ICML Workshop on Graph Representation Learning and Beyond

Deep Graph Contrastive Representation Learning

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Joint work with Yichen XU, Feng YU, Qiang LIU, Shu WU, and Liang WANG
Outline

1. Preamble
2. The Proposed Method
3. Experiments
4. Concluding Remarks
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3. Experiments
4. Concluding Remarks
Representation Learning on Graphs

• Goal: efficient feature learning for machine learning on graphs

\[ f : \mathbb{R}^F \times \{0, 1\}^N \rightarrow \mathbb{R}^{F'} \]

• 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

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

Remove edges
Mask node features

$\tilde{\mathcal{G}}_1 = (\tilde{\mathbf{X}}_1, \tilde{\mathbf{A}}_1)$

Anchor

$\tilde{\mathcal{G}}_2 = (\tilde{\mathbf{X}}_2, \tilde{\mathbf{A}}_2)$

Remove edges
Mask node features

Original features
Corrupted features
Positive pairs
Negative pairs (intra-view)
Negative pairs (inter-view)
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.

\[
l(u_i, v_i) = \log \frac{e^{\theta(u_i, v_i)} / \tau}{e^{\theta(u_i, v_i)} / \tau + \sum_{k=1}^{N} \mathbb{1}_{[k \neq i]} e^{\theta(u_i, v_k)} / \tau + \sum_{k=1}^{N} \mathbb{1}_{[k \neq i]} e^{\theta(u_i, u_k)} / \tau}
\]
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.

\[ \tilde{A} = A \circ \tilde{R} \]

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

\[ \tilde{X} = [x_1 \circ \tilde{m}; x_2 \circ \tilde{m}; \cdots ; x_N \circ \tilde{m}]^T \]
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Experiment Setup

• Datasets

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

<table>
<thead>
<tr>
<th>Method</th>
<th>Training Data</th>
<th>Cora</th>
<th>Citeseer</th>
<th>Pubmed</th>
<th>DBLP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Raw features</td>
<td>$X$</td>
<td>64.8</td>
<td>64.6</td>
<td>84.8</td>
<td>71.6</td>
</tr>
<tr>
<td>node2vec</td>
<td>$A$</td>
<td>74.8</td>
<td>52.3</td>
<td>80.3</td>
<td>78.8</td>
</tr>
<tr>
<td>DeepWalk</td>
<td>$A$</td>
<td>75.7</td>
<td>50.5</td>
<td>80.5</td>
<td>75.9</td>
</tr>
<tr>
<td>DeepWalk + features</td>
<td>$X,A$</td>
<td>73.1</td>
<td>47.6</td>
<td>83.7</td>
<td>78.1</td>
</tr>
<tr>
<td>GAE</td>
<td>$X,A$</td>
<td>76.9</td>
<td>60.6</td>
<td>82.9</td>
<td>81.2</td>
</tr>
<tr>
<td>VGAE</td>
<td>$X,A$</td>
<td>78.9</td>
<td>61.2</td>
<td>83.0</td>
<td>81.7</td>
</tr>
<tr>
<td>DGI</td>
<td>$X,A$</td>
<td>82.6±0.4</td>
<td>68.8±0.7</td>
<td>86.0±0.1</td>
<td>83.2±0.1</td>
</tr>
<tr>
<td><strong>GRACE</strong></td>
<td>$X,A$</td>
<td><strong>83.3±0.4</strong></td>
<td><strong>72.1±0.5</strong></td>
<td><strong>86.7±0.1</strong></td>
<td><strong>84.2±0.1</strong></td>
</tr>
<tr>
<td>SGC</td>
<td>$X,A,Y$</td>
<td>80.6</td>
<td>69.1</td>
<td>84.8</td>
<td>81.7</td>
</tr>
<tr>
<td>GCN</td>
<td>$X,A,Y$</td>
<td>82.8</td>
<td>72.0</td>
<td>84.9</td>
<td>82.7</td>
</tr>
</tbody>
</table>
# Inductive Node Classification

<table>
<thead>
<tr>
<th>Method</th>
<th>Training Data</th>
<th>Reddit</th>
<th>PPI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Raw features</td>
<td>X</td>
<td>58.5</td>
<td>42.2</td>
</tr>
<tr>
<td>DeepWalk</td>
<td>A</td>
<td>32.4</td>
<td>—</td>
</tr>
<tr>
<td>DeepWalk + features</td>
<td>X, A</td>
<td>69.1</td>
<td>—</td>
</tr>
<tr>
<td>GraphSAGE-GCN</td>
<td>X, A</td>
<td>90.8</td>
<td>46.5</td>
</tr>
<tr>
<td>GraphSAGE-mean</td>
<td>X, A</td>
<td>89.7</td>
<td>48.6</td>
</tr>
<tr>
<td>GraphSAGE-LSTM</td>
<td>X, A</td>
<td>90.2</td>
<td>48.2</td>
</tr>
<tr>
<td>GraphSAGE-pool</td>
<td>X, A</td>
<td>89.2</td>
<td>50.2</td>
</tr>
<tr>
<td>DGI</td>
<td>X, A</td>
<td>94.0±0.1</td>
<td>63.8±0.2</td>
</tr>
<tr>
<td><strong>GRACE</strong></td>
<td>X, A</td>
<td><strong>94.2±0.0</strong></td>
<td><strong>66.1±0.1</strong></td>
</tr>
<tr>
<td>FastGCN</td>
<td>X, A, Y</td>
<td>93.7</td>
<td>—</td>
</tr>
<tr>
<td>GaAN-mean</td>
<td>X, A, Y</td>
<td>95.8±0.1</td>
<td>96.9±0.2</td>
</tr>
</tbody>
</table>
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.
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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.
Acknowledgements

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THANKS