The 37th AAAI Conference (AAAI 2023)

I’m Me, We’re Us, and I’m Us: Tri-directional Contrastive Learning on Hypergraphs

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Hypergraphs are Everywhere

- Many real-world interactions are group-wise.
  - Ex) Collaborations of researchers, interactions of proteins, co-purchases of items.
- A hypergraph can represent such group-wise interactions naturally.
  - A hypergraph is a set of hyperedges that allow containing any number of nodes.

Collaborations of researchers  
Joint interactions of proteins  
Hypergraph  

From wikipedia
Machine Learning on Hypergraphs

- Hypergraph-based ML approaches show its effectiveness on various tasks.
  - Methods: HGNN [Feng et al. 2019], HNHN [Dong, Sawin, and Bengio 2020], AllSet [Chien et al. 2022], etc.
  - Tasks: classification [Feng et al. 2019], clustering [Benson, Gleich, and Leskovec 2016], outlier detection [Lee, Choe, and Shin 2022], etc.

- Most hypergraph neural networks (HNNs) are trained in a (semi-)supervised way.
  - High-quality data labeling is time, resource, and labor-intensive.
  - HNNs trained in a supervised way may overfit and fail to generalize.

- Self-supervised learning, which does not require labels, has become popular, and especially contrastive learning (CL) has achieved great success.
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Contrastive Learning Paradigm

- CL aims to **maximize the agreement** between differently augmented views of the same input via a contrastive loss [Chen et al. 2020].
- CL has demonstrated its effectiveness in computer vision, NLP, and graph domains.
- CL on hypergraphs remains largely underexplored.
In This Work

• In this work, we propose **TriCL**, a novel hypergraph contrastive learning method, to answer the following questions.

Questions?

• (Q1) What to contrast?
• (Q2) How to augment a hypergraph?
• (Q3) How to select negative samples?
Road Map

• Preamble

• Proposed Method: TriCL

• Experiments

• Conclusion
Proposed Approach: TriCL

• **Goal:** to train a hypergraph encoder in a contrastive manner
Proposed Approach: TriCL

1. Hypergraph augmentation
Hypergraph Augmentation

- TriCL first generates two alternative views of the hypergraph $\mathcal{H}$, by applying stochastic hypergraph augmentation functions $\mathcal{T}_1$ and $\mathcal{T}_2$.
- Augmentation: **node feature masking** + **membership masking**.

Node feature masking

Column-wise masking

\[
\begin{array}{cccc}
v_1 & 0 & 0 & \cdots & 1 & 0 & 0 \\
v_2 & 1 & 1 & \cdots & 0 & 0 & 1 \\
v_3 & 1 & 0 & \cdots & 0 & 0 & 0 \\
v_4 & 0 & 0 & \cdots & 1 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 1 & 0 & \cdots & 0 & 0 & 0 \\
1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 1 & 0 & \cdots & 0 & 0 & 1 \\
\end{array}
\]

Corrupted feature matrix

Membership masking

\[
\begin{array}{ccc}
ev_1 & 0 & 0 & \cdots & 1 & 0 & 0 \\
ev_2 & 1 & 0 & \cdots & 0 & 0 & 1 \\
ev_3 & 1 & 0 & \cdots & 0 & 0 & 0 \\
ev_4 & 0 & 0 & \cdots & 1 & 1 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 1 & 0 & \cdots & 0 & 1 & 0 \\
0 & 0 & 1 & \cdots & 0 & 1 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 1 \\
\end{array}
\]

Corrupted incidence matrix
Proposed Approach: TriCL

Hypergraph encoder

\[ \mathcal{H} = (X, H) \]

\[ \mathcal{T}_1 \]

\[ \mathcal{T}_2 \]

Node-level contrast → Group-level contrast → Membership-level contrast
Hypergraph Encoder

• The encoder produces node and hyperedge representations, $P$ and $Q$, for two augmented views.

• TriCL uses a simple **mean pooling layer** as an encoder.

At layer $k$,

$$P^{(k)} = \sigma \left( D_V^{-1} H W Q^{(k)} \Theta_V^{(k)} + b_V^{(k)} \right)$$

$$Q^{(k)} = \sigma \left( D_E^{-1} H^T P^{(k-1)} \Theta_E^{(k)} + b_E^{(k)} \right)$$
Proposed Approach: TriCL

Node-level contrast ➔ Group-level contrast ➔ Membership-level contrast

Node feature masking
Membership masking

$H = (X, H)$

$H_1 = (X_1, H_1)$

$H_2 = (X_2, H_2)$

$\mathcal{T}_1$

$\mathcal{T}_2$

Hypergraph Encoder $f_\theta(\cdot)$

Shared weights

Hyperedge Projection Head

Hyperedge Encoder $g_\phi(\cdot)$

Node Projection Head

Hypergraph Encoder $g_\psi(\cdot)$

$P_1$

$Q_1$

$P_2$

$Q_2$

$Z_1$

$Y_1$

$Z_2$

$Y_2$

Projection head
Projection Head

- SimCLR [Chen et al. 2020] empirically demonstrates that including projection head helps to improve the quality of representations.
- Projection head: two-layer MLP and ELU activation.
Proposed Approach: TriCL

Tri-directional contrastive loss
Tri-directional Contrastive Loss

- Three contrastive objectives:
  1. **Node-level** contrast: discriminate the same node from other nodes.
  2. **Group-level** contrast: discriminate the same hyperedge from other hyperedges.
  3. **Membership-level** contrast: discriminate a ‘real’ membership from a ‘fake’ one.
Motivating Examples

Q) How can the three forms of contrast be helpful for representation learning?

① In node classification, **Information about a group of nodes could be helpful.**
   - Papers written by the same author are more likely to belong to the same field and cover similar topics (i.e., homophily exists in hypergraphs).
Q) How can the three forms of contrast be helpful for node representation learning?

① In node classification, Information about a group of nodes could be helpful.

② Leveraging node-hyperedge membership helps enrich the information of node and hyperedge.
Tri-directional Contrastive Loss

Node contrastive loss

- Discriminate the same node from other nodes.
- Embed \textit{microscopic structural information} into embeddings.

For node $i$: \[ \ell_n(z_{1,i}, z_{2,i}) = -\log \frac{e^{s(z_{1,i}, z_{2,i})/\tau_n}}{\sum_{k=1}^{|V|} e^{s(z_{1,i}, z_{2,k})/\tau_n}}, \]

For all nodes: \[ \mathcal{L}_n = \frac{1}{2|V|} \sum_{i=1}^{|V|} \left\{ \ell_n(z_{1,i}, z_{2,i}) + \ell_n(z_{2,i}, z_{1,i}) \right\} \]

(Proposed) Tri-directional contrastive loss:
\[ \mathcal{L} = \mathcal{L}_n + \omega_g \mathcal{L}_g + \omega_m \mathcal{L}_m \]
Tri-directional Contrastive Loss

Group contrastive loss

- Discriminate the same hyperedge from other hyperedges.
- Embed *group-level structural information* into embeddings.

For hyperedge $j$:  
$$\ell_g(y_{1,j}, y_{2,j}) = - \log \frac{e^{s(y_{1,j}, y_{2,j})/\tau_g}}{\sum_{k=1}^{|E|} e^{s(y_{1,j}, y_{2,k})/\tau_g}},$$

For all hyperedges:  
$$\mathcal{L}_g = \frac{1}{2|E|} \sum_{j=1}^{|E|} \{\ell_g(y_{1,j}, y_{2,j}) + \ell_g(y_{2,j}, y_{1,j})\}$$

(Proposed) Tri-directional contrastive loss:  
$$\mathcal{L} = \mathcal{L}_n + \omega_g \mathcal{L}_g + \omega_m \mathcal{L}_m$$
Tri-directional Contrastive Loss

Membership contrastive loss

- Discriminate a ‘real’ membership from a ‘fake’ one.
- Apply group-level constraints to nodes.

For membership \((i, j)\): 
\[
\ell_m(z_i, y_j) = - \log \frac{e^{D(z_i, y_j)/\tau_m}}{e^{D(z_i, y_j)/\tau_m} + \sum_{k:i \neq k} e^{D(z_i, y_k)/\tau_m}}
\]
when \(z_i\) is the anchor
\[
- \log \frac{e^{D(z_i, y_j)/\tau_m}}{e^{D(z_i, y_j)/\tau_m} + \sum_{k:k \neq j} e^{D(z_k, y_j)/\tau_m}}
\]
when \(y_j\) is the anchor

For all memberships: 
\[
\mathcal{L}_m = \frac{1}{2K} \sum_{i=1}^{V|} \sum_{j=1}^{E|} \mathbb{I}_{[h_{ij}=1]} \left\{ \ell_m(z_{1,i}, y_{2,j}) + \ell_m(z_{2,i}, y_{1,j}) \right\}
\]

(Proposed) Tri-directional contrastive loss: 
\[
\mathcal{L} = \mathcal{L}_n + \omega_g \mathcal{L}_g + \omega_m \mathcal{L}_m
\]
Road Map

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Datasets

• 10 commonly used benchmark datasets
  • **Co-citation**: Cora, Citeseer, and Pubmed [Sen et al. 2008]
  • **Co-authorship**: Cora and DBLP [Rossi and Ahmed 2015]
  • **Vision and graphics**: NTU2012 [Chen et al. 2003] and ModelNet40 [Wu et al. 2015]
  • **UCI repository**: Zoo, 20Newsgroups, and Mushroom [Dua and Graff 2017]

<table>
<thead>
<tr>
<th></th>
<th>Cora-C</th>
<th>Citeseer</th>
<th>Pubmed</th>
<th>Cora-A</th>
<th>DBLP</th>
<th>Zoo</th>
<th>20News</th>
<th>Mushroom</th>
<th>NTU2012</th>
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<td>43</td>
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<td>65,451</td>
<td>40,620</td>
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<td>3.03</td>
<td>3.20</td>
<td>4.35</td>
<td>4.28</td>
<td>4.45</td>
<td>39.93</td>
<td>654.51</td>
<td>136.31</td>
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<td>5</td>
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<tr>
<td>Avg. node degree</td>
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<td>2.37</td>
<td>9.02</td>
<td>1.92</td>
<td>2.41</td>
<td>17.00</td>
<td>4.03</td>
<td>5.00</td>
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<tr>
<td>Max. hyperedge size</td>
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<td>26</td>
<td>171</td>
<td>43</td>
<td>202</td>
<td>93</td>
<td>2241</td>
<td>1808</td>
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<tr>
<td>Max. node degree</td>
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<td>88</td>
<td>99</td>
<td>23</td>
<td>18</td>
<td>17</td>
<td>44</td>
<td>5</td>
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<td>7</td>
<td>6</td>
<td>7</td>
<td>4</td>
<td>2</td>
<td>67</td>
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</table>
Baselines

• 10 (semi-)supervised models:
  • MLP
  • Graph neural networks:
    • GCN [Kipf and Welling 2017]
    • GAT [Velickovic et al. 2018]
  • Hypergraph neural networks:
    • HGNN [Feng et al. 2019]
    • HyperConv [Bai, Zhang, and Torr 2021]
    • HNHN [Dong, Sawin, and Bengio 2020]
    • HyperGCN [Yadati et al. 2019]
    • HyperSAGE [Arya et al. 2020]
    • UniGCN [Huang and Yang 2021]
    • AllSetTransformer [Chien et al. 2022]

• 4 unsupervised models:
  • Network embedding method:
    • Node2vec [Grover and Leskovec 2016]
  • Graph CL methods:
    • DGI [Velickovic et al. 2018]
    • GRACE [Zhu et al. 2020]
  • Hypergraph CL method:
    • S²-HHGR [Zhang et al. 2021]

✔ For graph-based methods

Clique expansion

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Evaluation Protocol

Q) How to assess the quality of node representations learnt by TriCL?

• Task-1: Node classification
  • **Linear evaluation**: train the encoder unsupervised manner and then employ a $\ell_2$-regularized logistic regression model on top of the frozen representations.

• Task-2: Clustering
  • **k-means clustering**: train the encoder unsupervised manner and then employ k-means clustering on top of the frozen representations.
Performance on Node Classification

- **TriCL consistently outperforms its unsupervised baselines** by significant margins.
- It also outperforms the models trained with label supervision.

<table>
<thead>
<tr>
<th>Supervised</th>
<th>Method</th>
<th>Cora-C</th>
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<th>NTT2012</th>
<th>ModelNet40</th>
<th>A.R.</th>
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<tbody>
<tr>
<td>MLP</td>
<td>60.32 ± 1.5</td>
<td>62.06 ± 2.3</td>
<td>76.27 ± 1.1</td>
<td>64.05 ± 1.4</td>
<td>81.18 ± 0.2</td>
<td>75.62 ± 9.5</td>
<td>79.19 ± 0.5</td>
<td>99.58 ± 0.3</td>
<td>65.17 ± 2.3</td>
<td>93.75 ± 0.6</td>
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<td>GCN*</td>
<td>77.11 ± 1.8</td>
<td>66.07 ± 2.4</td>
<td>82.63 ± 0.6</td>
<td>73.66 ± 1.3</td>
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<td>OOM</td>
<td>OOM</td>
<td>71.17 ± 2.4</td>
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<td>GAT*</td>
<td>77.75 ± 2.1</td>
<td>67.62 ± 2.5</td>
<td>81.96 ± 0.7</td>
<td>74.52 ± 1.3</td>
<td>88.59 ± 0.1</td>
<td>36.48 ± 10.0</td>
<td>OOM</td>
<td>OOM</td>
<td>70.94 ± 2.6</td>
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<td>83.52 ± 0.7</td>
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<td>80.15 ± 0.3</td>
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<td>UniGCN</td>
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<td>82.15 ± 0.9</td>
<td>91.12 ± 0.1</td>
<td>80.25 ± 11.2</td>
<td>80.14 ± 0.2</td>
<td>99.83 ± 0.1</td>
<td>75.23 ± 2.4</td>
<td>97.08 ± 0.1</td>
<td>1.5</td>
<td></td>
</tr>
</tbody>
</table>

: The best performance
: The second-best performance
A.R.: Average rank
Ablation Study

- The more types of contrast we use, the better the performance tends to be.
- **Using all types of contrast achieves the best performance** in most cases as they are complementarily reinforcing each other.

<table>
<thead>
<tr>
<th>$L_n$</th>
<th>$L_g$</th>
<th>$L_m$</th>
<th>Cora-C</th>
<th>Citeseer</th>
<th>Pubmed</th>
<th>Cora-A</th>
<th>DBLP</th>
<th>Zoo</th>
<th>20News</th>
<th>Mushroom</th>
<th>NTU2012</th>
<th>ModelNet40</th>
<th>A.R.</th>
</tr>
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<tbody>
<tr>
<td>✓</td>
<td>-</td>
<td>-</td>
<td>80.23 ± 1.2</td>
<td>70.28 ± 1.5*</td>
<td>83.44 ± 0.6</td>
<td>81.94 ± 1.1</td>
<td>90.88 ± 0.1</td>
<td>79.94 ± 11.1</td>
<td><strong>80.18 ± 0.2</strong></td>
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<td>75.20 ± 2.6</td>
<td>97.01 ± 0.2</td>
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<td>79.69 ± 1.6</td>
<td>71.02 ± 1.3*</td>
<td>80.20 ± 1.3</td>
<td>78.98 ± 1.4</td>
<td>88.60 ± 0.2</td>
<td>79.31 ± 10.7</td>
<td>79.35 ± 0.4</td>
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<td>76.76 ± 1.8</td>
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<td>79.80 ± 11.0</td>
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<td><strong>80.18 ± 0.2</strong></td>
<td>99.81 ± 0.1</td>
<td><strong>75.25 ± 2.5</strong></td>
<td>97.02 ± 0.1</td>
<td>2.5</td>
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<td>-</td>
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<td>80.49 ± 1.3</td>
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<td>83.98 ± 0.7</td>
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<td>90.75 ± 0.1</td>
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<td>80.15 ± 0.2</td>
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<td>✓</td>
<td><strong>81.57 ± 1.1</strong></td>
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<td><strong>82.15 ± 0.9</strong></td>
<td><strong>91.12 ± 0.1</strong></td>
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<td>80.14 ± 0.2</td>
<td><strong>99.83 ± 0.1</strong></td>
<td><strong>75.23 ± 2.4</strong></td>
<td><strong>97.08 ± 0.1</strong></td>
<td><strong>1.4</strong></td>
</tr>
</tbody>
</table>

Robustness to the Number of Negatives

- TriCL-Subsampling ($k$) uses randomly subsampled $k$ negatives across the hypergraph to construct the node- and group-level contrastive loss.

- **TriCL is very robust** to the number of negatives.

- Even if only **two negatives** are used, the performance degradation is **<1%**.

### A.P.D: Average performance degradation

<table>
<thead>
<tr>
<th>Method</th>
<th>Cora-C</th>
<th>Citeseer</th>
<th>Pubmed</th>
<th>Cora-A</th>
<th>DBLP</th>
<th>Zoo</th>
<th>20News</th>
<th>Mushroom</th>
<th>NTU2012</th>
<th>ModelNet40</th>
<th>A.P.D.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S^2$-HHGR all negatives</td>
<td>78.08 ± 1.7</td>
<td>68.21 ± 1.8</td>
<td>82.13 ± 0.6</td>
<td>78.15 ± 1.1</td>
<td>88.69 ± 0.2</td>
<td>80.06 ± 11.1</td>
<td>79.75 ± 0.3</td>
<td>97.15 ± 0.5</td>
<td>73.95 ± 2.4</td>
<td>93.26 ± 0.2</td>
<td>-</td>
</tr>
<tr>
<td>TriCL-Subsampling ($k = 2$)</td>
<td>80.62 ± 1.3</td>
<td>71.95 ± 1.3</td>
<td>83.22 ± 0.7</td>
<td>81.25 ± 1.0</td>
<td>90.66 ± 0.2</td>
<td>80.10 ± 11.1</td>
<td>80.03 ± 0.2</td>
<td>99.82 ± 0.1</td>
<td>74.95 ± 2.6</td>
<td>97.02 ± 0.1</td>
<td>0.49%</td>
</tr>
<tr>
<td>TriCL-Subsampling ($k = 4$)</td>
<td>81.15 ± 1.2</td>
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<td>80.12 ± 0.2</td>
<td>99.84 ± 0.1</td>
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<td>0.14%</td>
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<td>81.57 ± 1.1</td>
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<td>82.15 ± 0.9</td>
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<td>75.23 ± 2.4</td>
<td>97.08 ± 0.1</td>
<td>-</td>
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</table>
Performance on Clustering

- TriCL achieves strong clustering performance in terms of NMI and F1.
- Why? The node embeddings learned by TriCL **simultaneously preserve local and community structural information** by fully utilizing group-level contrast.

### A.R.: Average rank

<table>
<thead>
<tr>
<th>Method</th>
<th>Cora-C NMI↑</th>
<th>Cora-C F1↑</th>
<th>Citeseer NMI↑</th>
<th>Citeseer F1↑</th>
<th>Pubmed NMI↑</th>
<th>Pubmed F1↑</th>
<th>Cora-A NMI↑</th>
<th>Cora-A F1↑</th>
<th>DBLP NMI↑</th>
<th>DBLP F1↑</th>
<th>Zoo NMI↑</th>
<th>Zoo F1↑</th>
<th>20News NMI↑</th>
<th>20News F1↑</th>
<th>Mushroom NMI↑</th>
<th>Mushroom F1↑</th>
<th>NTU2012 NMI↑</th>
<th>NTU2012 F1↑</th>
<th>ModelNet40 NMI↑</th>
<th>ModelNet40 F1↑</th>
<th>A.R.↓</th>
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<td>21.5</td>
<td>36.1</td>
<td>19.5</td>
<td><strong>53.4</strong></td>
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<td>15.7</td>
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<td><strong>36.6</strong></td>
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<td>40.1</td>
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<tr>
<td>S²-HHGR</td>
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<td><strong>91.1</strong></td>
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<td>60.6</td>
<td>82.7</td>
<td>71.2</td>
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<td><strong>71.5</strong></td>
<td><strong>95.7</strong></td>
<td><strong>94.7</strong></td>
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</tr>
</tbody>
</table>
Qualitative Analysis

• **TriCL gives more visually and numerically** (based on t-SNE plots and the Silhouette score) **distinguishable clusters** than its two variants.

<table>
<thead>
<tr>
<th></th>
<th>TriCL-N</th>
<th>TriCL-NG</th>
<th>TriCL</th>
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<td><strong>Citeseer</strong></td>
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<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
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<td>Silhouette score</td>
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<td><strong>Cora-C</strong></td>
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<td>Silhouette score</td>
<td>0.167</td>
<td>0.215</td>
<td>0.244</td>
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Road Map

• Preamble
• Proposed Method: TriCL
• Experiments
• Conclusion
Conclusion

• We proposed TriCL, a novel hypergraph contrastive learning method.
  (Q1) What to contrast?
  • (A) Tri-directional contrast: node, group, and membership contrast
  (Q2) How to augment a hypergraph?
  • (A) Node feature masking and membership masking
  (Q3) How to select negative samples?
  • (A) Uniform random sampling

Code and Data: https://github.com/wooner49/TriCL
The 37th AAAI Conference (AAAI 2023)

I’m Me, We’re Us, I’m Us: Tri-directional Contrastive Learning on Hypergraphs

Dongjin Lee

Kijung Shin