GOOD-D: On Unsupervised Graph Out-Of-Distribution Detection

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https://github.com/yixinliu233/G-OOD-D.

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Reported by Nengqiang Xiang

Introduction

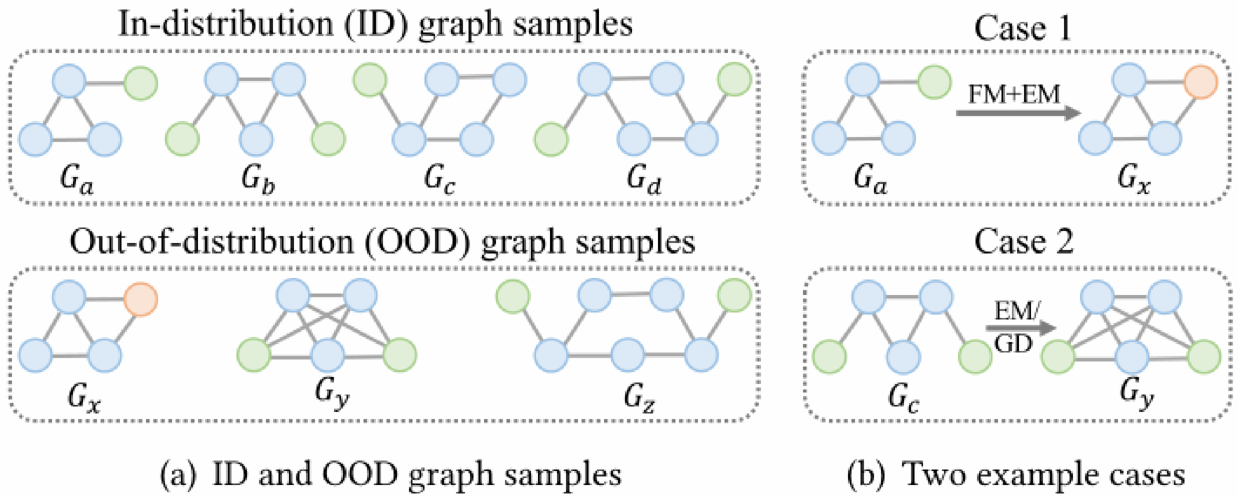


Figure 1: Toy examples of (a) ID graphs (G_a - G_d) and OOD graphs (G_x - G_z); and (b) perturbation-based augmentations (e.g., feature modification (FM), edge modification (EM), and graph diffusion (GD)) introducing OOD samples.

Current endeavors mostly focus on grid-structured data and its application for graph-structured data remains under-explored. Considering the fact that data labeling on graphs is commonly time-expensive and labor-intensive, the author studies the problem of unsupervised graph OOD detection,

To achieve this goal, the author develops a new graph contrastive learning framework GOOD-D for detecting OOD graphs without using any ground-truth labels.

Method

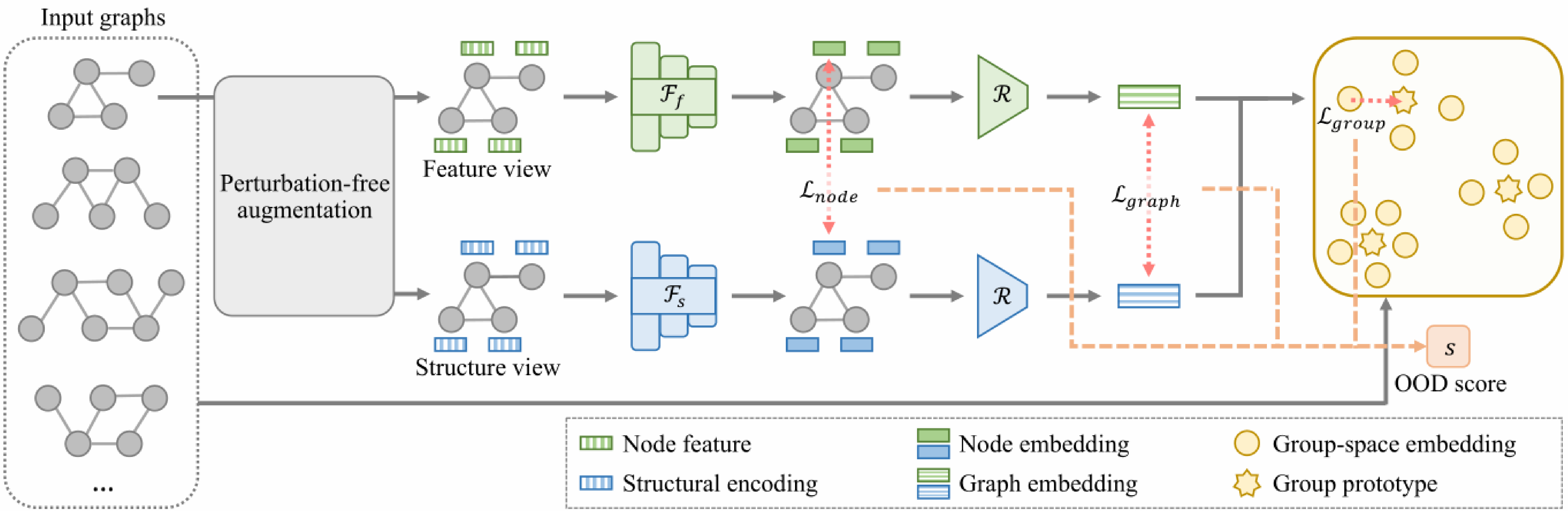
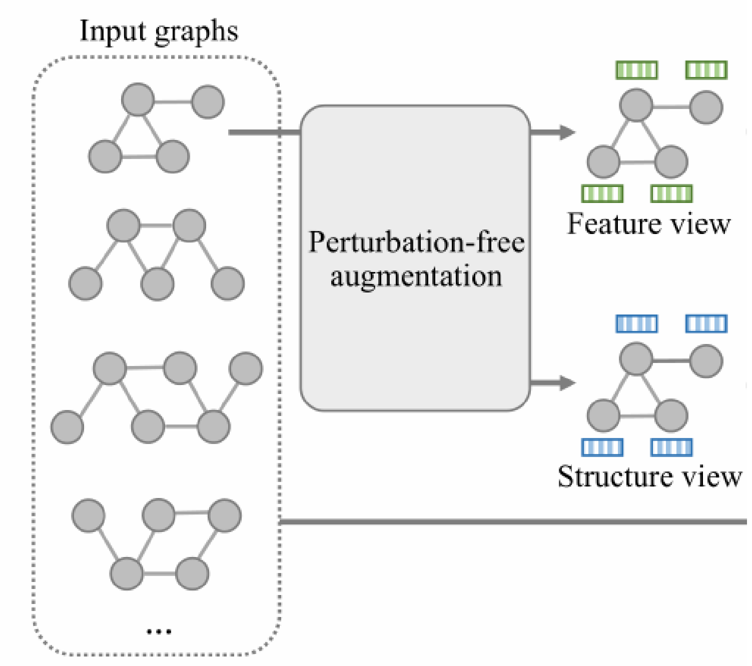


Figure 2: An overall illustration of the proposed method GOOD-D.

Method



PRELIMINARIES:

$$G = (\mathcal{V}, \mathcal{E}, \mathbf{X}) = (\mathbf{A}, \mathbf{X})$$

ID dataset $\mathcal{D}^{in} = \{G_1^{in}, \cdots G_{N_1}^{in}\} \in \mathbb{P}^{in}$

OOD dataset $\mathcal{D}^{out} = \{G_1^{out}, \cdots G_{N_2}^{out}\} \in \mathbb{P}^{out}$

Train: ID dataset $\mathcal{D}_{train}^{in} \subset \mathcal{D}^{in}$

Test: $\mathcal{D}_{test}^{in} \subset \mathcal{D}^{in} \, (\mathcal{D}_{test}^{in} \cap \mathcal{D}_{train}^{in} = \emptyset) \cup \mathcal{D}_{test}^{out} \subset \mathcal{D}^{out}$

Perturbation-free Graph Data Augmentation

$G_f = (\mathbf{A}, \mathbf{X}) \quad G_s = (\mathbf{A}, \mathbf{S})$

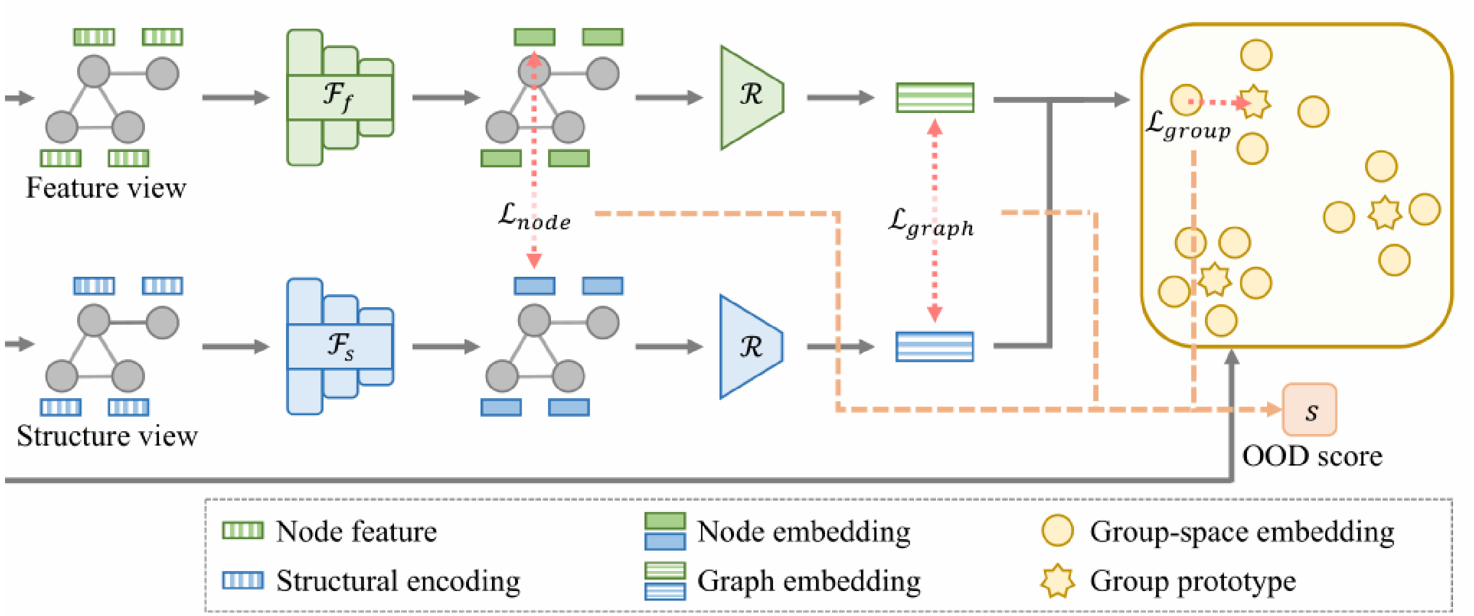
$$\mathbf{s}_i^{(rw)} = \left[\mathbf{T}_{ii}, \mathbf{T}_{ii}^2, \cdots, \mathbf{T}_{ii}^{d_s^{(rw)}} \right] \in \mathbb{R}^{d_s^{(rw)}}, \quad (1)$$

$\mathbf{T} = \mathbf{A}\mathbf{D}^{-1} \quad \mathbf{D}_{ii} = \sum_j \mathbf{A}_{ij}$

$$\mathbf{s}_{ik}^{(dg)} = \begin{cases} 1, k = \mathbf{D}_{ii} \text{ or } k = d_s^{(dg)} < \mathbf{D}_{ii} \\ 0, k \neq \mathbf{D}_{ii} \end{cases}, \quad (2)$$

$\mathbf{s}_i = [\mathbf{s}_i^{(rw)} || \mathbf{s}_i^{(dg)}]$

Method



graph embedding ⟵ readout function

$$\mathbf{h}_G^{(f)} = \sum_{v_i \in \mathcal{V}_G} \mathbf{h}_i^{(f)}, \quad \mathbf{h}_G^{(s)} = \sum_{v_i \in \mathcal{V}_G} \mathbf{h}_i^{(s)}, \tag{4}$$

Hierarchical Graph Contrastive Learning

GNN encoders and readout function：

$$\mathbf{h}_i^{(f,l)} = \mathrm{MLP}^{(f,l)}\left(\mathbf{h}_i^{(f,l-1)} + \sum_{v_j \in \mathcal{N}(v_i)} \mathbf{h}_j^{(f,l-1)}\right), \tag{3}$$

$$\mathbf{h}_i^{(f)} = [\mathbf{h}_i^{(f,1)} || \cdots || \mathbf{h}_i^{(f,L)}]$$

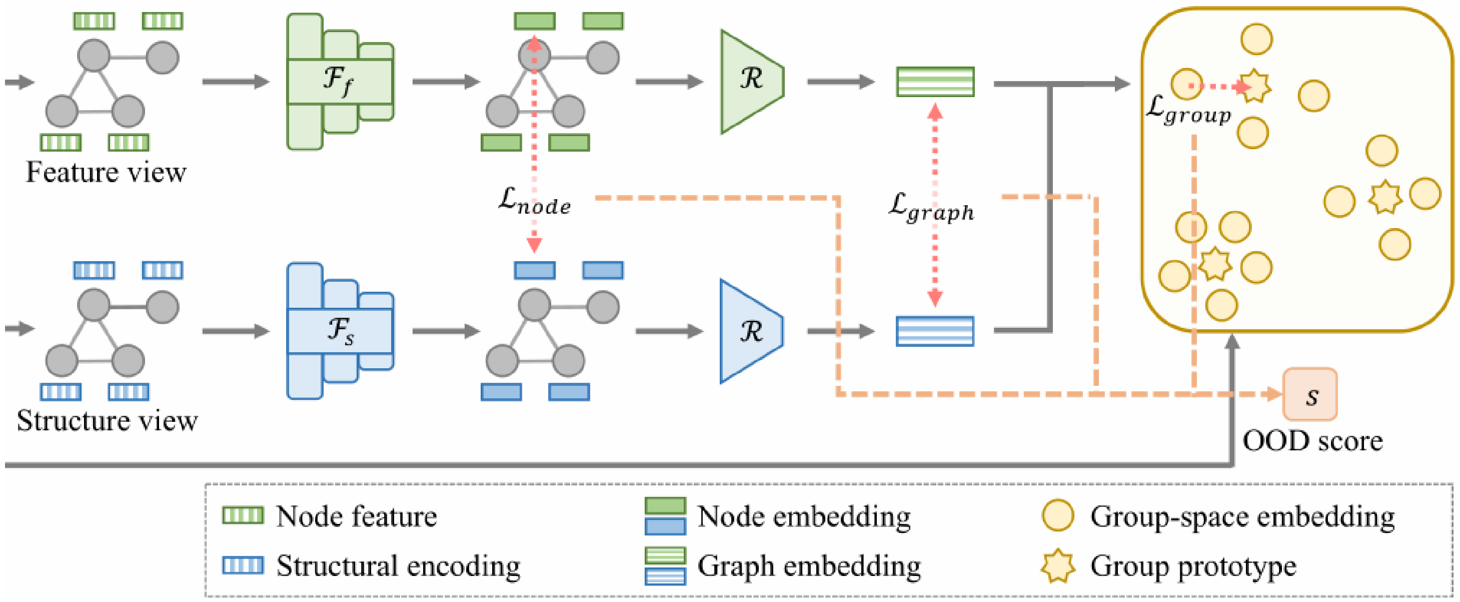
Node-levelcontrast：

$$\mathbf{h}_i^{(f)} \text{ and } \mathbf{h}_i^{(s)} \longrightarrow \mathbf{z}_i^{(f)} \text{ and } \mathbf{z}_i^{(s)}$$

$$\mathcal{L}_{node} = \frac{1}{|\mathcal{B}|} \sum_{G_j \in \mathcal{B}} \frac{1}{2|\mathcal{V}_{G_j}|} \sum_{v_i \in \mathcal{V}_{G_j}} \left[\ell(\mathbf{z}_i^{(f)}, \mathbf{z}_i^{(s)}) + \ell(\mathbf{z}_i^{(s)}, \mathbf{z}_i^{(f)})\right],$$

$$\ell(\mathbf{z}_i^{(f)}, \mathbf{z}_i^{(s)}) = -\log \frac{e^{\mathrm{sim}(\mathbf{z}_i^{(f)}, \mathbf{z}_i^{(s)})/\tau}}{\sum_{v_k \in \mathcal{V}_{G_j} \setminus v_i} e^{\mathrm{sim}(\mathbf{z}_i^{(f)}, \mathbf{z}_k^{(s)})/\tau}}, \tag{5}$$

Method



Graph-level contrast:

$$\mathbf{h}_G^{(f)} \text{ and } \mathbf{h}_G^{(s)} \longrightarrow \mathbf{z}_G^{(f)} \text{ and } \mathbf{z}_G^{(s)}$$

$$\mathcal{L}_{graph} = \frac{1}{2|\mathcal{B}|} \sum_{G_i \in \mathcal{B}} \left[\ell(\mathbf{z}_{G_i}^{(f)}, \mathbf{z}_{G_i}^{(s)}) + \ell(\mathbf{z}_{G_i}^{(s)}, \mathbf{z}_{G_i}^{(f)}) \right],$$

$$\ell(\mathbf{z}_{G_i}^{(f)}, \mathbf{z}_{G_i}^{(s)}) = -\log \frac{e^{\mathrm{sim}(\mathbf{z}_{G_i}^{(f)}, \mathbf{z}_{G_i}^{(s)})/\tau}}{\sum_{G_j \in \mathcal{B} \setminus G_i} e^{\mathrm{sim}(\mathbf{z}_{G_i}^{(f)}, \mathbf{z}_{G_j}^{(s)})/\tau}}, \quad (6)$$

Group-level contrast:

$$\text{concatenate } \mathbf{h}_{G_i}^{(f)} \text{ with } \mathbf{h}_{G_i}^{(s)} \longrightarrow \mathbf{z}_{G_i} \xrightarrow{\text{K-means}} C = \{\mathbf{c}_i\}_{i=1}^{K}$$

$$\mathcal{L}_{group} = -\frac{1}{|\mathcal{B}|} \sum_{G_i \in \mathcal{B}} \log \frac{e^{\mathrm{sim}(\mathbf{z}_{G_i}, \mathbf{c}_j)/\tau_j}}{\sum_{c_k \in C \setminus c_j} e^{\mathrm{sim}(\mathbf{z}_{G_i}, \mathbf{c}_k)/\tau_k}}, \quad (7)$$

$$\mathcal{L} = \mathcal{L}_{node} + \mathcal{L}_{graph} + \mathcal{L}_{group}. \quad (8)$$

Adaptive Training and OOD Scoring

$$s_{G_i} = s_{G_i}^{(node)} + s_{G_i}^{(graph)} + s_{G_i}^{(group)} \quad (9)$$

$$\mathcal{L} = (\sigma_{node})^{\alpha} \mathcal{L}_{node} + (\sigma_{graph})^{\alpha} \mathcal{L}_{graph} + (\sigma_{group})^{\alpha} \mathcal{L}_{group}, \quad (10)$$

$$s_{G_i} = \frac{s_{G_i}^{(node)} - \mu_{node}}{\sigma_{node}} + \frac{s_{G_i}^{(graph)} - \mu_{graph}}{\sigma_{graph}} + \frac{s_{G_i}^{(group)} - \mu_{group}}{\sigma_{group}}, \quad (11)$$

Experiments

Table 1: OOD detection results in terms of AUC (in percent, mean ± std). The best and runner-up results are highlighted with bold and underline, respectively.

ID dataset	BZR	PTC-MR	AIDS	ENZYMES	IMDB-M	Tox21	FreeSolv	BBBP	ClinTox	Esol	Avg.
OOD dataset	COX2	MUTAG	DHFR	PROTEIN	IMDB-B	SIDER	ToxCast	BACE	LIPO	MUV	Rank
PK-LOF	42.22±8.39	51.04±6.04	50.15±3.29	50.47±2.87	48.03±2.53	51.33±1.81	49.16±3.70	53.10±2.07	50.00±2.17	50.82±1.48	11.9
PK-OCSVM	42.55±8.26	49.71±6.58	50.17±3.30	50.46±2.78	48.07±2.41	51.33±1.81	48.82±3.29	53.05±2.10	50.06±2.19	51.00±1.33	11.8
PK-iF	51.46±1.62	54.29±4.33	51.10±1.43	51.67±2.69	50.67±2.47	49.87±0.82	52.28±1.87	51.47±1.33	50.81±1.10	50.85±3.51	10.1
WL-LOF	48.99±6.20	53.31±8.98	50.77±2.87	52.66±2.47	52.28±4.50	51.92±1.58	51.47±4.23	52.80±1.91	51.29±3.40	51.26±1.31	9.3
WL-OCSVM	49.16±4.51	53.31±7.57	50.98±2.71	51.77±2.21	51.38±2.39	51.08±1.46	50.38±3.81	52.85±2.00	50.77±3.69	50.97±1.65	10.0
WL-iF	50.24±2.49	51.43±2.02	50.10±0.44	51.17±2.01	51.07±2.25	50.25±0.96	52.60±2.38	50.78±0.75	50.41±2.17	50.61±1.96	11.3
InfoGraph-iF	63.17±9.74	51.43±5.19	93.10±1.35	60.00±1.83	58.73±1.96	56.28±0.81	56.92±1.69	53.68±2.90	48.51±1.87	54.16±5.14	7.4
InfoGraph-MD	86.14±6.77	50.79±8.49	69.02±11.67	55.25±3.51	**81.38**±1.14	59.97±2.06	58.05±5.46	70.49±4.63	48.12±5.72	77.57±1.69	6.5
GraphCL-iF	60.00±3.81	50.86±4.30	92.90±1.21	61.33±2.27	59.67±1.65	56.81±0.97	55.55±2.71	59.41±3.58	47.84±0.92	62.12±4.01	7.7
GraphCL-MD	83.64±6.00	73.03±2.38	93.75±2.13	52.87±6.11	79.09±2.73	58.30±1.52	60.31±5.24	75.72±1.54	51.58±3.64	78.73±1.40	4.3
OCGIN	76.66±4.17	80.38±6.84	86.01±6.59	57.65±2.96	67.93±3.86	46.09±1.66	59.60±4.78	61.21±8.12	49.13±4.13	54.04±5.50	6.9
GLocalKD	75.75±5.99	70.63±3.54	93.67±1.24	57.18±2.03	78.25±4.35	66.28±0.98	64.82±3.31	73.15±1.26	55.71±3.81	86.83±2.35	4.1
GOOD-D$_{simp}$	93.00±3.20	78.43±2.67	98.91±0.41	**61.89**±2.51	79.71±1.19	65.30±1.27	70.48±2.75	81.56±1.97	66.13±2.98	91.39±0.46	2.2
GOOD-D	**94.99**±2.25	**81.21**±2.65	**99.07**±0.40	61.84±1.94	79.94±1.09	**66.50**±1.35	**80.13**±3.43	**82.91**±2.58	**69.18**±3.61	**91.52**±0.70	**1.2**

Experiments

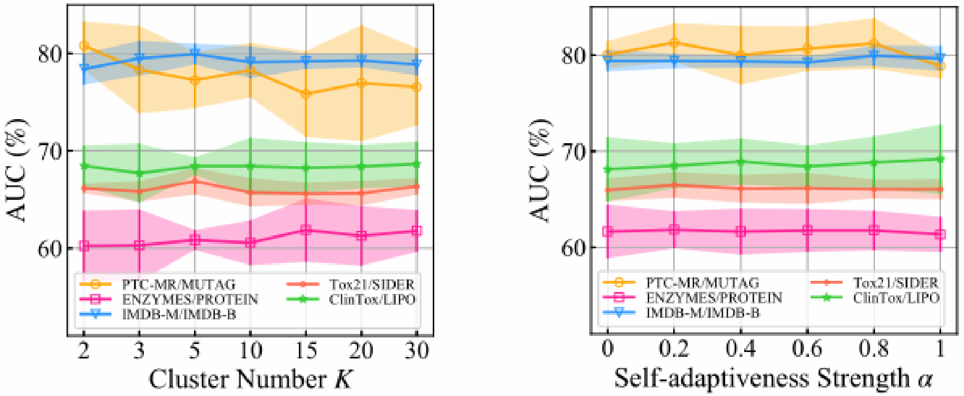
Table 2: Anomaly detection results in terms of AUC (in percent, mean ± std). The best and runner-up results are highlighted with bold and underline, respectively.

Method	PK-OCSVM	PK-iF	WL-OCSVM	WL-iF	InfoGraph-iF	GraphCL-iF	OCGIN	GLocalKD	GOOD-D$_{simp}$	GOOD-D
PROTEINS-full	50.49±4.92	60.70±2.55	51.35±4.35	61.36±2.54	57.47±3.03	60.18±2.53	70.89±2.44	**77.30±5.15**	74.74±2.28	71.97±3.86
ENZYMES	53.67±2.66	51.30±2.01	55.24±2.66	51.60±3.81	53.80±4.50	53.60±4.88	58.75±5.98	61.39±8.81	61.23±4.58	**63.90±3.69**
AIDS	50.79±4.30	51.84±2.87	50.12±3.43	61.13±0.71	70.19±5.03	79.72±3.98	78.16±3.05	93.27±4.19	94.09±1.75	**97.28±0.69**
DHFR	47.91±3.76	52.11±3.96	50.24±3.13	50.29±2.77	52.68±3.21	51.10±2.35	49.23±3.05	56.71±3.57	**62.71±3.38**	62.67±3.11
BZR	46.85±5.31	55.32±6.18	50.56±5.87	52.46±3.30	63.31±8.52	60.24±5.37	65.91±1.47	69.42±7.78	74.48±4.91	**75.16±5.15**
COX2	50.27±7.91	50.05±2.06	49.86±7.43	50.27±0.34	53.36±8.86	52.01±3.17	53.58±5.05	59.37±12.67	60.46±12.34	**62.65±8.14**
DD	48.30±3.98	71.32±2.41	47.99±4.09	70.31±1.09	55.80±1.77	59.32±3.92	72.27±1.83	**80.12±5.24**	72.24±1.82	73.25±3.19
NCI1	49.90±1.18	50.58±1.38	50.63±1.22	50.74±1.70	50.10±0.87	49.88±0.53	**71.98±1.21**	68.48±2.39	59.56±1.62	61.12±2.21
IMDB-B	50.75±3.10	50.80±3.17	54.08±5.19	50.20±0.40	56.50±3.58	56.50±4.90	60.19±8.90	52.09±3.41	65.49±1.06	**65.88±0.75**
REDDIT-B	45.68±2.24	46.72±3.42	49.31±2.33	48.26±0.32	68.50±5.56	71.80±4.38	75.93±8.65	77.85±2.62	87.87±1.38	**88.67±1.24**
COLLAB	49.59±2.24	50.49±1.72	52.60±2.56	50.69±0.32	46.27±0.73	47.61±1.29	60.70±2.97	52.94±0.85	62.10±0.63	**72.08±0.90**
HSE	57.02±8.42	56.87±10.51	62.72±10.13	53.02±5.12	53.56±3.98	51.18±2.71	64.84±4.70	59.48±1.44	69.18±1.89	**69.65±2.14**
MMP	46.65±6.31	50.06±3.73	55.24±3.26	52.68±3.34	54.59±2.01	54.54±1.86	**71.23±0.16**	67.84±0.59	70.18±1.14	70.51±1.56
p53	46.74±4.88	50.69±2.02	54.59±4.46	50.85±2.16	52.66±1.95	53.29±2.32	58.50±0.37	64.20±0.81	**66.48±0.56**	62.99±1.55
PPAR-gamma	53.94±6.94	45.51±2.58	57.91±6.13	49.60±0.22	51.40±2.53	50.30±1.56	**71.19±4.28**	64.59±0.67	66.85±2.19	67.34±1.71
Avg. Rank	8.7	7.7	6.9	7.5	6.5	6.9	3.5	3.1	2.3	**1.7**

Experiments

Table 3: Ablation study results of GOOD-D$_{simp}$ and its variants in terms of AUC (in percent, mean ± std).

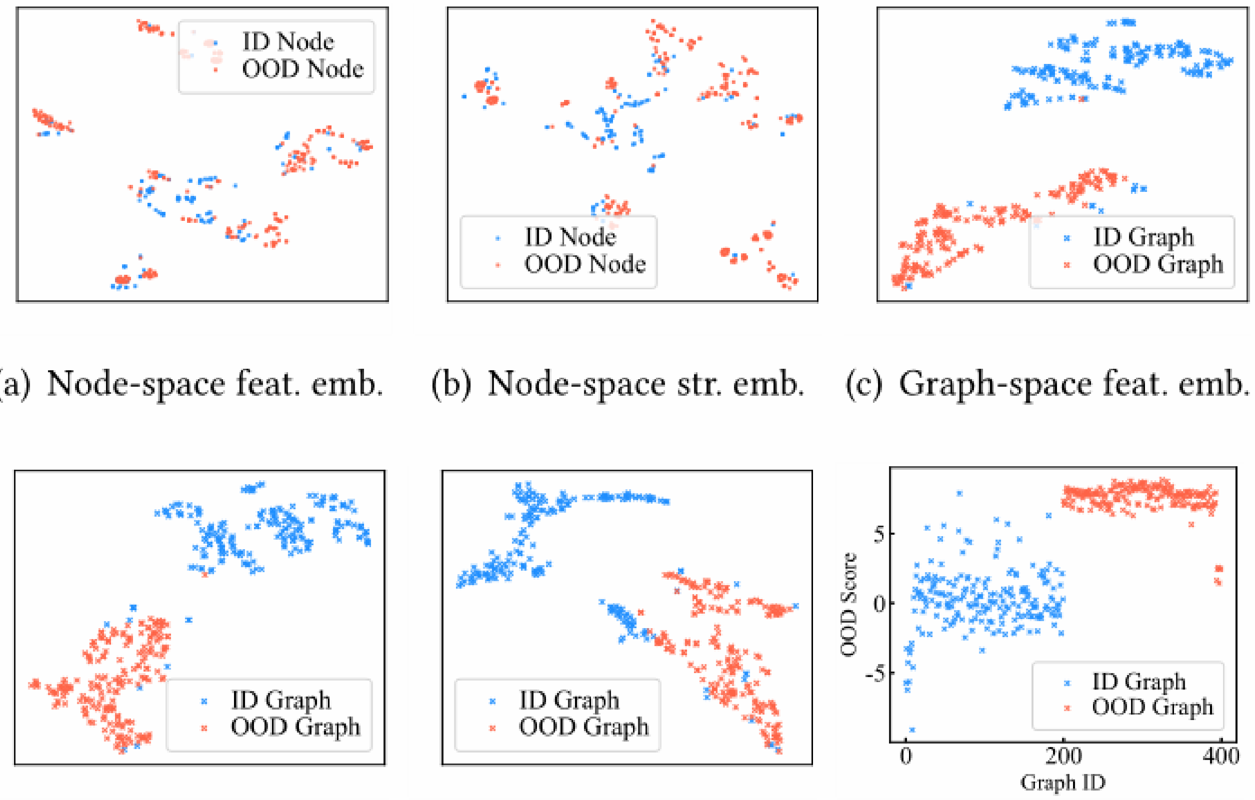
$\mathcal{L}_{node}$	$\mathcal{L}_{graph}$	$\mathcal{L}_{group}$	BZR / COX2	PTC-MR / MUTAG	AIDS / DHFR	ENZYMES / PROTEIN	IMDB-M / IMDB-B	Tox21 / SIDER	FreeSolv / ToxCast	BBBP / BACE	ClinTox / LIPO	Esol / MUV
✓	-	-	83.51±4.14	72.48±3.77	96.84±0.58	60.85±2.95	79.34±1.81	62.58±0.67	59.48±2.20	69.53±2.29	53.29±4.32	86.49±1.20
-	✓	-	87.44±4.66	77.84±3.71	97.60±1.05	56.74±1.96	75.22±1.91	65.07±1.32	**78.40**±6.44	77.66±2.29	70.11±2.44	89.57±2.80
-	-	✓	79.21±5.60	74.83±8.54	89.47±1.85	50.43±7.41	72.91±2.75	54.84±2.56	58.16±6.23	58.09±5.43	58.46±5.35	83.35±2.71
✓	✓	-	**93.14**±3.63	77.53±4.02	98.90±0.42	61.48±3.46	79.55±1.35	65.44±1.13	71.45±4.23	80.43±2.57	65.89±4.57	90.94±1.16
✓	-	✓	85.01±3.05	76.10±3.01	96.87±0.52	59.69±1.89	79.69±1.67	63.01±0.97	56.30±5.33	69.66±2.45	54.14±4.01	86.31±1.99
-	✓	✓	86.59±5.24	77.97±4.00	97.22±1.35	55.51±4.39	76.17±1.65	**65.48**±0.78	77.38±5.19	79.77±4.39	**70.20**±1.01	88.33±1.35
✓	✓	✓	93.00±3.20	**78.43**±2.67	**98.91**±0.41	**61.89**±2.51	**79.71**±1.19	65.30±1.27	70.48±2.75	**81.56**±1.97	66.13±2.98	**91.39**±0.46



(a) Sensitivity of K (b) Sensitivity of α

Figure 3: Parameter sensitivity of K and α.

Experiments



(a) Node-space feat. emb. (b) Node-space str. emb. (c) Graph-space feat. emb.

(d) Graph-space str. emb. (e) Group-space emb. (f) OOD score

Figure 4: Visualization on AIDS/DHFR dataset pair. (a)-(e): t-SNE visualization of testing sample embeddings (emb.) of feature (feat.) or structure (str.) view at different embedding spaces. (f): OOD scores of GOOD-D on testing samples.