# Generative Semi-supervised Graph Anomaly Detection

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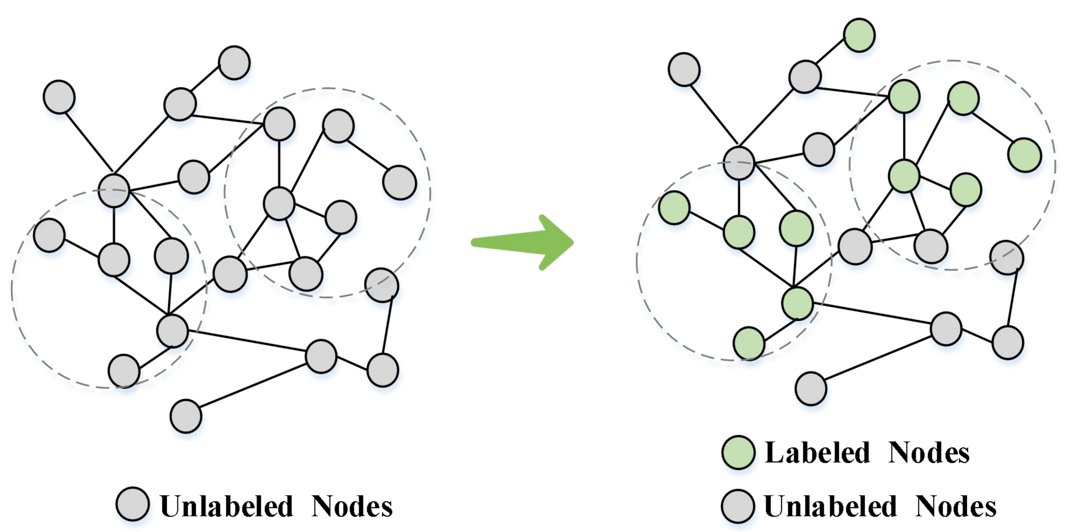
## Motivation

This work considers a practical **semi-supervised graph anomaly detection (GAD) scenario**, where part of the nodes in a graph are known to be normal, contrasting to the extensively explored unsupervised setting with a fully unlabeled graph.

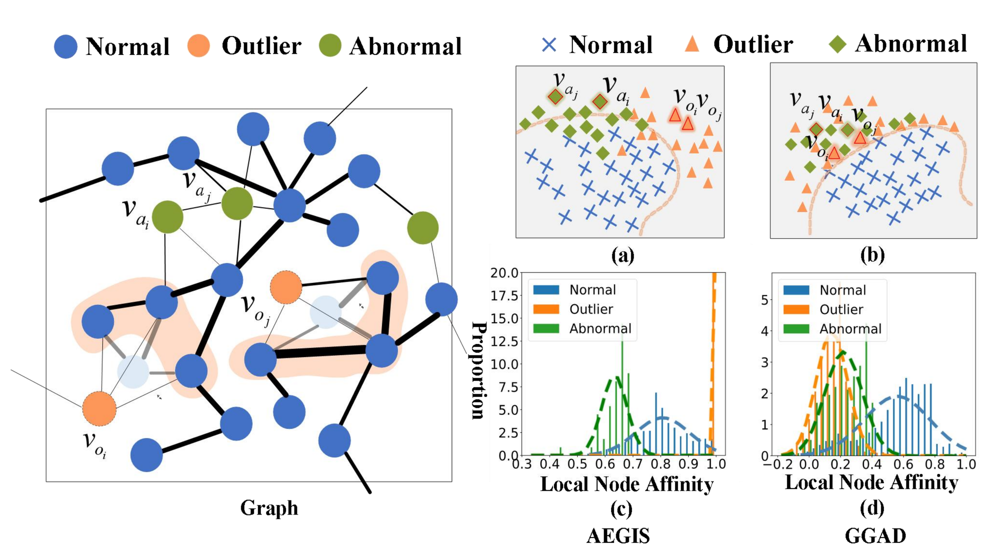




Unsupervised

Partial Normal Labeled Supervised

Randomly sample some nodes from the graph as the normal nodes, without any human manual labeling (the same labeling cost as unsupervised GAD).

## Two Important Priors about Anomalies




**Asymmetric local affinity**

The affinity between normal nodes is typically significantly stronger than that between normal and abnormal nodes.

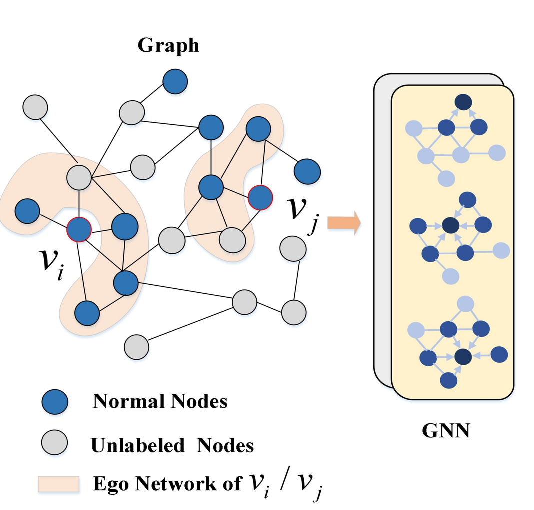
**Egocentric closeness**

The outliers should be closed to the normal nodes that share similar local structure due to subtle abnormality or adversarial camouflage.

## Key idea

The key idea is to generate pseudo anomaly nodes, referred to as 'outlier nodes', for providing effective negative node samples in training a discriminative one-class classifier.

## Graph Neural Network for Node Representation




$$\mathbf{H}^{(l)} = GNN(\mathbf{A},\mathbf{H}^{(l-1)};\mathbf{W}^{(l-1)}) \quad \mathbf{H}^{(l)}\in\mathbb{R}^{N\times h^{(l)}}, \mathbf{H}^{(l-1)}\in\mathbb{R}^{N\times h^{(l-1)}}$$

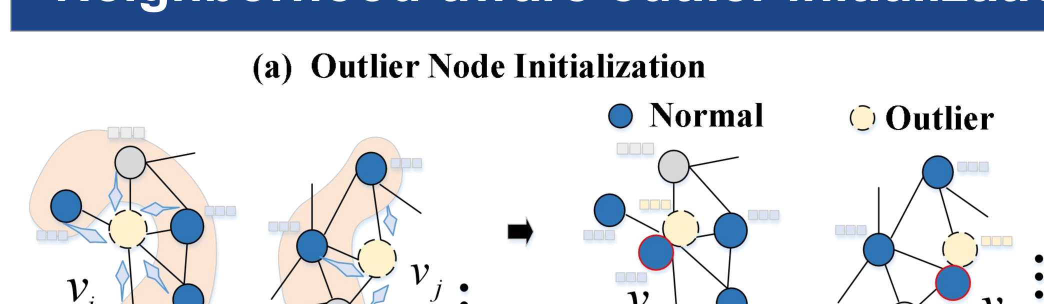
$\mathbf{W}^{(l)}$ learnable parameters $\quad \mathbf{H}^{(0)} = \mathbf{X}$

$\mathbf{H}_i^{(l)}$ are the embeddings of node $v_i$

Employ a 2-layer GCN due to its high efficiency

$$\mathbf{H}^{(\ell)} = \phi\left(\mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}}\mathbf{H}^{(\ell-1)}\mathbf{W}^{(\ell-1)}\right)$$

## Neighborhood-aware outlier initialization

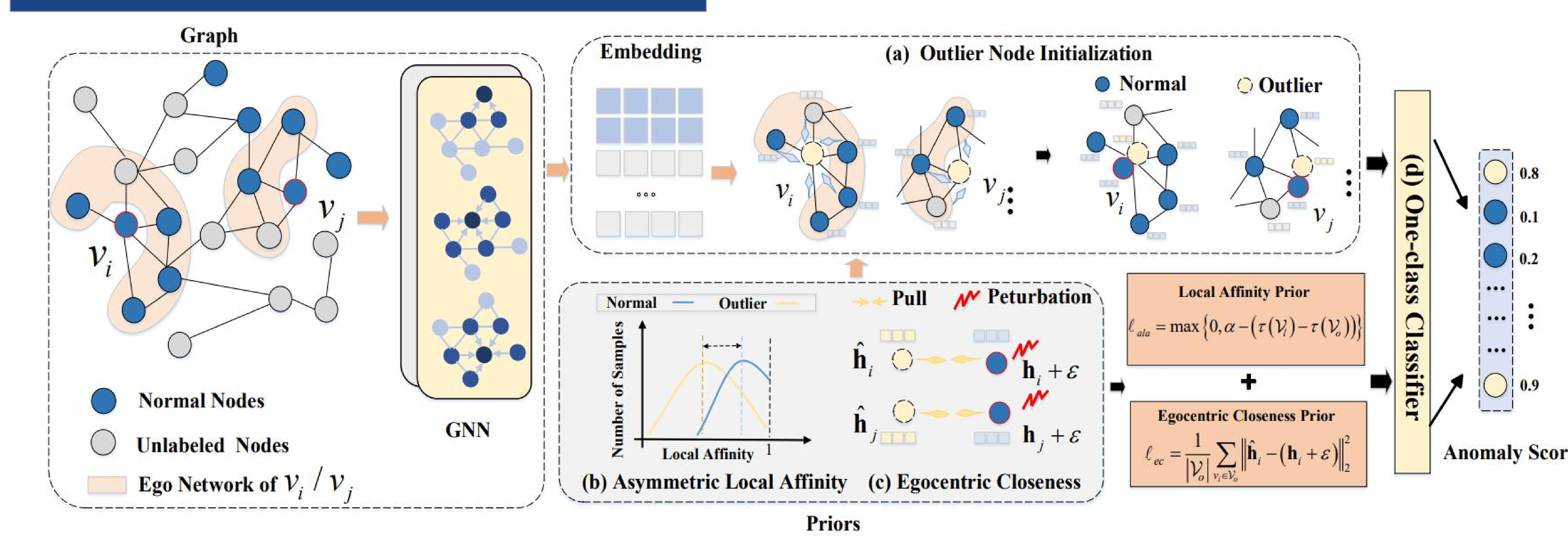



We sample a set of normal nodes from normal set and respectively generate an outlier node for each of them based on its ego network.

$$\hat{\mathbf{h}}_i = \Psi(v_i, \mathcal{N}(v_i);\Theta_g) = \frac{1}{|\mathcal{N}(v_i)|}\sum_{v_j\in\mathcal{N}(v_i)} \sigma(\widetilde{\mathbf{W}}\mathbf{h}_j)$$

$\Psi$ is a mapping function determined by parameters $\Theta_g$ and $\widetilde{\mathbf{W}}\in\mathbb{R}^{d\times d}$ are the learnable parameter

## The Framework of GGAD




## Incorporating the Asymmetric Local Affinity Prior

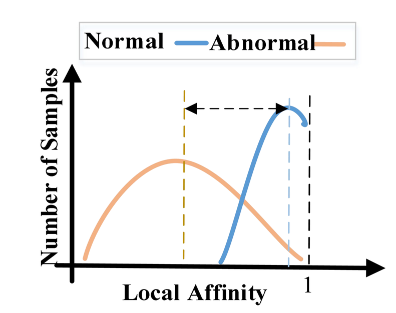
- **Local Node Affinity Calculation**

$$\tau(v_i) = \frac{1}{|\mathcal{N}(v_i)|}\sum_{v_j\in\mathcal{N}(v_i)} \mathrm{sim}(\mathbf{h}_i,\mathbf{h}_j) \qquad \tau(\mathcal{V}_l) = \frac{1}{|\mathcal{V}_l|}\sum_{v_i\in\mathcal{V}_l}\tau(v_i) \qquad \tau(\mathcal{V}_o) = \frac{1}{|\mathcal{V}_o|}\sum_{v_i\in\mathcal{V}_o}\tau(v_i)$$

$\mathcal{V}_o$ and $\mathcal{V}_l$ are the sets of abnormal nodes and normal nodes

- **Enforcing the Structural Affinity Prior**

$$\ell_{ala} = \max\{0, \alpha - (\tau(\mathcal{V}_l) - \tau(\mathcal{V}_o))\}$$ Margin loss function




Asymmetric Local Affinity

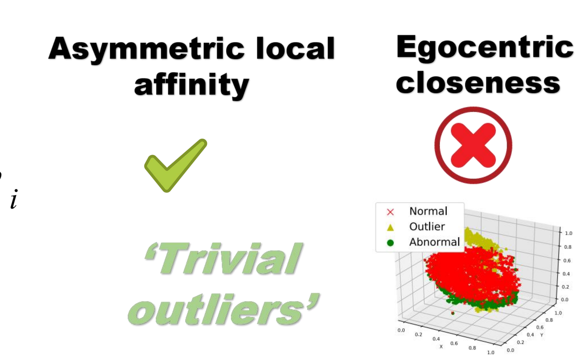
## Incorporating the Egocentric Closeness Prior

Solely using this local affinity prior may distribute far away from the normal nodes in the representation space.

$$\ell_{ec} = \frac{1}{|\mathcal{V}_o|}\sum_{v_i\in\mathcal{V}_o}\left\|\hat{\mathbf{h}}_i - (\mathbf{h}_i + \varepsilon)\right\|_2^2$$

$\mathbf{h}_i$ and $\hat{\mathbf{h}}_i$ are the representations of the normal node $v_i$ and its corresponding generated outliers

$\varepsilon$ is a noise perturbation generated from a Gaussian distribution to guarantee separability




## Training and Inference

- **Binary cross-entropy loss function**

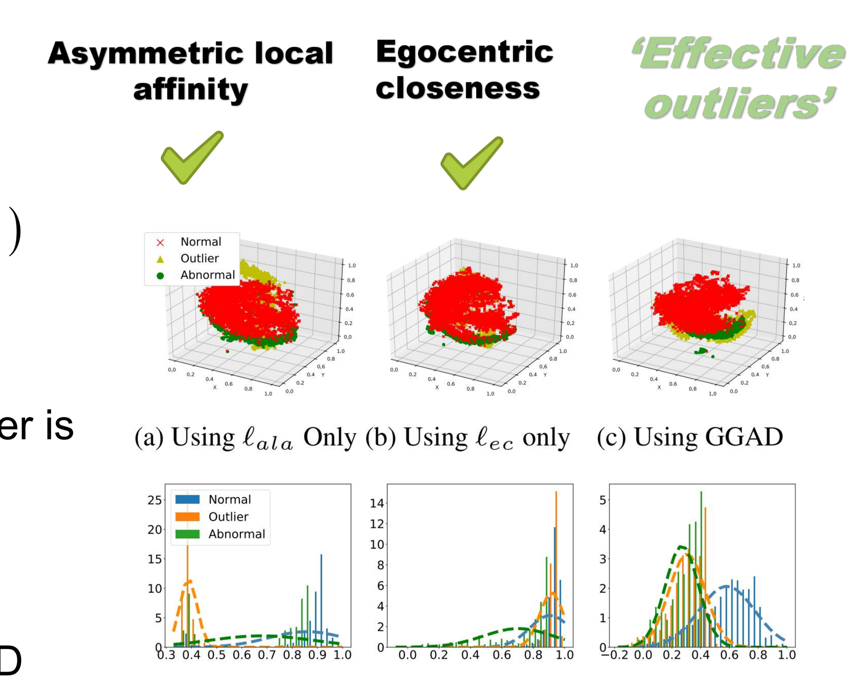
$$\ell_{bce} = \sum_{i}^{|\mathcal{V}_o|+|\mathcal{V}_l|} y_i\log(p_i) + (1-y_i)\log(1-p_i)$$

$$\ell_{total} = \ell_{bce} + \beta\ell_{ala} + \lambda\ell_{ec}$$

The inverse prediction of the one-class classifier is used as the anomaly score

$$\mathrm{score}(v_j) = 1 - \eta(\mathbf{h}_j;\Theta^*)$$

where $\Theta^*$ is the learned parameters of GGAD




(a) Using $\ell_{ala}$ Only (b) Using $\ell_{ec}$ only (c) Using GGAD

(d) Using $\ell_{ala}$ Only (e) Using $\ell_{ec}$ Only (f) Using GGAD

## Main Comparison Restult

| Setting | Method | AUROC Amazon | AUROC T-Finance | AUROC Reddit | AUROC Elliptic | AUROC Photo | AUROC DGraph | AUPRC Amazon | AUPRC T-Finance | AUPRC Reddit | AUPRC Elliptic | AUPRC Photo | AUPRC DGraph |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Unsupervised | DOMINANT | 0.7025 | 0.6087 | 0.5105 | 0.2960 | 0.5136 | 0.5738 | 0.1315 | 0.0536 | 0.0380 | 0.0454 | 0.1039 | 0.0075 |
| | AnomalyDAE | 0.7783 | 0.5809 | 0.5091 | 0.4963 | 0.5069 | 0.5763 | 0.1429 | 0.0491 | 0.0319 | 0.0872 | 0.0987 | 0.0070 |
| | OCGNN | 0.7165 | 0.4732 | 0.5246 | 0.2581 | 0.5307 | / | 0.1352 | 0.0392 | 0.0375 | 0.0616 | 0.0965 | / |
| | AEGIS | 0.6059 | 0.6496 | 0.5349 | 0.4553 | 0.5516 | 0.4509 | 0.1200 | 0.0622 | 0.0413 | 0.0827 | 0.0972 | 0.0053 |
| | GAAN | 0.6513 | 0.3091 | 0.5216 | 0.2590 | 0.4296 | / | 0.0852 | 0.0283 | 0.0348 | 0.0436 | 0.0767 | / |
| | TAM | 0.8303 | 0.6175 | 0.6062 | 0.4039 | 0.5675 | / | 0.4024 | 0.0547 | 0.0437 | 0.0502 | 0.1013 | / |
| Semi-supervised | DOMINANT | 0.8867 | 0.6167 | 0.5194 | 0.3256 | 0.5314 | 0.5851 | 0.7289 | 0.0542 | 0.0414 | 0.0652 | 0.1283 | 0.0076 |
| | AnomalyDAE | 0.9171 | 0.6027 | 0.5280 | 0.5409 | 0.5272 | 0.5866 | 0.7748 | 0.0538 | 0.0362 | 0.0949 | 0.1177 | 0.0071 |
| | OCGNN | 0.8810 | 0.5742 | 0.5622 | 0.2881 | 0.6461 | / | 0.7538 | 0.0492 | 0.0400 | 0.0640 | **0.1501** | / |
| | AEGIS | 0.7593 | 0.6728 | 0.5605 | 0.5132 | 0.5936 | 0.4450 | 0.2616 | 0.0685 | 0.0441 | 0.0912 | 0.1110 | 0.0058 |
| | GAAN | 0.6531 | 0.3636 | 0.5349 | 0.2724 | 0.4355 | / | 0.0856 | 0.0324 | 0.0362 | 0.0611 | 0.0768 | / |
| | TAM | 0.8405 | 0.5923 | 0.5829 | 0.4150 | 0.6013 | / | 0.5183 | 0.0551 | 0.0446 | 0.0552 | 0.1087 | / |
| | **GGAD (Ours)** | **0.9443** | **0.8228** | **0.6354** | **0.7290** | **0.6476** | **0.5943** | **0.7922** | **0.1825** | **0.0610** | **0.2425** | 0.1442 | **0.0082** |

## Ablation Study

- By unifying both priors through the two losses, the generated outlier nodes can be thought as hard anomalies that lie at the fringe of normal nodes in the feature representation space

Ablation study on our two priors

| Metric | $\ell_{ala}$ | $\ell_{ec}$ | Amazon | T-Finance | Reddit | Elliptic | Photo | DGraph |
|---|---|---|---|---|---|---|---|---|
| AUROC | | ✓ | 0.8871 | 0.8149 | 0.5839 | 0.6863 | 0.5762 | 0.5891 |
| | ✓ | | 0.7250 | 0.6994 | 0.5230 | 0.7001 | 0.6103 | 0.5513 |
| | ✓ | ✓ | **0.9324** | **0.8228** | **0.6354** | **0.7290** | **0.6476** | **0.5943** |
| AUPRC | | ✓ | 0.6643 | 0.1739 | 0.0409 | 0.1954 | 0.1137 | 0.0076 |
| | ✓ | | 0.1783 | 0.0800 | 0.0398 | **0.2683** | 0.1186 | 0.0063 |
| | ✓ | ✓ | **0.7843** | **0.1924** | **0.0610** | 0.2425 | **0.1442** | **0.0087** |

GGAD vs. alternative outlier generators

| Metric | Method | Amazon | T-Finance | Reddit | Elliptic | Photo | DGraph |
|---|---|---|---|---|---|---|---|
| AUROC | Random | 0.7263 | 0.4613 | 0.5227 | 0.6856 | 0.5678 | 0.5712 |
| | NLO | 0.8613 | 0.6179 | 0.5638 | 0.6787 | 0.5307 | 0.5538 |
| | Noise | 0.8508 | 0.8204 | 0.5285 | 0.6786 | 0.5940 | 0.5779 |
| | GaussianP | 0.2279 | 0.6659 | 0.5235 | 0.6715 | 0.5925 | 0.5862 |
| | VAE | 0.8984 | 0.6674 | 0.6175 | 0.7055 | 0.6222 | 0.5801 |
| | GAN | 0.8288 | 0.5487 | 0.5378 | 0.6256 | 0.6032 | 0.5101 |
| | **GGAD (Ours)** | **0.9324** | **0.8228** | **0.6354** | **0.7290** | **0.6476** | **0.5943** |
| AUPRC | Random | 0.1755 | 0.0402 | 0.0394 | 0.1981 | 0.1063 | 0.0061 |
| | NLO | 0.4696 | 0.1364 | 0.0495 | 0.1750 | 0.1092 | 0.0065 |
| | Noise | 0.5384 | 0.1762 | 0.0381 | 0.1924 | 0.1200 | 0.0076 |
| | GaussianP | 0.0397 | 0.0677 | 0.0376 | 0.1682 | 0.1194 | 0.0078 |
| | VAE | 0.6111 | 0.0652 | 0.0528 | 0.2344 | 0.1272 | 0.0063 |
| | GAN | 0.3715 | 0.0461 | 0.0433 | 0.1263 | 0.1143 | 0.0051 |
| | **GGAD (Ours)** | **0.7843** | **0.1924** | **0.0610** | **0.2425** | **0.1442** | **0.0087** |

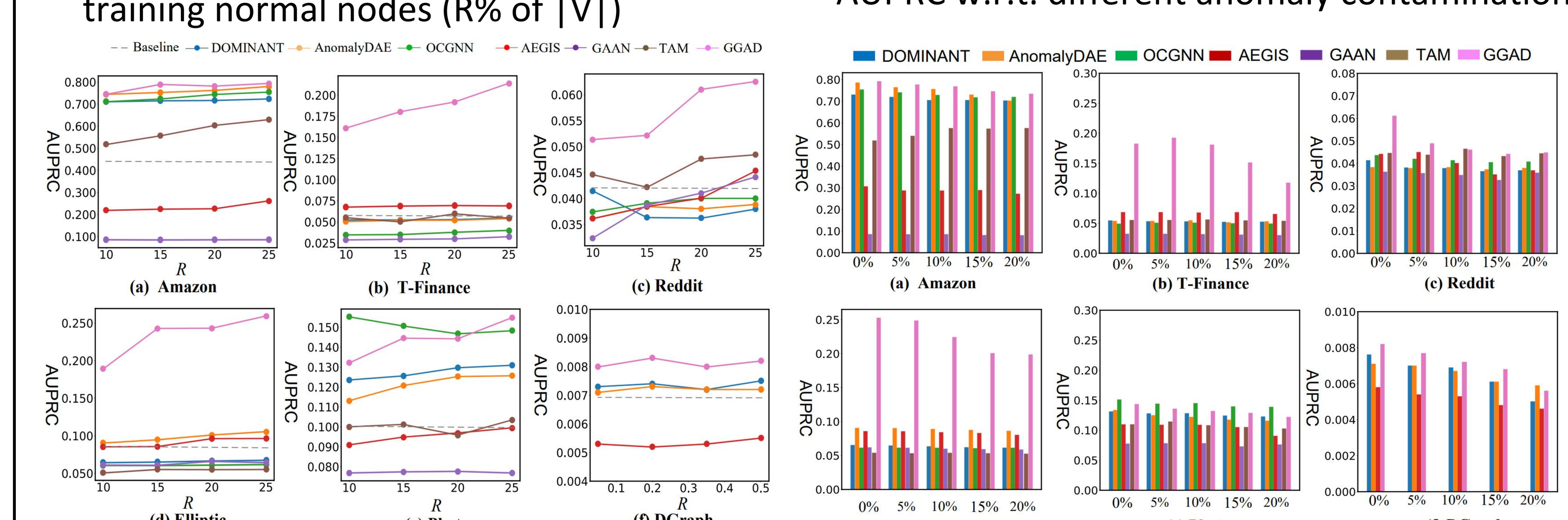
- Random
- Nonlearnable Outliers (NLO)
- Gaussian Perturbation
- Noise and GaussianP
- VAE and GAN

## Performance w.r.t. Training Size and Anomaly Contamination

- With increasing training samples of normal nodes, the performance of all methods generally gets improved
- GGAD consistently maintains the best performance under different contamination rates, showing good robustness w.r.t. the contamination

AUPRC results w.r.t. different number of training normal nodes (R% of |V|)

AUPRC w.r.t. different anomaly contamination




## GGAD enabled Unsupervised Methods

- We incorporate the outlier generation into existing unsupervised method demonstrating the generation in GGAD can also benefit the existing unsupervised methods

GGAD enabled unsupervised methods

| Metric | Method | Amazon | T-Finance | Elliptic |
|---|---|---|---|---|
| #Anomalies/#Top-K Nodes | | 387/500 | 351/1000 | 1448/2000 |
| AUROC | DOMINATE | 0.7025 | 0.6087 | 0.2960 |
| | GGAD-enabled DOMINATE | 0.8186 | 0.6275 | 0.2986 |
| | OCGNN | 0.7165 | 0.4732 | 0.2581 |
| | GGAD-enabled OCGNN | 0.8692 | 0.5931 | 0.2638 |
| | AEGIS | 0.6059 | 0.6496 | 0.4553 |
| | GGAD-enabled AEGIS | 0.8395 | 0.7024 | 0.5036 |
| | GGAD | 0.9431 | 0.8108 | 0.7225 |
| AUPRC | DOMINATE | 0.1315 | 0.0536 | 0.0454 |
| | GGAD-enabled DOMINATE | 0.3462 | 0.0585 | 0.0613 |
| | OCGNN | 0.1352 | 0.0392 | 0.0616 |
| | GGAD-enabled OCGNN | 0.3950 | 0.0480 | 0.0607 |
| | AEGIS | 0.1200 | 0.0622 | 0.0827 |
| | GGAD-enabled AEGIS | 0.3833 | 0.0784 | 0.0910 |
| | GGAD | 0.7769 | 0.1734 | 0.2484 |

- The distribution of the generated outliers have much smaller MMD distance

Analysis of the generated outliers using MMD distance

| Metric | Amazon | T-Finance | Elliptic | Photo | Reddit |
|---|---|---|---|---|---|
| with Abnormal Node | **0.1980** | **0.0784** | **0.1094** | **0.3703** | **0.3409** |
| with Normal Node | 0.2318 | 0.1040 | 0.1304 | 0.3880 | 0.3605 |

## Computational Efficiency Analysis

- GGAD is generally more efficient than existing unsupervised GAD methods

Runtimes (in seconds) on the six datasets on CPU

| Method | Amazon | T-Finance | Reddit | Elliptic | Photo | DGraph |
|---|---|---|---|---|---|---|
| DOMINANT | 1592 | 10721 | 125 | 1119 | 437 | 388 |
| AnomalyDAE | 1656 | 18560 | 161 | 8296 | 445 | 457 |
| OCGNN | 765 | 5717 | 162 | 3517 | 125 | / |
| AEGIS | 1121 | 15258 | 166 | 5638 | 417 | 1022 |
| GAAN | 1678 | 12120 | 94 | 1866 | 307 | / |
| TAM | 4516 | 17360 | 432 | 13200 | 165 | / |
| **GGAD (Ours)** | 658 | 9345 | 368 | 5146 | 106 | 488 |