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Engineering

Graph Contrastive Learning with Augmentations

Yuning You[1*], Tianlong Chen[2*], Yongduo Sui[3], Ting Chen[4], Zhangyang Wang[2], Yang Shen[1]

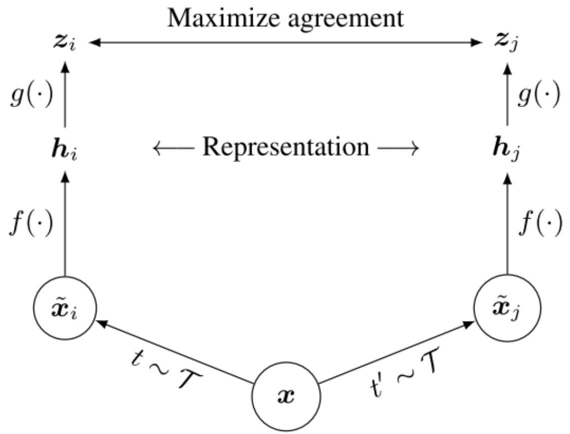
[1]Texas A&M University, [2]University of Texas at Austin,
[3]University of Science and Technology of China, [4]Google Research, Brain Team,
[*]Equal contribution, __Speaker

Background

- Pre-training graph neural networks (GNNs) is under-explored with some exceptions, while its necessity emerges in recent years;

- Designing GNN pre-training schemes is challenging due to the dataset diversity;

- Recent surge of interest in contrastive learning in computer vision provides us a potential methodology for designing GNN pre-training schemes.



Methods: Data Augmentation for Graphs

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- Data augmentation: creating novel and realistically rational data via certain transformation without affecting the semantics label;
- Little exploration on data augmentations on graphs;
- We propose four general data augmentations for graph-structured data and discuss the intuitive priors that they introduce.

Table 1: Overview of data augmentations for graphs.

Data augmentation	Type	Underlying Prior
Node dropping	Nodes, edges	Vertex missing does not alter semantics.
Edge perturbation	Edges	Semantic robustness against connectivity variations.
Attribute masking	Nodes	Semantic robustness against losing partial attributes per node.
Subgraph	Nodes, edges	Local structure can hint the full semantics.

Methods: Graph Contrastive Learning (GraphCL)

- GraphCL: maximizing agreement between two augmented views of graph via a contrastive loss in the latent space.

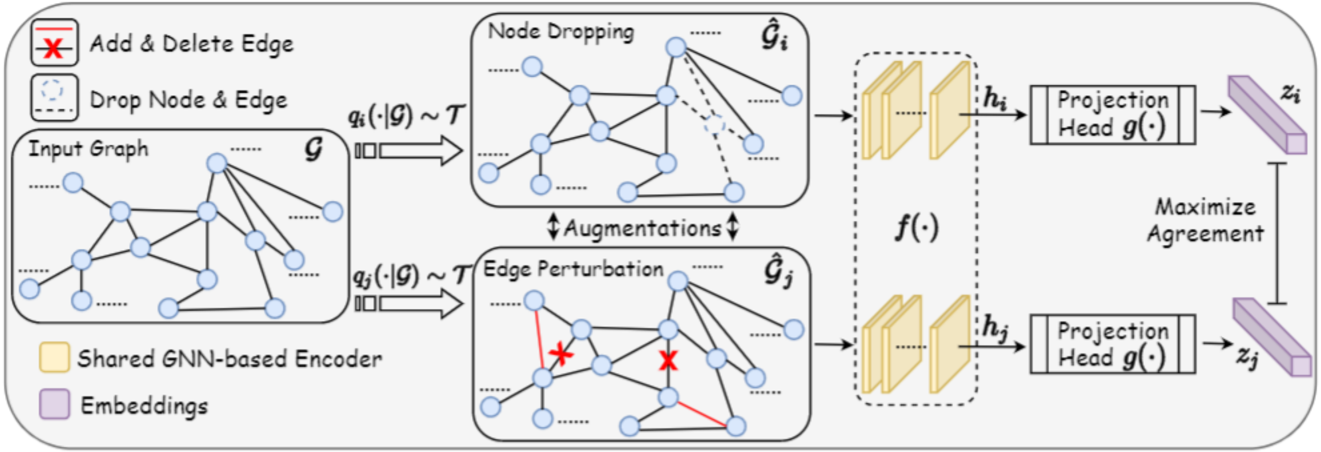

Figure 1: A framework of graph contrastive learning. Two graph augmentations $q_i(\cdot|\mathcal{G})$ and $q_j(\cdot|\mathcal{G})$ are sampled from an augmentation pool $\mathcal{T}$ and applied to input graph $\mathcal{G}$. A shared GNN-based encoder $f(\cdot)$ and a projection head $g(\cdot)$ are trained to maximize the agreement between representations z_i and z_j via a contrastive loss.

The Role of Data Augmentation in GraphCL

Table 2: Datasets statistics.

Datasets	Category	Graph Num.	Avg. Node	Avg. Degree
NCI1	Biochemical Molecules	4110	29.87	1.08
PROTEINS	Biochemical Molecules	1113	39.06	1.86
COLLAB	Social Networks	5000	74.49	32.99
RDT-B	Social Networks	2000	429.63	1.15

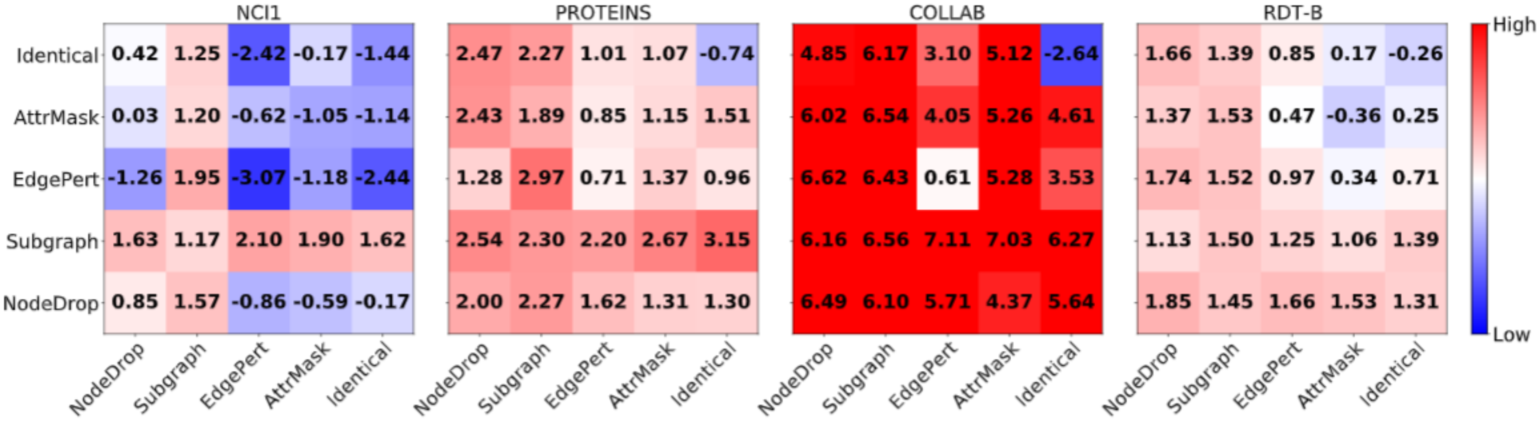

Figure 2: Semi-supervised learning accuracy gain (%) when contrasting different augmentation pairs, compared to training from scratch, under four datasets: NCI1, PROTEINS, COLLAB, and RDT-B. Pairing "Identical" stands for a no-augmentation baseline for contrastive learning, where the positive pair diminishes and the negative pair consists of two non-augmented graphs. Warmer colors indicate better performance gains. The baseline training-from-scratch accuracies are 60.72%, 70.40%, 57.46%, 86.63% for the four datasets respectively.

The Role of Data Augmentation in GraphCL

- Obs. 1. Data augmentations are crucial in graph contrastive learning;
- Obs. 2. Composing different augmentations benefits more;
- Obs. 3. Edge perturbation benefits social networks but hurts some biochemical molecules;
- Obs. 4. Applying attribute masking achieves better performance in denser graphs;
- Obs. 5. Node dropping and subgraph are generally beneficial across datasets.

Comparison with the State-of-the-art Methods

- Semi-supervised learning:

Table 3: Semi-supervised learning with pre-training & finetuning. Red numbers indicate the best performance and the number that overlap with the standard deviation of the best performance (comparable ones). 1% or 10% is label rate; baseline and Aug. represents training from scratch without and with augmentations, respectively.

Dataset	NCI1	PROTEINS	DD	COLLAB	RDT-B	RDT-M5K	GITHUB	MNIST	CIFAR10
1% baseline	60.72±0.45	-	-	57.46±0.25	-	-	54.25±0.22	60.39±1.95	27.36±0.75
1% Aug.	60.49±0.46	-	-	58.40±0.97	-	-	56.36±0.42	67.43±0.36	27.39±0.44
1% GAE	61.63±0.84	-	-	63.20±0.67	-	-	59.44±0.44	57.58±2.07	21.09±0.53
1% Infomax	62.72±0.65	-	-	61.70±0.77	-	-	58.99±0.50	63.24±0.78	27.86±0.43
1% GraphCL	62.55±0.86	-	-	64.57±1.15	-	-	58.56±0.59	83.41±0.33	30.01±0.84
10% baseline	73.72±0.24	70.40±1.54	73.56±0.41	73.71±0.27	86.63±0.27	51.33±0.44	60.87±0.17	79.71±0.65	35.78±0.81
10% Aug.	73.59±0.32	70.29±0.64	74.30±0.81	74.19±0.13	87.74±0.39	52.01±0.20	60.91±0.32	83.99±2.19	34.24±2.62
10% GAE	74.36±0.24	70.51±0.17	74.54±0.68	75.09±0.19	87.69±0.40	53.58±0.13	63.89±0.52	86.67±0.93	36.35±1.04
10% Infomax	74.86±0.26	72.27±0.40	75.78±0.34	73.76±0.29	88.66±0.95	53.61±0.31	65.21±0.88	83.34±0.24	41.07±0.48
10% GraphCL	74.63±0.25	74.17±0.34	76.17±1.37	74.23±0.21	89.11±0.19	52.55±0.45	65.81±0.79	93.11±0.17	43.87±0.77

- Unsupervised representation learning:

Table 4: Comparing classification accuracy on top of graph representations learned from graph kernels, SOTA representation learning methods, and GIN pre-trained with GraphCL. The compared numbers are from the corresponding papers under the same experiment setting.

Dataset	NCI1	PROTEINS	DD	MUTAG	COLLAB	RDT-B	RDT-M5K	IMDB-B
GL	-	-	-	81.66±2.11	-	77.34±0.18	41.01±0.17	65.87±0.98
WL	80.01±0.50	72.92±0.56	-	80.72±3.00	-	68.82±0.41	46.06±0.21	72.30±3.44
DGK	80.31±0.46	73.30±0.82	-	87.44±2.72	-	78.04±0.39	41.27±0.18	66.96±0.56
node2vec	54.89±1.61	57.49±3.57	-	72.63±10.20	-	-	-	-
sub2vec	52.84±1.47	53.03±5.55	-	61.05±15.80	-	71.48±0.41	36.68±0.42	55.26±1.54
graph2vec	73.22±1.81	73.30±2.05	-	83.15±9.25	-	75.78±1.03	47.86±0.26	71.10±0.54
InfoGraph	76.20±1.06	74.44±0.31	72.85±1.78	89.01±1.13	70.65±1.13	82.50±1.42	53.46±1.03	73.03±0.87
GraphCL	77.87±0.41	74.39±0.45	78.62±0.40	86.80±1.34	71.36±1.15	89.53±0.84	55.99±0.28	71.14±0.44

Comparison with the State-of-the-art Methods

- Transfer learning:

Table 5: Transfer learning comparison with different manually designed pre-training schemes.

Dataset	BBBP	Tox21	ToxCast	SIDER	ClinTox	MUV	HIV	BACE	PPI
No Pre-Train	65.8±4.5	74.0±0.8	63.4±0.6	57.3±1.6	58.0±4.4	71.8±2.5	75.3±1.9	70.1±5.4	64.8±1.0
Infomax	68.8±0.8	75.3±0.5	62.7±0.4	58.4±0.8	69.9±3.0	75.3±2.5	76.0±0.7	75.9±1.6	64.1±1.5
EdgePred	67.3±2.4	76.0±0.6	64.1±0.6	60.4±0.7	64.1±3.7	74.1±2.1	76.3±1.0	79.9±0.9	65.7±1.3
AttrMasking	64.3±2.8	76.7±0.4	64.2±0.5	61.0±0.7	71.8±4.1	74.7±1.4	77.2±1.1	79.3±1.6	65.2±1.6
ContextPred	68.0±2.0	75.7±0.7	63.9±0.6	60.9±0.6	65.9±3.8	75.8±1.7	77.3±1.0	79.6±1.2	64.4±1.3
GraphCL	69.68±0.67	73.87±0.66	62.40±0.57	60.53±0.88	75.99±2.65	69.80±2.66	78.47±1.22	75.38±1.44	67.88±0.85

- Adversarial robustness.

Table 6: Adversarial performance under three adversarial attacks for GNN with different depth (following the protocol in [60]). Red numbers indicate the best performance.

Methods	Two-Layer		Three-Layer		Four-Layer	
	No Pre-Train	GraphCL	No Pre-Train	GraphCL	No Pre-Train	GraphCL
Unattack	93.20	94.73	98.20	98.33	98.87	99.00
RandSampling	78.73	80.68	92.27	92.60	95.13	97.40
GradArgmax	69.47	69.26	64.60	89.33	95.80	97.00
RL-S2V	42.93	42.20	41.93	61.66	70.20	84.86

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Thank you for listening!