao Han, Xiyang Hu, Hailiang Huang, Minqi Jiang, and Yue Zhao. Adbench: Anomaly detection benchmark. In Sanmi Koyejo, S. Mohamed, A. Agarwal, Danielle Belgrave, K. Cho, and A. Oh (eds.), Advances in Neural Information Processing Systems 35: Annual Conference on Neural Information Processing Systems 2022, NeurIPS 2022, New Orleans, LA, USA, November 28 December 9, 2022, 2022a.
- Kizewen Han, Huangjie Zheng, and Mingyuan Zhou. CARD: classification and regression diffusion models. In Sanmi Koyejo, S. Mohamed, A. Agarwal, Danielle Belgrave, K. Cho, and A. Oh (eds.), Advances in Neural Information Processing Systems 35: Annual Conference on Neural Information Processing Systems 2022, NeurIPS 2022, New Orleans, LA, USA, November 28 -December 9, 2022, 2022b.
- Junwei He, Qianqian Xu, Yangbangyan Jiang, Zitai Wang, and Qingming Huang. ADA-GAD: anomaly-denoised autoencoders for graph anomaly detection. In Michael J. Wooldridge, Jennifer G. Dy, and Sriraam Natarajan (eds.), *Thirty-Eighth AAAI Conference on Artificial Intelligence, AAAI 2024, Thirty-Sixth Conference on Innovative Applications of Artificial Intelligence, IAAI 2024, Fourteenth Symposium on Educational Advances in Artificial Intelligence, EAAI 2014, February 20-27, 2024, Vancouver, Canada*, pp. 8481–8489. AAAI Press, 2024.
- Mingguo He, Zhewei Wei, Zengfeng Huang, and Hongteng Xu. Bernnet: Learning arbitrary graph spectral filters via bernstein approximation. In Marc'Aurelio Ranzato, Alina Beygelzimer, Yann N. Dauphin, Percy Liang, and Jennifer Wortman Vaughan (eds.), Advances in Neural Information Processing Systems 34: Annual Conference on Neural Information Processing Systems 2021, NeurIPS 2021, December 6-14, 2021, virtual, pp. 14239–14251, 2021.
- Jonathan Ho, Ajay Jain, and Pieter Abbeel. Denoising diffusion probabilistic models. In Hugo
  Larochelle, Marc'Aurelio Ranzato, Raia Hadsell, Maria-Florina Balcan, and Hsuan-Tien Lin
  (eds.), Advances in Neural Information Processing Systems 33: Annual Conference on Neural
  Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual, 2020.
- Kuanwen Huang, Yang Yang, Yang Wang, Chunping Wang, Zhisheng Zhang, Jiarong Xu, Lei Chen, and Michalis Vazirgiannis. Dgraph: A large-scale financial dataset for graph anomaly detection. In Sanmi Koyejo, S. Mohamed, A. Agarwal, Danielle Belgrave, K. Cho, and A. Oh (eds.), Advances in Neural Information Processing Systems 35: Annual Conference on Neural Information Processing Systems 2022, NeurIPS 2022, New Orleans, LA, USA, November 28 - December 9, 2022, 2022.
- Jaehyeong Jo, Seul Lee, and Sung Ju Hwang. Score-based generative modeling of graphs via the system of stochastic differential equations. In Kamalika Chaudhuri, Stefanie Jegelka, Le Song, Csaba Szepesvári, Gang Niu, and Sivan Sabato (eds.), *International Conference on Machine Learning, ICML 2022, 17-23 July 2022, Baltimore, Maryland, USA*, volume 162 of *Proceedings of Machine Learning Research*, pp. 10362–10383. PMLR, 2022.
- Thomas N. Kipf and Max Welling. Semi-supervised classification with graph convolutional net works. In 5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings. OpenReview.net, 2017.

688

689

690

691

692

- Lingkai Kong, Jiaming Cui, Haotian Sun, Yuchen Zhuang, B. Aditya Prakash, and Chao Zhang. Autoregressive diffusion model for graph generation. In Andreas Krause, Emma Brunskill, Kyunghyun Cho, Barbara Engelhardt, Sivan Sabato, and Jonathan Scarlett (eds.), *International Conference on Machine Learning, ICML 2023, 23-29 July 2023, Honolulu, Hawaii, USA*, volume 202 of *Proceedings of Machine Learning Research*, pp. 17391–17408. PMLR, 2023.
- Srijan Kumar, Xikun Zhang, and Jure Leskovec. Predicting dynamic embedding trajectory in temporal interaction networks. In Ankur Teredesai, Vipin Kumar, Ying Li, Rómer Rosales, Evimaria Terzi, and George Karypis (eds.), *Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, KDD 2019, Anchorage, AK, USA, August 4-8, 2019*, pp. 1269–1278. ACM, 2019.
- Ao Li, Zhou Qin, Runshi Liu, Yiqun Yang, and Dong Li. Spam review detection with graph convolutional networks. In Wenwu Zhu, Dacheng Tao, Xueqi Cheng, Peng Cui, Elke A. Rundensteiner, David Carmel, Qi He, and Jeffrey Xu Yu (eds.), *Proceedings of the 28th ACM International Conference on Information and Knowledge Management, CIKM 2019, Beijing, China, November 3-7, 2019*, pp. 2703–2711. ACM, 2019.
- Kuan Li, Chunjing Xiao, Ziliang Feng, Shikang Pang, Wenxin Tai, and Fan Zhou. Controlled graph
   neural networks with denoising diffusion for anomaly detection. *Expert Syst. Appl.*, 237(Part B):
   121533, 2024.
- Can Liu, Li Sun, Xiang Ao, Jinghua Feng, Qing He, and Hao Yang. Intention-aware heterogeneous graph attention networks for fraud transactions detection. In Feida Zhu, Beng Chin Ooi, and Chunyan Miao (eds.), *KDD '21: The 27th ACM SIGKDD Conference on Knowledge Discovery and Data Mining, Virtual Event, Singapore, August 14-18, 2021*, pp. 3280–3288. ACM, 2021a.
- Jenny Liu, Aviral Kumar, Jimmy Ba, Jamie Kiros, and Kevin Swersky. Graph normalizing flows.
  In Hanna M. Wallach, Hugo Larochelle, Alina Beygelzimer, Florence d'Alché-Buc, Emily B.
  Fox, and Roman Garnett (eds.), Advances in Neural Information Processing Systems 32: Annual
  Conference on Neural Information Processing Systems 2019, NeurIPS 2019, December 8-14,
  2019, Vancouver, BC, Canada, pp. 13556–13566, 2019.
- Kay Liu, Hengrui Zhang, Ziqing Hu, Fangxin Wang, and Philip S. Yu. Data augmentation for supervised graph outlier detection with latent diffusion models. *CoRR*, abs/2312.17679, 2023.
- Kay Liu, Huijun (Lona) Yu, Yao Yan, Ziqing Hu, Pankaj Rajak, Amila Weerasinghe, Olcay
  Boz, Deepayan Chakrabarti, and Fei Wang. Graph diffusion models for anomaly detection. In WSDM 2024, 2024. URL https://www.amazon.science/publications/
  graph-diffusion-models-for-anomaly-detection.
- Yang Liu, Xiang Ao, Zidi Qin, Jianfeng Chi, Jinghua Feng, Hao Yang, and Qing He. Pick and choose: A gnn-based imbalanced learning approach for fraud detection. In Jure Leskovec, Marko Grobelnik, Marc Najork, Jie Tang, and Leila Zia (eds.), WWW '21: The Web Conference 2021, Virtual Event / Ljubljana, Slovenia, April 19-23, 2021, pp. 3168–3177. ACM / IW3C2, 2021b.
  - Zhiwei Liu, Yingtong Dou, Philip S. Yu, Yutong Deng, and Hao Peng. Alleviating the inconsistency problem of applying graph neural network to fraud detection. In Jimmy X. Huang, Yi Chang, Xueqi Cheng, Jaap Kamps, Vanessa Murdock, Ji-Rong Wen, and Yiqun Liu (eds.), Proceedings of the 43rd International ACM SIGIR conference on research and development in Information Retrieval, SIGIR 2020, Virtual Event, China, July 25-30, 2020, pp. 1569–1572. ACM, 2020.
- Kiaoxiao Ma, Ruikun Li, Fanzhen Liu, Kaize Ding, Jian Yang, and Jia Wu. Graph anomaly detection
  with few labels: A data-centric approach. In Ricardo Baeza-Yates and Francesco Bonchi (eds.), *Proceedings of the 30th ACM SIGKDD Conference on Knowledge Discovery and Data Mining, KDD 2024, Barcelona, Spain, August 25-29, 2024*, pp. 2153–2164. ACM, 2024a.
- Kiaoxiao Ma, Ruikun Li, Fanzhen Liu, Kaize Ding, Jian Yang, and Jia Wu. New recipes for graph anomaly detection: Forward diffusion dynamics and graph generation, 2024b.
- 701 Chenhao Niu, Yang Song, Jiaming Song, Shengjia Zhao, Aditya Grover, and Stefano Ermon. Permutation invariant graph generation via score-based generative modeling. In Silvia Chiappa and

735

743

Roberto Calandra (eds.), *The 23rd International Conference on Artificial Intelligence and Statistics, AISTATS 2020, 26-28 August 2020, Online [Palermo, Sicily, Italy]*, volume 108 of *Proceedings of Machine Learning Research*, pp. 4474–4484. PMLR, 2020.

Kushagra Pandey, Avideep Mukherjee, Piyush Rai, and Abhishek Kumar. Diffusevae: Efficient, controllable and high-fidelity generation from low-dimensional latents. *Trans. Mach. Learn. Res.*, 2022, 2022.

Shikang Pang, Chunjing Xiao, Wenxin Tai, Zhangtao Cheng, and Fan Zhou. Graph anomaly detection with diffusion model-based graph enhancement (student abstract). In Michael J. Wooldridge, Jennifer G. Dy, and Sriraam Natarajan (eds.), *Thirty-Eighth AAAI Conference on Artificial Intelligence, AAAI 2024, Thirty-Sixth Conference on Innovative Applications of Artificial Intelligence, IAAI 2024, Fourteenth Symposium on Educational Advances in Artificial Intelligence, EAAI 2014, February 20-27, 2024, Vancouver, Canada*, pp. 23610–23612. AAAI Press, 2024.

716 Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, Alban Desmaison, Andreas Köpf, Ed-717 ward Z. Yang, Zachary DeVito, Martin Raison, Alykhan Tejani, Sasank Chilamkurthy, Benoit 718 Steiner, Lu Fang, Junjie Bai, and Soumith Chintala. Pytorch: An imperative style, high-719 performance deep learning library. In Hanna M. Wallach, Hugo Larochelle, Alina Beygelzimer, 720 Florence d'Alché-Buc, Emily B. Fox, and Roman Garnett (eds.), Advances in Neural Informa-721 tion Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, 722 NeurIPS 2019, December 8-14, 2019, Vancouver, BC, Canada, pp. 8024–8035, 2019. 723

- Fabian Pedregosa, Gaël Varoquaux, Alexandre Gramfort, Vincent Michel, Bertrand Thirion, Olivier
  Grisel, Mathieu Blondel, Peter Prettenhofer, Ron Weiss, Vincent Dubourg, Jake VanderPlas,
  Alexandre Passos, David Cournapeau, Matthieu Brucher, Matthieu Perrot, and Edouard Duchesnay. Scikit-learn: Machine learning in python. *J. Mach. Learn. Res.*, 12:2825–2830, 2011.
- Oleg Platonov, Denis Kuznedelev, Michael Diskin, Artem Babenko, and Liudmila Prokhorenkova.
   A critical look at the evaluation of gnns under heterophily: Are we really making progress? In *The Eleventh International Conference on Learning Representations, ICLR 2023, Kigali, Rwanda, May 1-5, 2023*. OpenReview.net, 2023.
- Hezhe Qiao, Qingsong Wen, Xiaoli Li, Ee-Peng Lim, and Guansong Pang. Generative semi supervised graph anomaly detection. *CoRR*, abs/2402.11887, 2024.
- Aditya Ramesh, Prafulla Dhariwal, Alex Nichol, Casey Chu, and Mark Chen. Hierarchical textconditional image generation with CLIP latents. *CoRR*, abs/2204.06125, 2022.
- Shebuti Rayana and Leman Akoglu. Collective opinion spam detection: Bridging review networks and metadata. In Longbing Cao, Chengqi Zhang, Thorsten Joachims, Geoffrey I. Webb, Dragos D. Margineantu, and Graham Williams (eds.), *Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, Sydney, NSW, Australia, August 10-13, 2015*, pp. 985–994. ACM, 2015.
- Robin Rombach, Andreas Blattmann, Dominik Lorenz, Patrick Esser, and Björn Ommer. Highresolution image synthesis with latent diffusion models. In *IEEE/CVF Conference on Computer Vision and Pattern Recognition, CVPR 2022, New Orleans, LA, USA, June 18-24, 2022*, pp. 10674–10685. IEEE, 2022.
- Jiaming Song, Chenlin Meng, and Stefano Ermon. Denoising diffusion implicit models. In 9th International Conference on Learning Representations, ICLR 2021, Virtual Event, Austria, May 3-7, 2021. OpenReview.net, 2021a.
- Yang Song and Stefano Ermon. Generative modeling by estimating gradients of the data distribution.
  In Hanna M. Wallach, Hugo Larochelle, Alina Beygelzimer, Florence d'Alché-Buc, Emily B.
  Fox, and Roman Garnett (eds.), *Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, December 8-14, 2019, Vancouver, BC, Canada*, pp. 11895–11907, 2019.

- Yang Song, Jascha Sohl-Dickstein, Diederik P. Kingma, Abhishek Kumar, Stefano Ermon, and Ben Poole. Score-based generative modeling through stochastic differential equations. In 9th International Conference on Learning Representations, ICLR 2021, Virtual Event, Austria, May 3-7, 2021. OpenReview.net, 2021b.
- Jianheng Tang, Jiajin Li, Ziqi Gao, and Jia Li. Rethinking graph neural networks for anomaly detection. In Kamalika Chaudhuri, Stefanie Jegelka, Le Song, Csaba Szepesvári, Gang Niu, and Sivan Sabato (eds.), *International Conference on Machine Learning, ICML 2022, 17-23 July 2022, Baltimore, Maryland, USA*, volume 162 of *Proceedings of Machine Learning Research*, pp. 21076–21089. PMLR, 2022.
- Jianheng Tang, Fengrui Hua, Ziqi Gao, Peilin Zhao, and Jia Li. Gadbench: Revisiting and benchmarking supervised graph anomaly detection. In Alice Oh, Tristan Naumann, Amir Globerson,
  Kate Saenko, Moritz Hardt, and Sergey Levine (eds.), Advances in Neural Information Processing Systems 36: Annual Conference on Neural Information Processing Systems 2023, NeurIPS 2023, New Orleans, LA, USA, December 10 16, 2023, 2023.
- Petar Velickovic, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua
  Bengio. Graph attention networks. In *6th International Conference on Learning Representations, ICLR 2018, Vancouver, BC, Canada, April 30 May 3, 2018, Conference Track Proceedings.*OpenReview.net, 2018.
- Clément Vignac, Igor Krawczuk, Antoine Siraudin, Bohan Wang, Volkan Cevher, and Pascal Frossard. Digress: Discrete denoising diffusion for graph generation. In *The Eleventh International Conference on Learning Representations, ICLR 2023, Kigali, Rwanda, May 1-5, 2023.*OpenReview.net, 2023.
- Daixin Wang, Yuan Qi, Jianbin Lin, Peng Cui, Quanhui Jia, Zhen Wang, Yanming Fang, Quan Yu, Jun Zhou, and Shuang Yang. A semi-supervised graph attentive network for financial fraud detection. In Jianyong Wang, Kyuseok Shim, and Xindong Wu (eds.), 2019 IEEE International Conference on Data Mining, ICDM 2019, Beijing, China, November 8-11, 2019, pp. 598–607. IEEE, 2019a.
- Jianyu Wang, Rui Wen, Chunming Wu, Yu Huang, and Jian Xiong. Fdgars: Fraudster detection via graph convolutional networks in online app review system. In Sihem Amer-Yahia, Mohammad Mahdian, Ashish Goel, Geert-Jan Houben, Kristina Lerman, Julian J. McAuley, Ricardo Baeza-Yates, and Leila Zia (eds.), *Companion of The 2019 World Wide Web Conference, WWW 2019, San Francisco, CA, USA, May 13-17, 2019*, pp. 310–316. ACM, 2019b.
- Yanling Wang, Jing Zhang, Shasha Guo, Hongzhi Yin, Cuiping Li, and Hong Chen. Decoupling representation learning and classification for gnn-based anomaly detection. In Fernando Diaz, Chirag Shah, Torsten Suel, Pablo Castells, Rosie Jones, and Tetsuya Sakai (eds.), *SIGIR '21: The 44th International ACM SIGIR Conference on Research and Development in Information Retrieval, Virtual Event, Canada, July 11-15, 2021*, pp. 1239–1248. ACM, 2021.
- Mark Weber, Giacomo Domeniconi, Jie Chen, Daniel Karl I. Weidele, Claudio Bellei, Tom Robin son, and Charles E. Leiserson. Anti-money laundering in bitcoin: Experimenting with graph
   convolutional networks for financial forensics. *CoRR*, abs/1908.02591, 2019.
- Chunjing Xiao, Shikang Pang, Xovee Xu, Xuan Li, Goce Trajcevski, and Fan Zhou. Counterfactual data augmentation with denoising diffusion for graph anomaly detection. *CoRR*, abs/2407.02143, 2024.
- Fan Xu, Nan Wang, Hao Wu, Xuezhi Wen, Xibin Zhao, and Hai Wan. Revisiting graph-based
  fraud detection in sight of heterophily and spectrum. In Michael J. Wooldridge, Jennifer G. Dy,
  and Sriraam Natarajan (eds.), *Thirty-Eighth AAAI Conference on Artificial Intelligence, AAAI*2024, *Thirty-Sixth Conference on Innovative Applications of Artificial Intelligence, IAAI 2024, Fourteenth Symposium on Educational Advances in Artificial Intelligence, EAAI 2014, February*20-27, 2024, *Vancouver, Canada*, pp. 9214–9222. AAAI Press, 2024.
- Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? In 7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019. OpenReview.net, 2019.

- 810 Yang Yang, Yuhong Xu, Yizhou Sun, Yuxiao Dong, Fei Wu, and Yueting Zhuang. Mining fraudsters 811 and fraudulent strategies in large-scale mobile social networks. IEEE Trans. Knowl. Data Eng., 812 33(1):169–179, 2021.
- Kai Yi, Bingxin Zhou, Yiqing Shen, Pietro Lió, and Yuguang Wang. Graph denoising diffusion for 814 inverse protein folding. In Alice Oh, Tristan Naumann, Amir Globerson, Kate Saenko, Moritz 815 Hardt, and Sergey Levine (eds.), Advances in Neural Information Processing Systems 36: Annual 816 Conference on Neural Information Processing Systems 2023, NeurIPS 2023, New Orleans, LA, 817 USA, December 10 - 16, 2023, 2023. 818
- 819 Ge Zhang, Jia Wu, Jian Yang, Amin Beheshti, Shan Xue, Chuan Zhou, and Quan Z. Sheng. FRAU-820 DRE: fraud detection dual-resistant to graph inconsistency and imbalance. In James Bailey, Pauli 821 Miettinen, Yun Sing Koh, Dacheng Tao, and Xindong Wu (eds.), IEEE International Conference 822 on Data Mining, ICDM 2021, Auckland, New Zealand, December 7-10, 2021, pp. 867–876. IEEE, 823 2021.
- Tong Zhao, Tianwen Jiang, Neil Shah, and Meng Jiang. A synergistic approach for graph anomaly 825 detection with pattern mining and feature learning. IEEE Trans. Neural Networks Learn. Syst., 826 33(6):2393-2405, 2022.
  - Jiong Zhu, Yujun Yan, Lingxiao Zhao, Mark Heimann, Leman Akoglu, and Danai Koutra. Beyond homophily in graph neural networks: Current limitations and effective designs. In Hugo Larochelle, Marc'Aurelio Ranzato, Raia Hadsell, Maria-Florina Balcan, and Hsuan-Tien Lin (eds.), Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual, 2020.
  - COMMON PROCESS OF DIFFUSION PROBABILISTIC MODEL А

Here we show the common steps in the diffusion model as follows:

1

- Forward process: Given an input data sample  $x_0 \sim q(x_0)$ , the forward process constructs the latent variables  $x_{1:T}$  in a Markov chain by progressively adding Gaussian noises over T steps. Specifically, the forward transition  $x_{t-1} \rightarrow x_t$  is defined as  $q(x_t|x_{t-1}) =$  $\mathcal{N}(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$ , where  $t \in \{1, ..., T\}$  refers to the diffusion step,  $\mathcal{N}$  denotes the Gaussian distribution, and  $\beta_t \in (0,1)$  regulates the noise scales added at step t. If  $T \to \infty$ ,  $x_T$ approaches a standard Gaussian distribution (Ho et al., 2020).
- **Reverse process:** Diffusion models (DMs) aim to remove the added noises from  $x_t$  to recover  $x_{t-1}$  in the reverse step, striving to capture minor alterations in the complex generation process. Formally, taking  $x_T$  as the initial state, DMs learn the denoising process  $x_t \to x_{t-1}$  iteratively by  $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma_{\theta}(x_t, t))$ , where  $\mu_{\theta}(x_t, t)$  and  $\Sigma_{\theta}(x_t, t)$  are the mean and covariance of the Gaussian distribution predicted by a neural network with parameters  $\theta$ .
- **Optimization:** DMs are optimized by maximizing the Evidence Lower Bound (ELBO) of the likelihood of observed input data  $x_0$ . Denote  $\mathbb{D}_{KL}(p||q)$  as the Kullback–Leibler (KL) divergence from distribution p to distribution q:

$$\log p(x_0) = \log \int p(x_{0:T}) dx_{1:T} = \log \mathbb{E}_{q(x_{1:T}|x_0)} \left[ \frac{p(x_{0:T})}{q(x_{1:T}|x_0)} \right]$$

$$\geq \mathbb{E}_{q(x_{1:T}|x_0)} \left[ \frac{p(x_{0:T})}{q(x_{1:T}|x_0)} \right]$$

$$= \mathbb{E}_{q(x_1|x_0)} \left[ \log p_{\theta}(x_0|x_1) \right] - \mathbb{D}_{KL}(q(x_T|x_0)||p(x_T))$$

$$- \sum_{t=2}^{T} \mathbb{E}_{q(x_t|x_0)} \left[ \mathbb{D}_{KL}(q(x_{t-1}|x_t, x_0)||p_{\theta}(x_{t-1}|x_t)) \right]$$

$$(16)$$

861 862 863

813

824

827

829

830

831

832 833 834

835 836

837 838

839

840

841

842

843

844

845

846

847

848

849

850

851

852 853 854

855 856 857

858 859

> • Inference: After training  $\theta$ , DMs can draw  $x_T \sim \mathcal{N}(0, I)$  and use  $p_{\theta}(x_{t-1}|x_t)$  to iteratively repeat the generation process  $x_T \to x_{T-1} \to \ldots \to x_0$ .

## **B** POSTERIOR COEFFICIENTS DERIVATION

Similar to Han et al. (2022b), here we give the detailed derivation of Equation 6 and 7.

 $q(\mathbf{y}_{t-1}|\mathbf{y}_{t},\mathbf{y}_{0},\mathcal{E},\mathbf{X}) = q(\mathbf{y}_{t-1}|\mathbf{y}_{t},\mathbf{y}_{0},g_{\phi}(\mathcal{E},\mathbf{X})) \propto q(\mathbf{y}_{t}|\mathbf{y}_{t-1},g_{\phi}(\mathcal{E},\mathbf{X}))q(\mathbf{y}_{t-1}|\mathbf{y}_{0},g_{\phi}(\mathcal{E},\mathbf{X}))$   $\propto \exp\left(-\frac{1}{2}\left(\frac{(\mathbf{y}_{t}-(1-\sqrt{\alpha_{t}})g_{\phi}(\mathcal{E},\mathbf{X})-\sqrt{\alpha_{t}}\mathbf{y}_{t-1})^{2}}{1-\bar{\alpha}_{t-1}}\right)\right)$   $\approx \exp\left(-\frac{1}{2}\left(\frac{\alpha_{t}\mathbf{y}_{t-1}^{2}-2\sqrt{\alpha_{t}}\left(\mathbf{y}_{t}-(1-\sqrt{\alpha_{t}})g_{\phi}(\mathcal{E},\mathbf{X})\right)\mathbf{y}_{t-1}}{\beta_{t}}\right)$   $+\frac{\mathbf{y}_{t-1}^{2}-2\left(\sqrt{\bar{\alpha}_{t-1}}\mathbf{y}_{0}+(1-\sqrt{\bar{\alpha}_{t-1}})g_{\phi}(\mathcal{E},\mathbf{X})\right)\mathbf{y}_{t-1}}{1-\bar{\alpha}_{t-1}}\right)$   $=\exp(-\frac{1}{2}\left((\frac{\alpha_{t}}{\beta_{t}}+\frac{1}{1-\bar{\alpha}_{t-1}})\mathbf{y}_{t}^{2}-1\right)$   $-2\left(\underbrace{\sqrt{\alpha_{t-1}}}_{1-\bar{\alpha}_{t-1}}\mathbf{y}_{0}+\frac{\sqrt{\alpha_{t}}}{\beta_{t}}\mathbf{y}_{t}+\left(\frac{\sqrt{\alpha_{t}}\left(\sqrt{\alpha_{t}}-1\right)}{\beta_{t}}+\frac{1-\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\right)g_{\phi}(\mathcal{E},\mathbf{X})\mathbf{y}_{t-1})\right),$   $\operatorname{Term 2}$  (17)

where

Term 1 = 
$$\frac{\alpha_t (1 - \bar{\alpha}_{t-1}) + \beta_t}{\beta_t (1 - \bar{\alpha}_{t-1})} = \frac{1 - \bar{\alpha}_t}{\beta_t (1 - \bar{\alpha}_{t-1})},$$
 (18)

$$\tilde{\beta}_t = \frac{1}{(1)} = \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t} \beta_t,$$
(19)

Afterwards, we divide each coefficient in Term 2 by Term 1.

$$\gamma_0 = \frac{\sqrt{\bar{\alpha}_{t-1}}}{1 - \bar{\alpha}_{t-1}} / 1 = \frac{\sqrt{\bar{\alpha}_{t-1}}}{1 - \bar{\alpha}_t} \beta_t \tag{20}$$

$$\gamma_1 = \frac{\sqrt{\alpha_t}}{\beta_t} / 1 = \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t} \sqrt{\alpha_t},\tag{21}$$

901 and

$$\gamma_{2} = \left(\frac{\sqrt{\alpha_{t}}\left(\sqrt{\alpha_{t}}-1\right)}{\beta_{t}} + \frac{1-\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\right)/1$$

$$= \frac{\alpha_{t}-\bar{\alpha}_{t}-\sqrt{\alpha_{t}}\left(1-\bar{\alpha}_{t-1}\right)+\beta_{t}-\beta_{t}\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t}}$$

$$= 1 + \frac{\left(\sqrt{\bar{\alpha}_{t}}-1\right)\left(\sqrt{\alpha_{t}}+\sqrt{\bar{\alpha}_{t-1}}\right)}{1-\bar{\alpha}_{t}}.$$
(22)

Finally, we put every  $\gamma_0$ ,  $\gamma_1$ , and  $\gamma_2$  together and obtain Equation 6 and 7.

 $\tilde{\boldsymbol{\mu}}\left(\boldsymbol{y}_{t}, \boldsymbol{y}_{0}, g_{\phi}(\boldsymbol{\mathcal{E}}, \mathbf{X})\right) = \gamma_{0}\boldsymbol{y}_{0} + \gamma_{1}\boldsymbol{y}_{t} + \gamma_{2}g_{\phi}(\boldsymbol{\mathcal{E}}, \mathbf{X})$ (23)

### C DERIVATION OF CONDITIONAL NON-MARKOVIAN REVERSE PROCESS

Following DDIM, we formally carry out the derivation of discarding the Markov constraint introduced by Equation 4 in our prior-conditional reverse step Equation 6. First, let's organize our target: given  $q(\mathbf{y}_t | \mathbf{y}_0, g_{\phi}(\mathcal{E}, \mathbf{X}))$  and  $q(\mathbf{y}_{t-1} | \mathbf{y}_0, g_{\phi}(\mathcal{E}, \mathbf{X}))$ , without  $q(\mathbf{y}_t | \mathbf{y}_{t-1})$ , we aim to find  $q(\mathbf{y}_{t-1} | \mathbf{y}_t, \mathbf{y}_0, g_{\phi}(\mathcal{E}, \mathbf{X}))$ . Here we assume that  $\mathbf{y}_{t-1}$  is a linear combination of  $\mathbf{y}_t$ ,  $\mathbf{y}_0$  and prior  $g_{\phi}(\mathcal{E}, \mathbf{X})$  with coefficients denoted as  $m_t$ ,  $n_t$  and  $o_t$ , respectively. That is,

$$\mathbf{y}_{t-1} = m_t \mathbf{y}_t + n_t \mathbf{y}_0 + o_t g_\phi(\mathcal{E}, \mathbf{X}) + \sigma_t \epsilon_1$$
(24)

We also know that

$$\mathbf{y}_t = \sqrt{\bar{\alpha}_t} \mathbf{y}_0 + (1 - \sqrt{\bar{\alpha}_t}) g_\phi(\mathcal{E}, \mathbf{X}) + \sqrt{1 - \bar{\alpha}_t} \epsilon_2,$$
(25)

$$\mathbf{y}_{t-1} = \sqrt{\bar{\alpha}_{t-1}} \mathbf{y}_0 + (1 - \sqrt{\bar{\alpha}_{t-1}}) g_\phi(\mathcal{E}, \mathbf{X}) + \sqrt{1 - \bar{\alpha}_{t-1}} \epsilon_3.$$
(26)

Here, the subscripts of  $\epsilon_n$  are used to distinguish different samples from the Gaussian distribution. Substituting Equation 25 into Equation 24, we get

$$\mathbf{y}_{t-1} = m_t \left( \sqrt{\bar{\alpha}_t} \mathbf{y}_0 + (1 - \sqrt{\bar{\alpha}_t}) g_\phi(\mathcal{E}, \mathbf{X}) + \sqrt{1 - \bar{\alpha}_t} \epsilon_2 \right) + n_t \mathbf{y}_0 + o_t g_\phi(\mathcal{E}, \mathbf{X}) + \sigma_t \epsilon_1$$
(27)

$$= \left(m_t \sqrt{\bar{\alpha}_t} + n_t\right) \mathbf{y}_0 + \left(m_t - m_t \sqrt{\bar{\alpha}_t} + o_t\right) g_\phi(\mathcal{E}, \mathbf{X}) + m_t \sqrt{1 - \bar{\alpha}_t} \epsilon_2 + \sigma_t \epsilon_1$$
(28)

Therefore, we have

$$m_t \sqrt{\bar{\alpha}_t} + n_t = \sqrt{\bar{\alpha}_{t-1}},\tag{29}$$

$$m_t^2 (1 - \alpha_t) + \sigma_t^2 = 1 - \bar{\alpha}_{t-1}, \tag{30}$$

$$m_t - m_t \sqrt{\bar{\alpha}_t} + o_t = 1 - \sqrt{\bar{\alpha}_{t-1}} \tag{31}$$

Immediately, we can calculate  $m_t$  and  $n_t$ :

$$m_t = \sqrt{\frac{1 - \bar{\alpha}_{t-1} - \sigma_t^2}{1 - \bar{\alpha}_t}},$$
(32)

$$n_{t} = \sqrt{\bar{\alpha}_{t-1}} - \sqrt{\frac{\bar{\alpha}_{t}}{1 - \bar{\alpha}_{t}} \left(1 - \bar{\alpha}_{t-1} - \sigma_{t}^{2}\right)},$$
(33)

$$o_t = 1 - \sqrt{\bar{\alpha}_{t-1}} - \sqrt{\frac{1 - \bar{\alpha}_{t-1} - \sigma_t^2}{1 - \bar{\alpha}_t}} (1 - \sqrt{\bar{\alpha}_t}).$$
(34)

Substituting back into Equation 24, we have

$$\mathbf{y}_{t-1} = \sqrt{\frac{1 - \bar{\alpha}_{t-1} - \sigma_t^2}{1 - \bar{\alpha}_t}} \mathbf{y}_t + \left(\sqrt{\bar{\alpha}_{t-1}} - \sqrt{\frac{\bar{\alpha}_t}{1 - \bar{\alpha}_t}} \left(1 - \bar{\alpha}_{t-1} - \sigma_t^2\right)\right) \mathbf{y}_0 + \left(1 - \sqrt{\bar{\alpha}_{t-1}} - \sqrt{\frac{1 - \bar{\alpha}_{t-1} - \sigma_t^2}{1 - \bar{\alpha}_t}} \left(1 - \sqrt{\bar{\alpha}_t}\right)\right) g_\phi(\mathcal{E}, \mathbf{X}) + \sigma_t \epsilon$$
(35)

$$+ (1 - \sqrt{\alpha_{t-1}} - \sqrt{\frac{1 - \bar{\alpha}_t}{1 - \bar{\alpha}_t}} (1 - \sqrt{\alpha_t}))g_{\phi}(\mathcal{E}, \mathbf{X}) + \sigma_t \epsilon$$
$$= \sqrt{\bar{\alpha}_{t-1}}\mathbf{y}_0 + (1 - \sqrt{\bar{\alpha}_{t-1}})g_{\phi}(\mathcal{E}, \mathbf{X})$$

$$+\sqrt{1-\bar{\alpha}_{t-1}-\sigma_t^2}\left(\frac{1}{\sqrt{1-\bar{\alpha}_t}}\mathbf{y}_t-\frac{\sqrt{\bar{\alpha}_t}}{\sqrt{1-\bar{\alpha}_t}}\mathbf{y}_0-\frac{1-\sqrt{\bar{\alpha}_t}}{\sqrt{1-\bar{\alpha}_t}}g_\phi(\mathcal{E},\mathbf{X})\right)+\sigma_t\epsilon \quad (36)$$

$$=\sqrt{\bar{\alpha}_{t-1}}\mathbf{y}_0 + (1-\sqrt{\bar{\alpha}_{t-1}})g_\phi(\mathcal{E},\mathbf{X})$$

$$+\sqrt{1-\bar{\alpha}_{t-1}-\sigma_t^2}\frac{\mathbf{y}_t-\sqrt{\bar{\alpha}_t}\mathbf{y}_0-(1-\sqrt{\bar{\alpha}_t})g_\phi(\mathcal{E},\mathbf{X})}{\sqrt{1-\bar{\alpha}_t}}+\sigma_t\epsilon$$
(37)

Substituting the model's predicted value, we have

$$\mathbf{y}_{t-1} = \sqrt{\bar{\alpha}_{t-1}} \hat{\mathbf{y}}_{0|t} + (1 - \sqrt{\bar{\alpha}_{t-1}}) g_{\phi}(\mathcal{E}, \mathbf{X}) + \sqrt{1 - \bar{\alpha}_{t-1} - \sigma_t^2 \epsilon_{\theta}(\mathbf{y}_t, t, \mathcal{E}, \mathbf{X})} + \sigma_t \epsilon$$
(38)

At this point, the derived result Equation 38 is completely consistent with Equation 14. That is, we use the two conditions  $q(\mathbf{y}_t | \mathbf{y}_0, g_{\phi}(\mathcal{E}, \mathbf{X}))$  and  $q(\mathbf{y}_{t-1} | \mathbf{y}_0, g_{\phi}(\mathcal{E}, \mathbf{X}))$ , without  $q(\mathbf{y}_t | \mathbf{y}_{t-1})$ , and obtain  $q(\mathbf{y}_{t-1} | \mathbf{y}_t, \mathbf{y}_0, g_{\phi}(\mathcal{E}, \mathbf{X}))$ . DDPM removes the condition  $q(\mathbf{y}_t | \mathbf{y}_{t-1})$ , leading to the more general DDIM sampling formula.

# 972 D BASELINES

In this section, we introduce the baseline models, which can be broadly bifurcated into two categories: (1) General-purpose graph neural networks, and (2) Techniques specifically designed for
graph anomaly detection. We have annotated each model with their respective categories for easy
differentiation.

- GCN (Kipf & Welling, 2017) (1): This technique employs the convolution operation on graphs to propagate information from a node to its adjacent nodes. This allows the network to learn a representation for each node, grounded on its local neighborhood.
- **GIN** (Xu et al., 2019) (1): A variant of GNN, GIN is designed to encapsulate the graph's structure while maintaining graph isomorphism. This implies that it yields identical embeddings for graphs that are structurally indistinguishable, irrespective of permutations in their node labels.
- **GraphSAGE** (Hamilton et al., 2017) (1): This is an inductive learning framework that generates node embeddings by sampling and aggregating features from a node's local neighborhood.
- **GAT** (Velickovic et al., 2018) (1): This GNN framework incorporates the attention mechanism, assigning varying degrees of importance to different nodes during the neighborhood information aggregation process. This enables the model to concentrate on the most informative neighbors.
  - GAS (Li et al., 2019) (2): This is a highly scalable technique for detecting spam reviews. It expands GCN to manage heterogeneous and heterophilic graphs and adapts to the graph structure of specific GAD applications using the KNN algorithm.
- **PCGNN** (Liu et al., 2021b) (2): This framework is designed for imbalanced GNN learning in fraud detection. It employs a label-balanced sampler to select nodes and edges for training, leading to a balanced label distribution in the induced sub-graph. Additionally, it uses a learnable parameterized distance function to select neighbors, filtering out superfluous links and incorporating beneficial ones for fraud prediction.
- BWGNN (Tang et al., 2022) (2): This technique is proposed to address the 'right-shift' phenomenon of graph anomalies, where the spectral energy distribution focuses less on low frequencies and more on high frequencies. It utilizes the Beta kernel to tackle higher frequency anomalies through multiple flexible, spatial/spectral-localized, and band-pass filters.
  - **GHRN** (Gao et al., 2023b) (2): This approach addresses the heterophily issue in the spectral domain of graph anomaly detection by pruning inter-class edges to highlight and outline the graph's high-frequency components.

# E CHALLENGE OF GRAPH ANOMALY DETECTION

Although GAD is essentially a binary node classification problem, it presents several unique chal-lenges. Firstly, anomalous nodes typically constitute a small fraction of the total nodes, leading to a significant data imbalance (Liu et al., 2021b). Secondly, graphs containing anomalies often exhibit strong heterophily, where connected nodes possess diverse features and labels (Gao et al., 2023b; Tang et al., 2023). This heterophily necessitates the development of methods that can effectively handle neighborhood feature disparities during message passing. Lastly, anomalous nodes tend to camouflage their features and connections, striving to blend in by mimicking normal patterns within the graph (Liu et al., 2020). 

## 1020 F DETAILS OF THE DATASETS

The detailed statistics of the datasets we used are in Table 3. In line with the data characteristics of anomaly detection, the selected datasets each contain over 100 anomaly points, and the proportion of anomalies does not exceed 25%, satisfying the inherent imbalance problem in graph anomaly detection (Tang et al., 2023). For each dataset, we randomly selected 20% of the points as training data, 10% of the points as validation data, and the remaining points as test data.

	#Nodes	#Edges	Feature Dim	Anomaly Ratio	Feature Type
Elliptic	203,769	234,355	166	9.8%	Timestamps and transaction information
Tolokers	11,758	519,000	10	21.8%	User profile with task performance statis
YelpChi	45,954	3,846,979	32	14.5%	Hand-crafted review features and statist
Questions	48,921	153,540	301	3.0%	FastText embeddings for user description
Reddit	10,984	168,016	64	3.3%	Hand-crafted review features and statist

Table 3: Descriptive statistics of the datasets.

#### IMPLEMENTATION OF TOPOLOGICAL-GUIDED DENOISING NETWORK G

Reflecting upon Equation 9, we initially extend the formula of graph convolution to matrix form to facilitate computation across the entire graph, as shown below:

$$\mathbf{H}^{l} = \sigma(\mathbf{W}^{l-1}(\mathbf{I} - \mathbf{D}^{-1}\mathbf{A}\mathbf{H}^{l-1}))$$

After conducting L rounds of convolution, we use weighted summation as our aggregation function for the hidden representations obtained from each layer of graph convolution. The formula is as follows: 

$$\mathbf{H}^{final} = AGG(\mathbf{H}^1, \mathbf{H}^2, \dots, \mathbf{H}^L) = \sum_{l=0}^L \alpha_l \mathbf{H}^l$$

Here,  $\alpha_l$  are the weights for each layer's representation, which can be learned during training. Hav-ing obtained the representation of nodes that integrates both topological structure and node features, we construct our denoising function  $\epsilon_{\theta}(\mathbf{y}_t, t, \mathbf{H}^{final})$  through a Multilayer Perceptron (MLP). Fol-lowing the original DDPM Ho et al. (2020), we also adopt position embedding to encode time t. Therefore, the denoising function  $\epsilon_{\theta}$  is as follows: 

 $\epsilon_{\theta} = MLP(\text{Concat}[Pos(\mathbf{t}), \mathbf{y}_t, \mathbf{H}^{final}])$ 

In this equation, Pos(t) represents the position embedding of time mathbft,  $y_t$  is the current representation of the nodes, and  $\mathbf{H}^{final}$  is the final aggregated representation after L layers of graph convolution. 

#### Η TRAINING OF CGADM

According to the loss in Equation 11, the pseudo algorithm for training is shown in Algorithm 2

Algorithm 2 CGADM Training

1: I	Pre-train $g_{\phi}(\mathcal{E}, \mathbf{X})$ that predicts the anomaly prior
2: 1	repeat
3:	Draw $\mathbf{t} \sim \text{Uniform}(\{1, \dots, T\})$
4:	Draw $\epsilon \sim \mathcal{N}(0, I)$
5:	Compute the noise estimation loss:
	$\mathcal{L}_{\epsilon} =   \epsilon - \epsilon_{\theta}(\sqrt{\bar{\alpha}_{t}}\mathbf{y}_{0} + (1 - \sqrt{\bar{\alpha}_{t}})g_{\phi}(\mathcal{E}, \mathbf{X}) + \sqrt{1 - \bar{\alpha}_{t}}\epsilon, t, \mathcal{E}, \mathbf{X})  ^{2}$
6:	Take a numerical optimization step on $\nabla_{\theta} L_{\epsilon}$
7: 1	until Convergence

#### INFERENCE WITH PRIOR-AWARE STRIDED SAMPLING Ι

We show the complete pseudo algorithm for inference with our prior-aware strided sampling strategy in Algorithm 3

1080 Algorithm 3 Inference for Anomaly Detection with Sampling Strategy 1: Initialize  $\mathbf{y}_T \sim \mathcal{N}(g_{\phi}(\mathcal{E}, \mathbf{X}), I)$ 1082 2: Compute K based on the prior confidence  $|g_{\phi}(\mathcal{E}, \mathbf{X}) - 0.5|$  using:  $K = \frac{r}{1 + \exp\left(\frac{|g_{\phi}(\mathcal{E}, \mathbf{X}) - 0.5|}{0.5}\right)} \times T$ 1084 where r is a hyperparameter. 1087 3: Generate sampling time steps  $\{\tau_i\}_{i=1}^K$ : 1088  $\tau_i = \left| 1 + \frac{(T-1)(i-1)}{K-1} \right|, \quad i = 1, \dots, K$ 1089 1090 4: for i = K to 1 do 5: Set  $t = \tau_i$ Calculate reparameterized  $\hat{\mathbf{y}}_0$  using Equation 12: 6: 1093 1094  $\hat{\mathbf{y}}_0 = rac{1}{\sqrt{ar{lpha}_t}} \left( \mathbf{y}_t - (1 - \sqrt{ar{lpha}_t}) g_{\phi}(\mathcal{E}, \mathbf{X}) - \sqrt{1 - ar{lpha}_t} \epsilon_{ heta}(\mathbf{y}_t, t, \mathcal{E}, \mathbf{X}) 
ight)$ 1095 if i > 1 then 7: 8: Draw  $z \sim \mathcal{N}(0, I)$ 9: Update  $y_{t-1}$  using the modified non-Markovian reverse process: 1099  $\mathbf{y}_{t-1} = \sqrt{\bar{\alpha}_{\tau_{i-1}}} \hat{\mathbf{y}}_0 + (1 - \sqrt{\bar{\alpha}_{\tau_{i-1}}}) g_{\phi}(\mathcal{E}, \mathbf{X}) + \sqrt{1 - \bar{\alpha}_{\tau_{i-1}} - \sigma_t^2} \epsilon_{\theta}(\mathbf{y}_t, t, \mathcal{E}, \mathbf{X}) + \sigma_t z$ 1100 1101 10: else 1102 11: Set  $\mathbf{y}_{t-1} = \hat{\mathbf{y}}_0$ 1103 12: end if 1104 13: end for 1105 14: return  $y_0$ 1106 1107

# <sup>1108</sup> J IMPLEMENTATION DETAIL

1109

All experiments were conducted on a Linux machine equipped with an Nvidia GeForce RTX 3090. The CUDA version used was 11.1, and the driver version was 455.45.01. We implemented our algorithm and the corresponding baseline methods using PyTorch (Paszke et al., 2019) and the graph computation framework Pytorch-Geometric (Fey & Lenssen, 2019). For the Random Forest (RF) and Extreme Gradient Boosting Tree (XGBT) that serve as conditional anomaly estimators, we used the RF version implemented in the Scikit-Learn library Pedregosa et al. (2011). For XGBoost Chen & Guestrin (2016), we utilized its official implementation.

We initialize the latent vectors for all models with a Gaussian Distribution, having a mean value of 0 and a standard deviation of 0.01. To ensure a level playing field, the dimension of the hidden layer for all baseline models, as well as our CGADM, is set to 64. We conducted a grid search for hyper-parameter tuning. The learning rates were selected from the set [0.005, 0.01, 0.02, 0.05]. To prevent overfitting, we incorporated an L2 norm with the coefficient tuned from the set [0.001, 0.005, 0.01, 0.02, 0.01].
1120 0.02, 0.1]. For all methods, we selected the best models by implementing early stopping when the AUROC on the validation set did not increase for five consecutive epochs.

1124

# 1125 K EFFICACY IN HIGHLY IMBALANCED SCENARIOS

1127

We conducted additional experiments on the DGraph dataset Huang et al. (2022), a highly imbalanced real-world financial fraud detection dataset where anomalies constitute only 1.3% of the data.
The results are presented in Table 4:

As Table 4 illustrates, CGADM consistently outperforms all baseline methods on both AUPRC and
 AUROC metrics in this extremely imbalanced setting. Notably, the AUPRC metric demonstrates
 CGADM's ability to handle rare event detection by excelling in anomaly-specific precision and
 recall. Similarly, the superior AUROC indicates robust overall discriminative performance.

Method	AUPRC	AUROC
GCN	3.66	74.97
GIN	3.22	73.14
GraphSAGE	3.43	73.81
GAT	3.65	75.17
GAS	2.91	71.21
PCGNN	2.82	71.78
BWGNN	3.63	75.16
GHRN	3.68	75.15
CGADM	3.83	76.43

Metric	Dataset	GODM	CGenGA	CGADM (Ours)
AUPRC	Ellip	85.89	87.36	97.03
	Tolo	46.15	44.89	46.02
	Yelp	51.77	52.76	76.54
	Quest	15.11	15.34	18.51
	Reddit	5.55	5.78	5.79
AUROC	Ellip	93.92	96.07	99.34
	Tolo	76.42	78.95	79.68
	Yelp	84.33	85.65	92.69
	Quest	68.86	68.46	69.41
	Reddit	62.10	64.78	65.85

Table 5: Comparisons with Diffusion-based Data-centric Approaches

#### COMPARISONS WITH DIFFUSION-BASED DATA-CENTRIC APPROACHES L

We have conducted experiments to compare CGADM against the methods in GODM (Ma et al., 2024a) and CGenGA (Liu et al., 2023) on five benchmark datasets (*Elliptic, Tolo, Yelp, Quest*, and *Reddit*). For fair comparisons, we implemented the diffusion-based data-centric approaches following the settings and optimal detector configurations specified in their respective papers. We summarize the results in terms of AUPRC and AUROC in Table 5:

Our results demonstrate that CGADM consistently outperforms GODM Ma et al. (2024a) and CGenGA Liu et al. (2023) across almost all datasets in both AUPRC and AUROC metrics. This superior performance underscores the advantages of our generative framework in directly modeling the joint anomaly distribution, as opposed to relying on downstream discriminative classifiers.

#### **EMPIRICAL RESULTS ON EFFICIENCY** Μ

To provide concrete evidence, we conducted experiments to compare memory usage and inference time with all the baselines specifically designed for anomaly detection on the *Elliptic* dataset, which contains 203,769 nodes and 234,355 edges. The results are summarized in Table 6:

180	Model	Memory (MB)	Inference Time (s)
181 182	GAS	1418	2.3865
183	PCGN	914	0.0827
184	BWGNN	446	0.1185
185	GHRN	924	0.1249
186	CGADM (ours)	1048	0.5691

Table 6: Memory usage and inference time comparison on the Elliptic dataset.

1188 We have the following observation:

- **Memory Efficiency:** The use of sparse matrix computations ensures that CGADM remains efficient in terms of memory usage, even for large-scale graphs. The marginal increase in memory usage is negligible compared to the scalability benefits.
- **Inference Time:** While our inference time is higher than most discriminative methods, the increase is justified given the novel generative anomaly detection paradigm. Considering the already low baseline inference time of anomaly detection tasks, the additional time overhead is acceptable, especially in scenarios where performance improvements are critical.

## N ADDITIONAL EXPERIMENT RESULTS

We have also conducted experiments comparing our Conditional Graph Anomaly Diffusion Model (CGADM) with XGBGraph (Tang et al., 2023) and CONSISGAD (Chen et al., 2024) on the same datasets. Below, we present the results in terms of AUPRC and AUROC in Table 7 and 8, two widely used metrics in the anomaly detection domain:

Model	Ellip	Tolo	Yelp	Quest	Reddit
XGBGraph	90.47	44.47	75.91	14.33	4.59
CONSISGAD	86.42	40.59	41.74	12.85	5.57
Ours (CGADM)	97.03	46.02	76.54	18.51	5.79

Table 7: Comparison of AUPRC results with XGBGraph and CONSISGAD.

Model	Ellip	Tolo	Yelp	Quest	Reddit
XGBGraph	94.35	77.28	91.85	64.90	60.58
CONSISGAD	96.38	76.03	79.35	70.54	66.99
Ours (CGADM)	99.34	79.68	92.69	69.41	65.85

Table 8: Comparison of AUROC results with XGBGraph and CONSISGAD.

We computed the **F1-scores** for our model and baseline methods across all datasets. These results further confirm the superior performance of our model. Table 9 presents the F1-scores, which show consistency with the experiment results in Table 1.

Model	Ellip	Tolo	Yelp	Quest	Reddi
GCN	73.672	47.376	27.658	6.856	7.794
GIN	75.338	49.443	42.214	10.288	6.443
GraphSAGE	81.096	50.226	43.949	12.041	10.075
GAŤ	80.498	50.878	48.891	11.157	8.432
GAS	77.844	48.253	43.404	10.867	9.071
PCGNN	45.090	47.213	44.608	5.796	6.981
BWGNN	83.134	49.983	47.323	12.788	6.501
GHRN	85.678	51.493	45.970	12.696	6.702
xGBGraph	87.555	51.079	65.121	16.088	2.954
CONSISGAD	79.120	49.762	41.606	9.848	6.443
Ours (CGADM)	93.390	51.595	69.396	17.162	9.754

Table 9: F1-scores comparison across datasets.

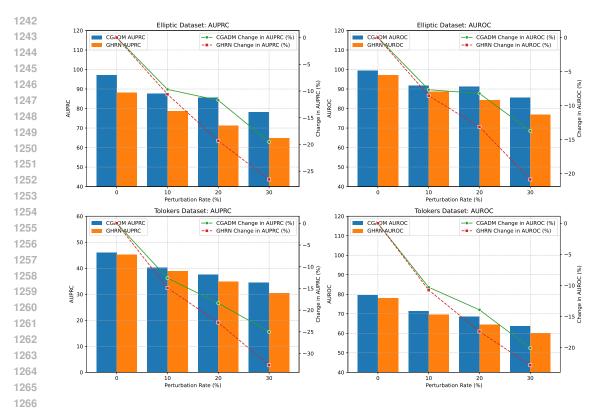


Figure 5: Robustness against Feature Manipulation

# O ROBUSTNESS OF CGADM AGAINST FEATURE MANIPULATION

To evaluate the robustness of CGADM against feature manipulation, we introduced feature perturbations in the Elliptic and Tolokers datasets. Specifically, we randomly perturbed the features of nodes with varying proportions (10%, 20%, and 30%) by randomly selecting values from their possible ranges with uniform probability. We then compared the performance of CGADM with GHRN (the best-performing baseline from our original experiments) under these conditions.

The results are summarized in Figure 5. As the proportion of perturbed nodes increases, the performance of both models decreases. However, CGADM consistently exhibits a slower decline compared to GHRN. This highlights CGADM's superior robustness to feature perturbations, which we attribute to its denoising reconstruction mechanism. This mechanism leverages information from neighboring nodes during the reverse diffusion process to iteratively restore the true anomaly signals.

# 1283 P EFFECT OF HIGH- AND LOW-FREQUENCY SIGNALS

To further substantiate that the high-frequency components are indeed reflected in the residual propagations, we designed an ablation study comparing our original CGADM (denoted as  $CGADM_{HP}$ ) with a variant (denoted as  $CGADM_{LP}$ ) that only propagates low-frequency sig-

$$\frac{1}{|\mathcal{N}(v)|+1} \left( \mathbf{h}_{v}^{l-1} + \sum_{u \in \mathcal{N}(v)} \mathbf{h}_{u}^{l-1} \right),$$
(39)

1288

1282

1267 1268 1269

1270

1291

where the feature representation is averaged across the node and its neighbors, propagating only low-frequency signals.

1295 We conducted experiments on the *Elliptic* and *YelpChi* datasets, varying the number of GNN layers in the denoiser module. The results are shown in Table 10:

GN	IN Layers	Model	AUPRC (Elliptic) %	AUROC (Elliptic) %	AUPRC (YelpChi) %	AUROC (Yelp(
	1	$CGADM_{HP}$	97.13	99.22	75.04	92.37
		$CGADM_{LP}$	95.71	98.43	72.23	91.88
	2	$CGADM_{HP}$	97.31	99.38	75.20	92.62
	2	$CGADM_{LP}$	93.73	97.60	70.92	90.88
	3	$CGADM_{HP}$	97.32	99.44	76.54	92.69
		$CGADM_{LP}$	90.83	95.58	71.43	89.64
	4	$CGADM_{HP}$	97.53	99.44	77.27	93.05
	-	$CGADM_{LP}$	87.12	92.60	69.98	87.71
	5	$CGADM_{HP}$	97.57	99.50	77.29	92.92
		$CGADM_{LP}$	81.20	89.49	68.71	86.08
Га	ole 10: I	Performance of	comparison of Co	$GADM_{HP}$ and $CC$	$GADM_{LP}$ with va	rying GNN l
Acc	ording t	o Table 10, w	e have the follow	ving observations:		
	fre acr inf	quency signa coss all metric formation for a	ls through residents and datasets. The	rvation Matters: ual propagation, consisting highlights the important of the second se	onsistently outperf	Forms CGAL ving high-fre
	-	•	-	~~ +	a	
				r $CGADM_{LP}$ , per		
	nu	mber of GNN	J layers increase	s. This is indicativ	ve of the well-kno	wn over-smo
				ow-pass filters cau		
				n. Conversely, $CG$		
	for	mance even i	mproves slightly	with additional lay	ers, demonstrating	the effective
				g over-smoothing.	,	
	res	iduai propaga	aton in initigating	5 over-smoothing.		
	3 Ito	rative Refine	ment Amplifier	<b>Over-Smoothing:</b>	In the context of c	ur diffusion
	the	: iterative refi	nement process i	repeatedly aggregat	tes neighborhood i	nformation,
	bat	ing the impac	t of over-smooth	ing in $CGADM_{LP}$	This leads to a fa	ilure to capt
				n stage of refineme		
	thi	s issue by leve	eraging high-free	quency signals to re	fine anomaly detec	ction through
	iter	rative process				-
		1				
Ç	Сом	PARISON W	/ітн Дата-аі	JGMENTATION ]	Methods	
C						
_			~~.~.			
'he	main di	istinction betw	ween CGADM a	nd the existing data	-augmentation me	thods lies in
lerl	ving and	proach to anor	naly detection. V	Vhile prior works fo	cus on using diffus	ion models f
				formance, CGADM		
				stribution of anoma	alles on the entire	graph. Belo
sum	marize	the key differ	ences:			
	~ ·		. 1 . 000 0	1 12	1.00	
				ses a graph-specific		
	fac	tual represent	tations by transfe	orming normal neig	ghbors into anomal	ous ones. T
				nique to enhance an		
	Cia	solution and and	,mentation techn	ique to enhance an	omary distinguishe	ionny.
	• "	GAD (Done )	at al 2024), Error	Nove diffusion mod	als to generate mor	inulated not
				ploys diffusion mod		
	enl	nancing graph	is by creating au	gmented data. This	technique is used	as a <b>data en</b>
				e learning framewo		
		mount w	a contrastiv	- isuning numewo		
	• Co	nGNN (Li et	al., 2024): Intro	oduces a generator	based on diffusion	n models to
			geregation and c	reate augmented d	iata for better ano	mary detecti
	for	mance.				
	• GE	) (Liu et al., 2	:024): Tackles th	e label imbalance p	roblem by generat	ting positive
				the latent space. The		
	- D14	ъ пяще я ан	asion model m t		ie prinning gour 18	
			1.	· · · · · · · · · · · · · · · · · · ·		
		t directly dete	ct anomalies.	<u>I</u>		
	not	t directly dete		-	1:66	
	not • Dit	t directly dete ffad (Ma et a	1., 2024b): Inves	stigates denoising d		synthesize
	not • Dit	t directly dete ffad (Ma et a	1., 2024b): Inves	stigates denoising d		synthesize
	not	t directly dete		-	diffusion models to	
	not • Dif str	t directly dete ffad (Ma et a r <b>uctures</b> and e	1., 2024b): Inves	stigates denoising c methods. This app		synthe

We have conducted a detailed experimental comparison of our proposed Conditional Graph Anomaly Diffusion Model (CGADM) with some diffusion-based data augmentation methods CA-GAD (Xiao et al., 2024), DEGAD (Pang et al., 2024), ConGNN (Li et al., 2024), GD (Liu et al., 2024), and Diffad (Ma et al., 2024b). We analyzed their performance across several standard bench-mark datasets (Elliptic, Tolokers, and YelpChi), and the key results are summarized below:

1355					
1356	Metric	Model	Ellip	Tolo	Yelp
1357		CAGAD	89.75	40.80	72.30
1358		DEGAD	93.86	43.51	75.11
1359	AUPRC	ConGNN	91.60	42.22	73.60
1360		GD	88.63	39.90	68.01
1361		Diffad	90.05	41.75	71.28
1362		CGADM	97.28	45.11	76.54
1363		CAGAD	94.82	72.22	90.34
1364		DEGAD	97.88	76.20	92.22
1365	AUROC	ConGNN	95.60	74.56	91.33
1366		GD	93.53	70.70	83.84
1367		Diffad	92.72	73.31	88.21
1368		CGADM	99.34	78.11	92.69

Table 11: AUPRC and AUROC comparison with Data Augmentation Methods

As shown in the Table 11, CGADM consistently outperforms the data-augmentation methods in both AUPRC and AUROC across all datasets. This underscores the efficacy of our generative framework in addressing graph anomaly detection challenges.