

CGMN: A Contrastive Graph Matching Network for Self-Supervised Graph Similarity Learning

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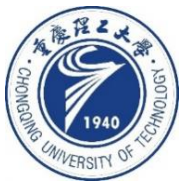
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IJCAI 2022

Code: None

2022. 06. 29 • ChongQing



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Reported by Chenghong Li

Introduction

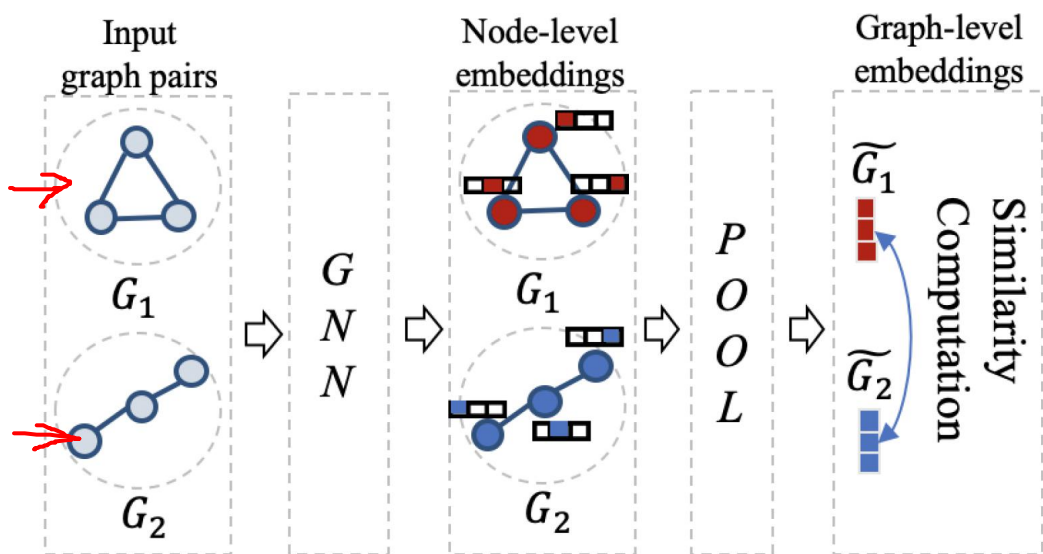


Figure 1: A view of the supervised graph similarity learning model.

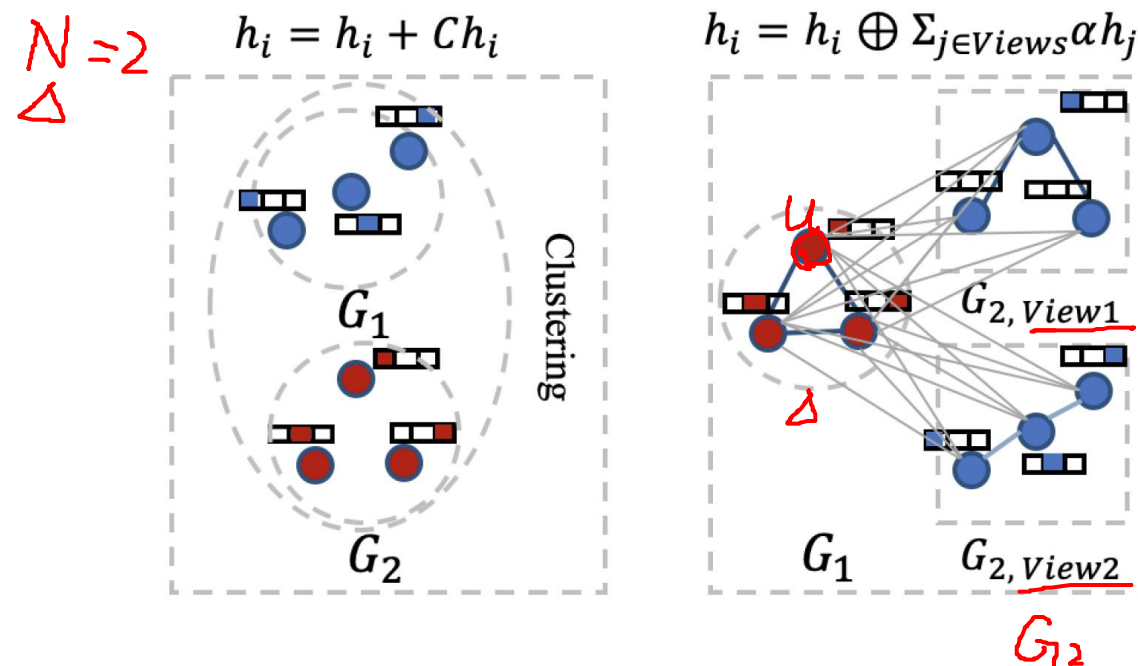


Figure 2: Comparison of node information update process. Left: Clustering-based unsupervised graph similarity learning. Right: Our proposed model CGMN. h_i denotes the embedding of node i . C represents the clustering weight, \oplus is concatenation, and α represents the cross-graph interaction weight.

Method

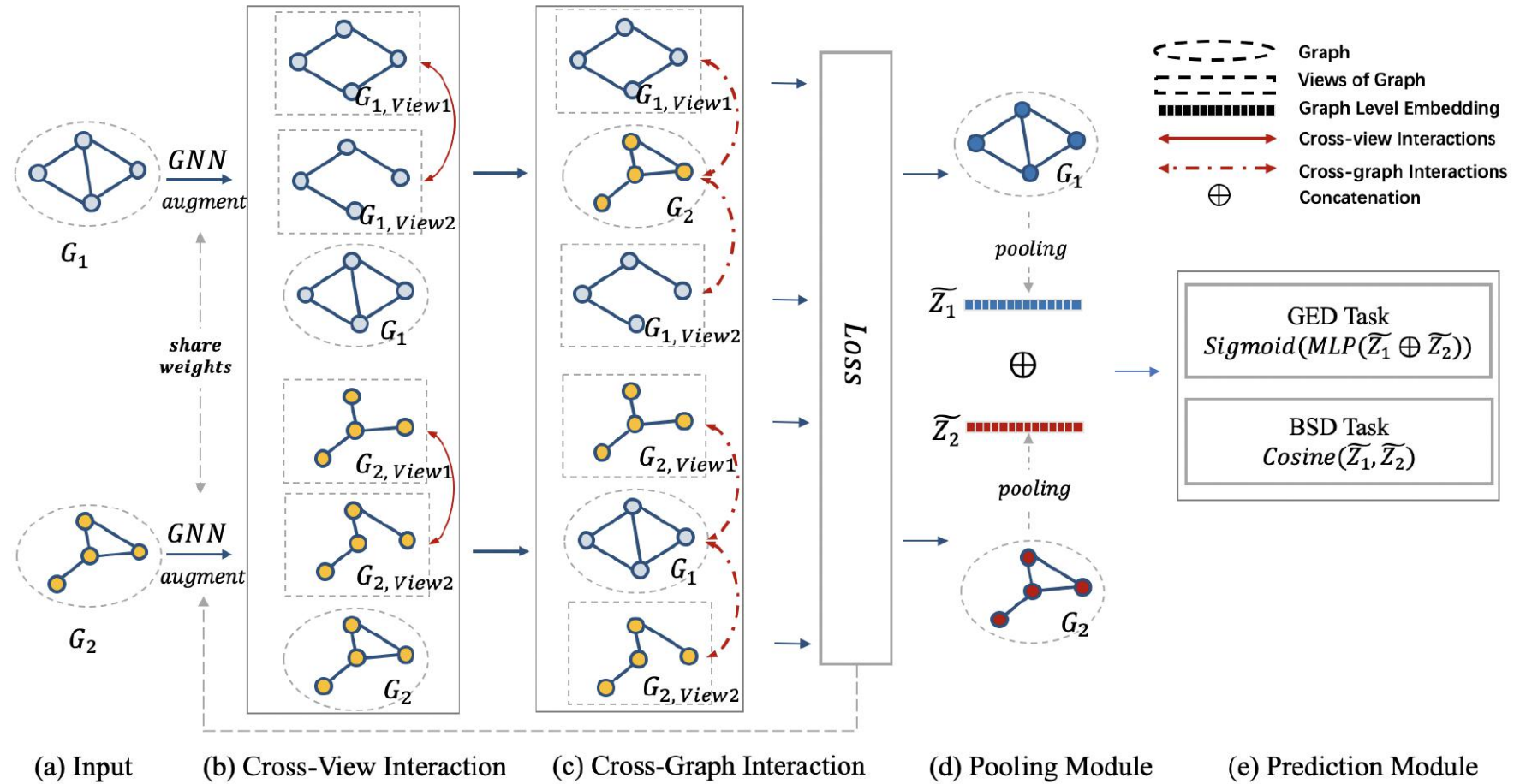
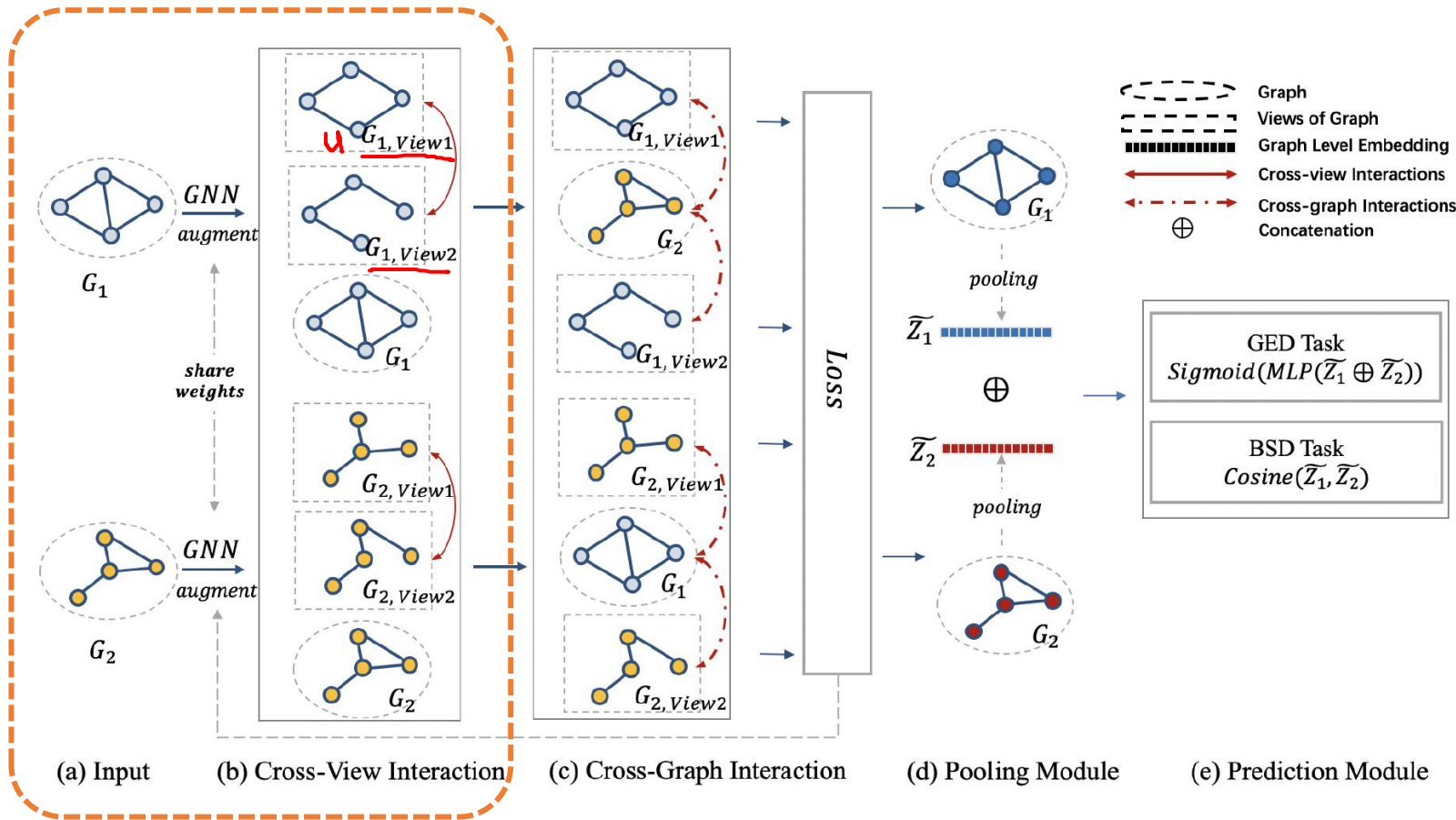


Figure 3: Overview of CGMN. First, we provide a framework to learn the embedding of each node. Second, we propose a cross-graph interaction strategy to match nodes in graph pairs. Third, we aggregate node embeddings to obtain the graph-level representations. Finally, we predict the similarity of graphs for different tasks.

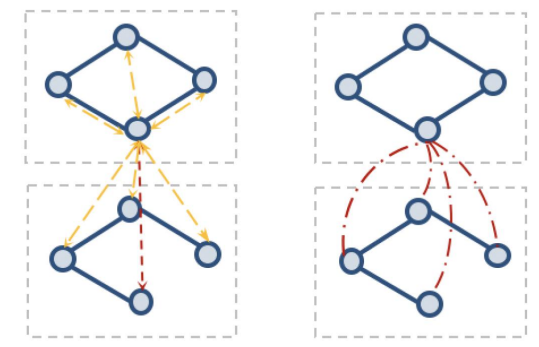
Method



$$H^l = \sigma(\tilde{A}H^{l-1}W^{l-1}), \quad (1)$$

$$\text{sim}(h_u, h_v) := \exp(\cos(h_u, h_v) / \tau), \quad (2)$$

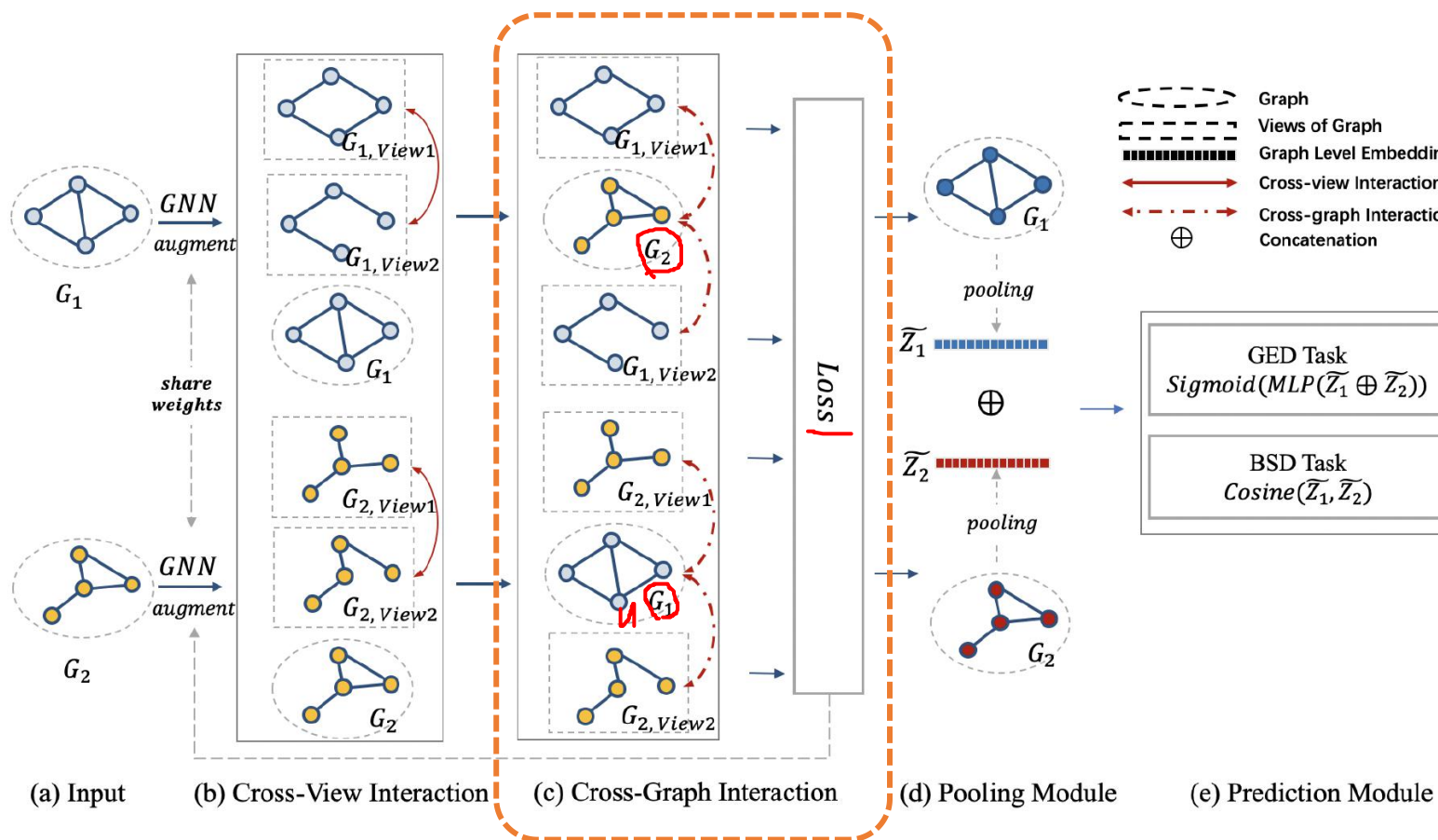
$$\hat{h}_u = h_u \oplus \sum_{v \in G_1, View2} \cos(h_u, h_v) h_v, \quad (3)$$



Legend for interaction types:
 Push away (yellow arrow), Pull closer (red arrow), Interaction (red dashed arrow)
 (a) Contrastive learning. (b) Cross-view interaction.

Figure 4: Difference between (a) contrastive learning and (b) cross-view interaction.

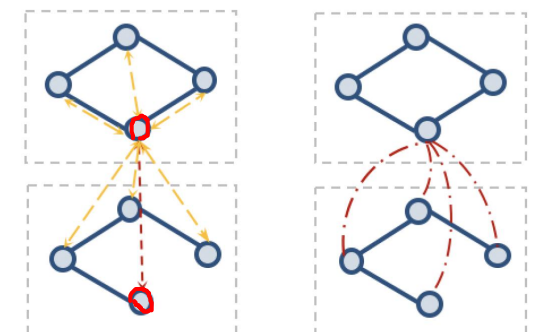
Method



$$\Rightarrow h_u^* = \hat{h}_u \oplus \sum_{i \in G_{2,View1}} \frac{\cos(\hat{h}_u, \hat{h}_i)}{\Delta} \hat{h}_i \oplus \sum_{j \in G_{2,View2}} \frac{\cos(\hat{h}_u, \hat{h}_j)}{\Delta} \hat{h}_j \quad (4)$$

$$loss(h_u^*, h_v^*) = -\log \frac{\text{sim}(h_u^*, h_v^*)}{\text{sim}(h_u^*, h_v^*) + \sum_{k=1}^N \text{sim}(h_u^*, h_k^*)} \quad (5)$$

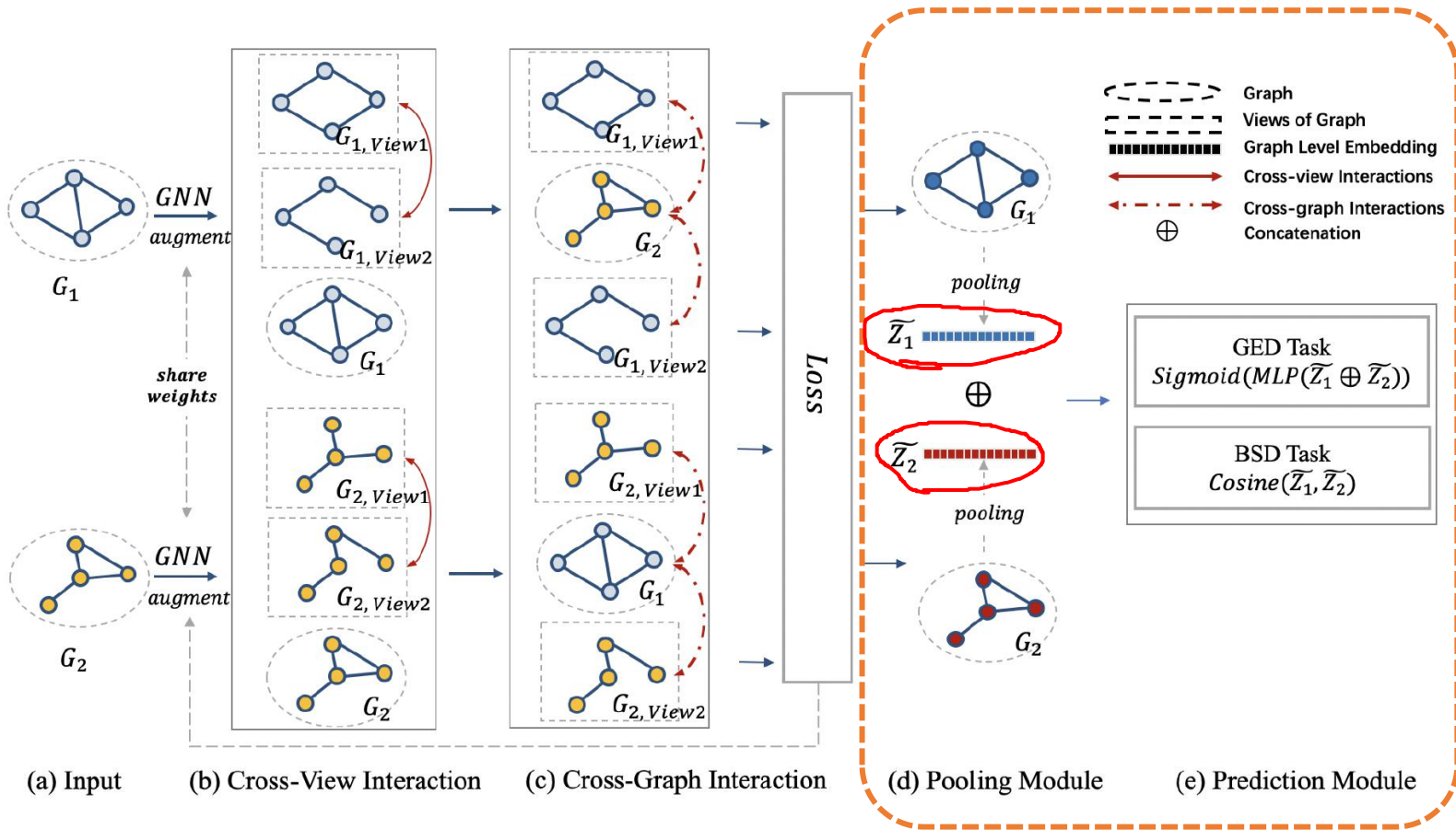
$$\mathcal{L} = \frac{1}{2} [loss(h_u^*, h_v^*) + loss(h_v^*, h_u^*)] \quad (6)$$



Legend for symbols:
 Push away (yellow arrow), Pull closer (red dashed arrow), Interaction (red dashed double-headed arrow)
 (a) Contrastive learning. (b) Cross-view interaction.

Figure 4: Difference between (a) contrastive learning and (b) cross-view interaction.

Method



$$\tilde{Z} = \text{AVG}(h_u : u \in G), \quad (7)$$

$$y = \text{sigmoid}(\text{MLP}(\tilde{Z}_1 \oplus \tilde{Z}_2)). \quad (8)$$

$$y = \text{cos}(\tilde{Z}_1, \tilde{Z}_2). \quad (9)$$



Experiments

	Datasets	Graphs	AvgN	AvgE	Classes
	Aids700nef	700	8.90	8.80	-
	Linux1000	1000	7.58	6.94	-
OpenSSL (OS)	OS [3, 200]	73,953	15.73	21.97	4,249
	OS [20, 200]	15,800	44.89	67.15	1,073
	OS [50, 200]	4,308	83.68	127.75	338
FFmpeg (FF)	FF [3, 200]	83,008	18.83	27.02	10,376
	FF [20, 200]	31,696	51.02	75.88	7,668
	FF [50, 200]	10,824	90.93	136.83	3,178

Table 1: Statistics of the datasets.

Experiments

 Spearman's Rank Correlation Coefficient (ρ)

 Kendall's Rank Correlation Coefficient (τ)

Datasets	Methods	MSE (10^{-3})	ρ	τ	p@10	p@20
Aids700nef	GCN	11.395±1.315	0.577±0.021	0.418±0.018	0.041±0.002	0.077±0.003
	GIN	9.280±0.163	0.629±0.020	0.462±0.016	0.044±0.018	0.096±0.021
	DGI	15.009±0.347	0.231±0.093	0.164±0.061	0.039±0.006	0.076±0.001
	GRACE	12.176±1.693	0.366±0.186	0.261±0.134	0.038±0.004	0.072±0.018
	ScGSLC	13.060±0.193	0.394±0.133	0.281±0.097	0.080±0.026	0.142±0.044
	CGMN	6.641±2.227	0.674±0.129	0.502±0.107	0.084±0.019	0.140±0.024
Linux1000	GCN	11.986±1.532	0.569±0.033	0.411±0.028	0.043±0.005	0.071±0.001
	GIN	22.188±5.259	0.647±0.112	0.484±0.099	0.081±0.018	0.084±0.025
	DGI	33.854±0.013	0.052±0.018	0.039±0.002	0.035±0.020	0.073±0.016
	GRACE	14.180±2.080	0.852±0.019	0.673±0.025	0.443±0.155	0.452±0.175
	ScGSLC	13.423±2.038	0.840±0.010	0.658±0.021	0.192±0.095	0.213±0.120
	CGMN	10.514±1.178	0.873±0.013	0.700±0.015	0.307±0.071	0.330±0.091

Table 2: Experimental results on the GED datasets in terms of five evaluation metrics.

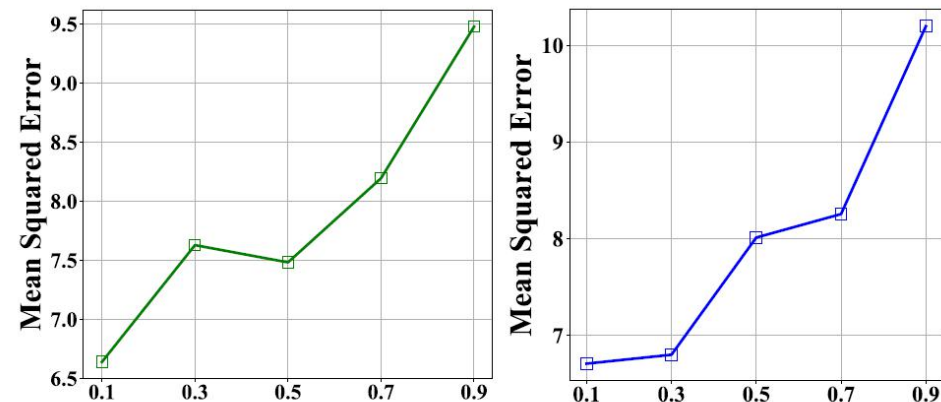
Methods	OS [50, 200]	OS [20, 200]	OS [3, 200]	FF [50, 200]	FF [20, 200]	FF [3, 200]
GCN	67.24±1.14	68.09±1.01	73.51±0.72	78.41±0.49	79.47±0.08	80.88±0.18
GIN	66.60±0.10	63.85±0.56	75.65±0.30	78.38±0.20	81.25±0.57	81.82±0.25
DGI	67.55±2.76	63.58±1.96	72.58±2.36	86.10±0.66	80.82±2.22	66.28±0.30
GRACE	68.84±2.45	67.01±0.49	69.86±0.29	85.44±0.27	75.05±0.73	66.95±2.78
ScGSLC	67.43±0.82	61.46±0.33	63.28±0.09	87.57±0.82	83.27±0.71	69.80±1.22
CGMN	80.89±0.20	78.15±0.85	75.94±1.86	86.11±0.98	86.76±0.85	77.98±2.69

Table 3: Experimental results on the BSD datasets in terms of AUC scores (%).

Experiments

Methods	MSE	ρ	τ	p@10	p@20
CGMN <i>w/o</i> cross-view	8.239	0.614	0.451	0.064	0.114
CGMN <i>w/o</i> cross-graph	8.753	0.537	0.387	0.050	0.091
CGMN	6.641	0.674	0.502	0.084	0.140

Table 4: Ablation study on Aids700nef.



(a) Masking node features.

(b) Removing edges.

Figure 5: Influence on parameters.



Thanks