ICML Workshop on Graph Representation Learning and Beyond

Deep Graph Contrastive Representation Learning

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Outline

1. Preamble
2. The Proposed Method
3. Experiments
4. Concluding Remarks

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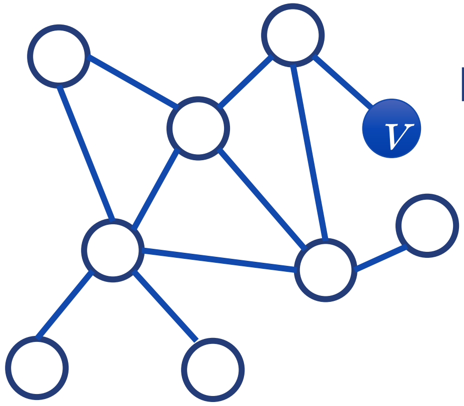
Representation Learning on Graphs

- Goal: efficient feature learning for machine learning on graphs



node 2 vec

$$f : \mathbb{R}^F \times \{0,1\}^N \to \mathbb{R}^{F'}$$

$\mathbb{R}^{F'}$ $\quad F' \ll F$

Node embeddings

- In reality, labels are not always available to models, which calls for training GNN in a self-supervised manner.

Contrastive Learning for GRL

- Node embedding approaches
  - Pioneering work of node embedding follows a contrastive framework originated in the skip-gram model.
  - For example, node2vec first samples short random walks and then enforces neighboring nodes on the same walk to share similar embeddings by contrasting them with other nodes.
- GNN-based approaches
  - GraphSAGE connects reconstruction objectives to GNN models, which excessively relies on the preset graph proximity matrix.
  - DGI firstly revitalizes InfoMax principle in the graph domain, which maximizes mutual information between node representations and global summary vectors.

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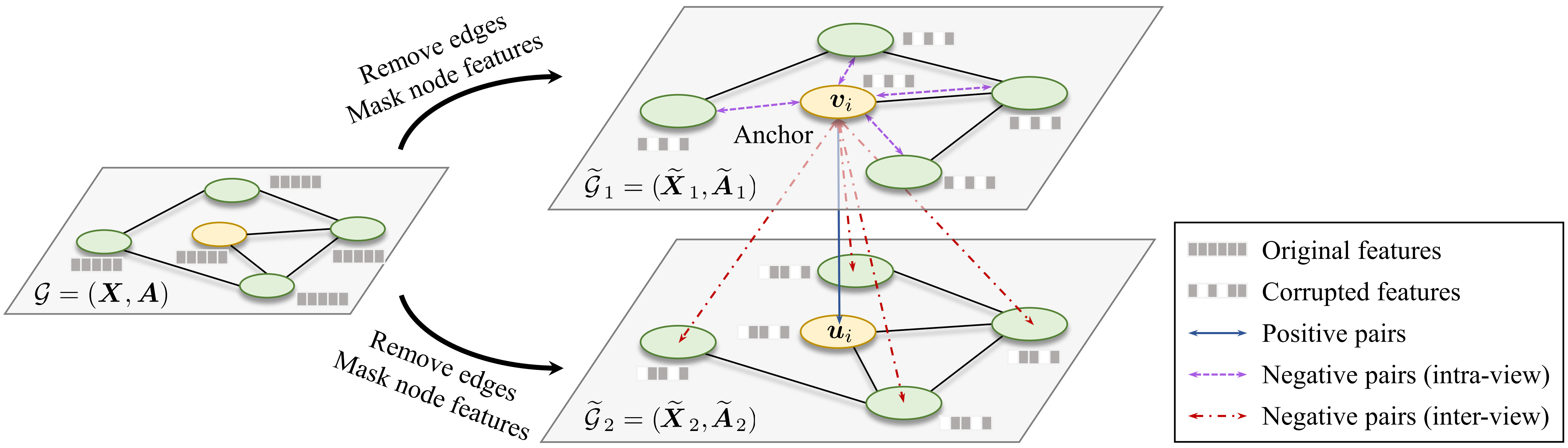
Model Illustration



Contrastive Learning Across Views

- We first generate two correlated graph views by randomly performing corruption.
- Then, we train the model using a contrastive loss to maximize the agreement between node embeddings in these two views.
  - Rather than contrasting node-level embeddings to global ones, we primarily focus on contrasting embeddings at the node level.

$$\ell(\boldsymbol{u}_i, \boldsymbol{v}_i) = \log \frac{e^{\theta(\boldsymbol{u}_i, \boldsymbol{v}_i)/\tau}}{\underbrace{e^{\theta(\boldsymbol{u}_i, \boldsymbol{v}_i)/\tau}}_{\text{the positive pair}} + \underbrace{\sum_{k=1}^{N} \mathbb{1}_{[k \neq i]} e^{\theta(\boldsymbol{u}_i, \boldsymbol{v}_k)/\tau}}_{\text{inter-view negative pairs}} + \underbrace{\sum_{k=1}^{N} \mathbb{1}_{[k \neq i]} e^{\theta(\boldsymbol{u}_i, \boldsymbol{u}_k)/\tau}}_{\text{intra-view negative pairs}}}$$

Hybrid Graph View Generation

- Appropriately choosing negative samples is important for InfoMax-based methods.
- We corrupt the original graph at both structure and attribute levels to construct diverse node contexts.
- **Removing edges (RE)**: randomly remove a portion of edges in the original graph.

$$\widetilde{\boldsymbol{A}} = \boldsymbol{A} \circ \widetilde{\boldsymbol{R}}$$

- **Masking node features (MF)**: randomly mask a fraction of dimensions with zeros in node features.

$$\widetilde{\boldsymbol{X}} = [\boldsymbol{x}_1 \circ \widetilde{\boldsymbol{m}}; \boldsymbol{x}_2 \circ \widetilde{\boldsymbol{m}}; \cdots; \boldsymbol{x}_N \circ \widetilde{\boldsymbol{m}}]^\top$$

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Experiment Setup

- Datasets

Dataset	Type	#Nodes	#Edges	#Features	#Classes
Cora	Transductive	2,708	5,429	1,433	7
Citeseer	Transductive	3,327	4,732	3,703	6
Pubmed	Transductive	19,717	44,338	500	3
DBLP	Transductive	17,716	105,734	1,639	4
Reddit	Inductive	231,443	11,606,919	602	41
PPI	Inductive	56,944 (24 graphs)	818,716	50	121 (multilabel)

Experiment Setup (cont.)

- Baselines:
  - Traditional methods DeepWalk and node2vec
  - GNN-based methods GAE, VGAE, GraphSAGE, and DGI
  - Representative semi-supervised methods
    - Transductive: GCN and SGC
    - Inductive: FastGCN and GaAN-mean

Transductive Node Classification

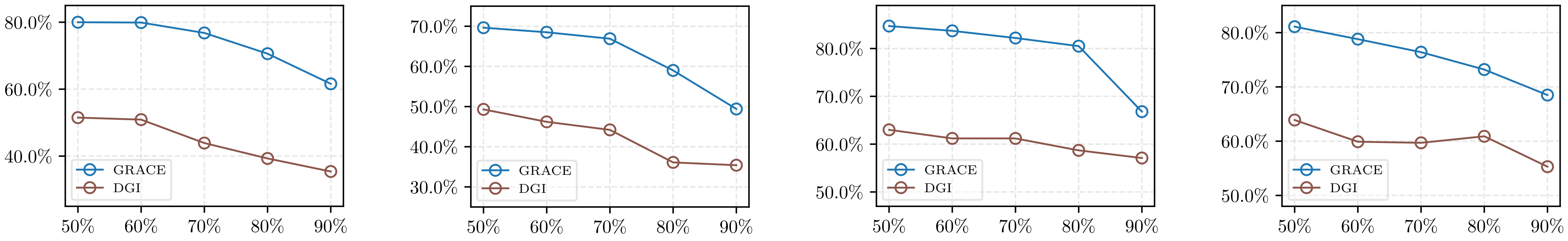
Method	Training Data	Cora	Citeseer	Pubmed	DBLP
Raw features	$\boldsymbol{X}$	64.8	64.6	84.8	71.6
node2vec	$\boldsymbol{A}$	74.8	52.3	80.3	78.8
DeepWalk	$\boldsymbol{A}$	75.7	50.5	80.5	75.9
DeepWalk + features	$\boldsymbol{X}, \boldsymbol{A}$	73.1	47.6	83.7	78.1
GAE	$\boldsymbol{X}, \boldsymbol{A}$	76.9	60.6	82.9	81.2
VGAE	$\boldsymbol{X}, \boldsymbol{A}$	78.9	61.2	83.0	81.7
DGI	$\boldsymbol{X}, \boldsymbol{A}$	82.6±0.4	68.8±0.7	86.0±0.1	83.2±0.1
GRACE	$\boldsymbol{X}, \boldsymbol{A}$	**83.3±0.4**	**72.1±0.5**	**86.7±0.1**	**84.2±0.1**
SGC	$\boldsymbol{X}, \boldsymbol{A}, \boldsymbol{Y}$	80.6	69.1	84.8	81.7
GCN	$\boldsymbol{X}, \boldsymbol{A}, \boldsymbol{Y}$	82.8	72.0	84.9	82.7

Inductive Node Classification

Method	Training Data	Reddit	PPI
Raw features	$\boldsymbol{X}$	58.5	42.2
DeepWalk	$\boldsymbol{A}$	32.4	—
DeepWalk + features	$\boldsymbol{X}, \boldsymbol{A}$	69.1	—
GraphSAGE-GCN	$\boldsymbol{X}, \boldsymbol{A}$	90.8	46.5
GraphSAGE-mean	$\boldsymbol{X}, \boldsymbol{A}$	89.7	48.6
GraphSAGE-LSTM	$\boldsymbol{X}, \boldsymbol{A}$	90.7	48.2
GraphSAGE-pool	$\boldsymbol{X}, \boldsymbol{A}$	89.2	50.2
DGI	$\boldsymbol{X}, \boldsymbol{A}$	94.0±0.1	63.8±0.2
GRACE	$\boldsymbol{X}, \boldsymbol{A}$	**94.2±0.0**	**66.1±0.1**
FastGCN	$\boldsymbol{X}, \boldsymbol{A}, \boldsymbol{Y}$	93.7	—
GaAN-mean	$\boldsymbol{X}, \boldsymbol{A}, \boldsymbol{Y}$	95.8±0.1	96.9±0.2

Robustness to Sparse Features

- Experiments with randomly contaminating the training data by masking a certain portion of the node features to zeros.
  - We vary the contamination rate of node features from 0.5 to 0.9 on four citation networks.



(a) Cora (b) Citeseer (c) Pubmed (d) DBLP

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Wrapping Up

1. We have developed a novel graph contrastive representation learning framework based on maximizing the agreement at the node level.
2. GRACE learns representations by first generating graph views using a hybrid scheme, removing edges and masking node features, and then applying a contrastive loss to maximize the agreement of node embeddings in these two views.
3. Experimental results demonstrate that GRACE can outperform existing state-of-the-art methods by large margins and even surpass supervised counterparts on transductive tasks.

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