





#### The 37<sup>TH</sup> AAAI Conference (AAAI 2023)

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



Dongjin Lee



Kijung Shin

## Hypergraphs are Everywhere

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



Collaborations of researchers



Joint interactions of proteins



Hypergraph

# 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 <u>contrastive learning (CL)</u> has achieved great success.

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#### **Contrastive Learning Paradigm**

- CL aims to <u>maximize the agreement</u> 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*.



#### **Proposed Approach: TriCL**



*(2)* Hypergraph encoder

## 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.



#### **Proposed Approach: TriCL**



**3** 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**



**(4)** Tri-directional contrastive loss

- Three contrastive objectives:
  - 1. <u>Node-level</u> contrast: discriminate the same node from other nodes.
  - 2. <u>Group-level</u> contrast: discriminate the same hyperedge from other hyperedges.
  - 3. <u>Membership-level</u> 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, <u>Information about a group of nodes could be helpful</u>.

• 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).



#### **Motivating Examples**

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

1 In node classification, <u>Information about a group of nodes could be helpful</u>.

 Leveraging node-hyperedge membership helps enrich the information of node and hyperedge.









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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]

	Cora-C	Citeseer	Pubmed	Cora-A	DBLP	Zoo	20News	Mushroom	NTU2012	ModelNet40
# Nodes	1,434	1,458	3,840	2,388	41,302	101	16,242	8,124	2,012	12,311
# Hyperedges	1,579	1,079	7,963	1,072	22,363	43	100	298	2,012	12,311
# Memberships	4,786	3,453	34,629	4,585	99,561	1,717	65,451	40,620	10,060	61,555
Avg. hyperedge size	3.03	3.20	4.35	4.28	4.45	39.93	654.51	136.31	5	5
Avg. node degree	3.34	2.37	9.02	1.92	2.41	17.00	4.03	5.00	5	5
Max. hyperedge size	5	26	171	43	202	93	2241	1808	5	5
Max. node degree	145	88	99	23	18	17	44	5	19	30
# Features	1,433	3,703	500	1,433	1,425	16	100	22	100	100
# Classes	7	6	3	7	6	7	4	2	67	40

#### **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:
    - S<sup>2</sup>-HHGR [Zhang et al. 2021]



#### **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 kmeans 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.

				: The	e best perf	ormance	:	A.R.: Averag	e rank			
	Method	Cora-C	Citeseer	Pubmed	Cora-A	DBLP	Zoo	20News	Mushroom	NTU2012	ModelNet40	A.R.↓
]	MLP	$60.32 \pm 1.5$	$62.06\pm2.3$	$76.27 \pm 1.1$	$64.05\pm1.4$	$81.18\pm0.2$	$75.62\pm9.5$	$\textbf{79.19} \pm \textbf{0.5}$	$99.58\pm0.3$	$65.17\pm2.3$	$93.75\pm0.6$	12.5
	GCN*	$77.11 \pm 1.8$	$66.07 \pm 2.4$	$82.63\pm0.6$	$73.66 \pm 1.3$	$87.58\pm0.2$	$36.79 \pm 9.6$	OOM	$92.47\pm0.9$	$71.17 \pm 2.4$	$91.67 \pm 0.2$	11.7
	GAT*	$77.75\pm2.1$	$67.62 \pm 2.5$	$81.96\pm0.7$	$74.52 \pm 1.3$	$88.59\pm0.1$	$36.48 \pm 10.0$	OOM	OOM	$70.94 \pm 2.6$	$91.43\pm0.3$	11
ed	HGNN	$77.50 \pm 1.8$	$66.16 \pm 2.3$	$83.52\pm0.7$	$74.38 \pm 1.2$	$88.32\pm0.3$	$78.58 \pm 11.1$	$80.15\pm0.3$	$98.59 \pm 0.5$	$72.03\pm2.4$	$92.23\pm0.2$	8.1
vis	HyperConv	$76.19\pm2.1$	$64.12\pm2.6$	$83.42\pm0.6$	$73.52 \pm 1.0$	$88.83\pm0.2$	$62.53 \pm 14.5$	$\textbf{79.83} \pm \textbf{0.4}$	$97.56\pm0.6$	$72.62\pm2.6$	$91.84\pm0.1$	9.8
pei	HNHN	$76.21 \pm 1.7$	$67.28 \pm 2.2$	$80.97\pm0.9$	$74.88 \pm 1.6$	$86.71 \pm 1.2$	$78.89 \pm 10.2$	$79.51 \pm 0.4  99.78 \pm 0.1$		$71.45\pm3.2$	$92.96\pm0.2$	8.9
Suj	HyperGCN	HyperGCN $64.11 \pm 7.4$		$78.40 \pm 9.2$ $60.65 \pm 9$		$76.59 \pm 7.6$	$40.86 \pm 2.1  77.31 \pm 6.0$		$48.26\pm0.3$	$46.05\pm3.9$	$69.23 \pm 2.8$	15.1
	HyperSAGE	$64.98 \pm 5.3$	$52.43\pm9.4$	$79.49 \pm 8.7$	$64.59\pm4.3$	$79.63\pm8.6$	$40.86\pm2.1$	OOT	OOT	OOT	OOT	14.7
	UniGCN	$77.91 \pm 1.9$	$66.40 \pm 1.9$	$84.08\pm0.7$	$77.30 \pm 1.4$	$90.31\pm0.2$	$72.10 \pm 12.1$	$\textbf{80.24} \pm \textbf{0.4}$	$98.84 \pm 0.5$	$73.27\pm2.7$	$94.62\pm0.2$	5.9
	AllSet	$76.21 \pm 1.7$	$67.83 \pm 1.8$	$\overline{82.85\pm0.9}$	$76.94 \pm 1.3$	$90.07\pm0.3$	$72.72 \pm 11.8$	$\textbf{79.90} \pm \textbf{0.4}$	$99.78\pm0.1$	$75.09 \pm 2.5$	$96.85\pm0.2$	6.2
	Node2vec*	$70.99 \pm 1.4$	$53.85 \pm 1.9$	$78.75\pm0.9$	$58.50\pm2.1$	$72.09\pm0.3$	$17.02\pm4.1$	$63.35 \pm 1.7$	$88.16 \pm 0.8$	$67.72\pm2.1$	$84.94\pm0.4$	15.6
р	DGI*	$78.17 \pm 1.4$	$68.81 \pm 1.8$	$80.83\pm0.6$	$76.94 \pm 1.1$	$88.00\pm0.2$	$36.54\pm9.7$	OOM	OOM	$72.01\pm2.5$	$92.18\pm0.2$	9.3
ise	<b>GRACE</b> *	$79.11 \pm 1.7$	$68.65 \pm 1.7$	$80.08\pm0.7$	$76.59 \pm 1.0$	OOM	$37.07\pm9.3$	OOM	OOM	$70.51\pm2.4$	$90.68\pm0.3$	10.4
erv	S <sup>2</sup> -HHGR	$78.08 \pm 1.7$	$68.21 \pm 1.8$	$82.13\pm0.6$	$78.15\pm1.1$	$88.69 \pm 0.2$	$80.06 \pm 11.1$	$\textbf{79.75} \pm \textbf{0.3}$	$97.15\pm0.5$	$73.95 \pm 2.4$	$93.26\pm0.2$	6.8
Ins	Random-Init	$63.62\pm3.1$	$60.44 \pm 2.5$	$67.49 \pm 2.2$	$66.27\pm2.2$	$76.57\pm0.6$	$78.43 \pm 11.0$	$77.14\pm0.6$	$97.40\pm0.6$	$74.39\pm2.6$	$96.29\pm0.3$	11.9
Un	TriCL-N	$80.23 \pm 1.2$	$70.28 \pm 1.5$	$83.44\pm0.6$	$81.94 \pm 1.1$	$90.88\pm0.1$	$79.94 \pm 11.1$	$80.18\pm0.2$	$99.76\pm0.2$	$75.20\pm2.6$	$97.01\pm0.2$	3.4
. –	TriCL-NG	$81.45 \pm 1.2$	$71.38 \pm 1.2$	$83.68\pm0.7$	$82.00\pm1.0$	$90.94\pm0.1$	$80.19 \pm 11.1$	$80.18\pm0.2$	$99.81\pm0.1$	$\textbf{75.25} \pm \textbf{2.5}$	$97.02\pm0.1$	2
	TriCL	$\overline{\textbf{81.57}\pm\textbf{1.1}}$	$\overline{\textbf{72.02} \pm \textbf{1.2}}$	$\textbf{84.26} \pm \textbf{0.6}$	$\overline{\textbf{82.15}\pm\textbf{0.9}}$	$\overline{\textbf{91.12}\pm\textbf{0.1}}$	$\overline{\textbf{80.25}\pm\textbf{11.2}}$	$\overline{80.14\pm0.2}$	$\overline{\textbf{99.83}\pm\textbf{0.1}}$	$\underline{75.23 \pm 2.4}$	$\overline{\textbf{97.08}\pm\textbf{0.1}}$	1.5

#### **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.

					: The best	performa	nce	: The second-best performance A.R.: Average ran							
$\mathcal{L}_n$	$\mathcal{L}_{g}$	$\mathcal{L}_m$	Cora-C	Citeseer	Pubmed	Cora-A	DBLP	Zoo	Zoo 20News		NTU2012	ModelNet40	A.R.↓		
1	-	-	$80.23 \pm 1.2$	$70.28 \pm 1.5*$	$83.44\pm0.6$	$81.94 \pm 1.1$	$90.88\pm0.1$	$79.94 \pm 11.1$	$\textbf{80.18} \pm \textbf{0.2}$	$99.76\pm0.2$	$75.20\pm2.6$	$97.01\pm0.2$	3.8		
-	1	-	$79.69 \pm 1.6$	$71.02 \pm 1.3 *$	$80.20 \pm 1.3$	$78.98 \pm 1.4$	$88.60\pm0.2$	$79.31 \pm 10.7$	$79.35\pm0.4$	$99.13\pm0.3$	$74.41 \pm 2.6$	$96.66\pm0.2$	5.7		
-	-	1	$76.76 \pm 1.8$	$63.98 \pm 2.0$	$79.86\pm0.9$	$76.77 \pm 1.1$	$63.95\pm7.2$	$79.80 \pm 11.0$	$\textbf{79.27} \pm \textbf{0.3}$	$94.87\pm0.7$	$73.11\pm2.8$	$96.57\pm0.2$	6.9		
1	1	-	$81.45 \pm 1.2$	$71.38 \pm 1.4$	$83.68\pm0.7$	$82.00 \pm 1.0$	$90.94 \pm 0.1$	$80.19 \pm 11.1$	$\textbf{80.18} \pm \textbf{0.2}$	$99.81\pm0.1$	$\textbf{75.25} \pm \textbf{2.5}$	$97.02\pm0.1$	<u>2.3</u>		
1	-	1	$80.49 \pm 1.3$	$70.46 \pm 1.5$	$83.98\pm0.7$	$\overline{81.62\pm1.0}$	$\overline{90.75\pm0.1}$	$80.19 \pm 11.1$	$80.15\pm0.2$	$\overline{99.74\pm0.2}$	$75.12\pm2.5$	$97.03 \pm 0.1$	3.6		
-	1	1	$80.80 \pm 1.1$	$71.73 \pm 1.4$	$82.81\pm0.7$	$80.24 \pm 1.0$	$90.17\pm0.1$	$\underline{80.20 \pm 11.1}$	$79.29\pm0.2$	$99.82\pm0.1$	$73.76\pm2.5$	$96.74 \pm 0.1$	4.1		
1	1	1	$\textbf{81.57} \pm \textbf{1.1}$	$\overline{\textbf{72.02}\pm\textbf{1.4}}$	$\textbf{84.26} \pm \textbf{0.6}$	$\textbf{82.15} \pm \textbf{0.9}$	$\textbf{91.12} \pm \textbf{0.1}$	$\overline{\textbf{80.25}\pm\textbf{11.2}}$	$80.14\pm0.2$	$\textbf{99.83} \pm \textbf{0.1}$	$\underline{75.23 \pm 2.4}$	$\textbf{97.08} \pm \textbf{0.1}$	1.4		

#### **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%.

Method	Cora-C	Citeseer	Pubmed	Cora-A	DBLP	Zoo	20News	Mushroom	NTU2012	ModelNet40	A.P.D.
S <sup>2</sup> -HHGR all negatives	$78.08 \pm 1.7$	$68.21 \pm 1.8$	$82.13\pm0.6$	$78.15\pm1.1$	$88.69 \pm 0.2$	$80.06 \pm 11.1$	$\textbf{79.75} \pm \textbf{0.3}$	$97.15\pm0.5$	$73.95\pm2.4$	$93.26\pm0.2$	-
TriCL-Subsampling $(k = 2)$	$80.62 \pm 1.3$	$71.95 \pm 1.3$	$83.22\pm0.7$	$81.25\pm1.0$	$90.66\pm0.2$	$80.10\pm11.1$	$80.03\pm0.2$	$99.82\pm0.1$	$74.95\pm2.6$	$97.02\pm0.1$	0.49%
TriCL-Subsampling $(k = 4)$	$81.15\pm1.2$	$\textbf{72.24} \pm \textbf{1.2}$	$83.91\pm0.7$	$81.85\pm0.9$	$90.83\pm0.1$	$80.16 \pm 11.3$	$80.08\pm0.2$	$\textbf{99.84} \pm \textbf{0.1}$	$75.02\pm2.6$	$97.05\pm0.1$	0.18%
TriCL-Subsampling $(k = 8)$	$81.32\pm1.2$	$72.04 \pm 1.3$	$83.88\pm0.7$	$82.05\pm0.9$	$90.93\pm0.1$	$80.14 \pm 11.2$	$80.12\pm0.2$	$99.84\pm0.1$	$75.09 \pm 2.5$	$97.05\pm0.1$	0.14%
TriCL-Subsampling $(k = 16)$	$81.49 \pm 1.1$	$72.02 \pm 1.2$	$84.23\pm0.7$	$82.10\pm0.9$	$90.97\pm0.1$	$80.10 \pm 11.1$	$80.13\pm0.2$	$99.84\pm0.1$	$75.16\pm2.5$	$97.07\pm0.1$	0.06%
TriCL all negatives	$\textbf{81.57} \pm \textbf{1.1}$	$72.02\pm1.2$	$\textbf{84.26} \pm \textbf{0.6}$	$\textbf{82.15} \pm \textbf{0.9}$	$\textbf{91.12} \pm \textbf{0.1}$	$\textbf{80.25} \pm \textbf{11.2}$	$\textbf{80.14} \pm \textbf{0.2}$	$99.83\pm0.1$	$\textbf{75.23} \pm \textbf{2.4}$	$\textbf{97.08} \pm \textbf{0.1}$	-

A.P.D: Average performance degradation

## **Performance on Clustering**

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

A.R.: Average rank

Method	Cora-C		Citeseer		Pubmed		Cora-A		DBLP		Zoo		20News		Mushroom		NTU2012		ModelNet40		
	NMI↑	F1↑	NMI↑	F1↑	NMI↑	F1↑	NMI↑	F1↑	NMI↑	F1↑	NMI↑	F1↑	NMI↑	F1↑	NMI↑	F1↑	NMI↑	F1↑	NMI↑	F1↑	А.К.↓
features	20.0	28.8	21.5	36.1	19.5	53.4	17.2	29.2	37.0	47.3	78.3	77.3	15.7	41.1	36.6	72.4	81.7	69.0	90.6	86.5	3.8
Node2vec*	39.1	44.5	24.5	38.5	23.1	40.1	16.0	34.1	32.4	37.8	11.5	41.6	8.7	26.6	1.6	44.0	78.3	57.7	72.9	53.1	5.0
DGI*	54.8	<u>60.1</u>	40.1	51.7	30.4	53.0	45.2	<u>52.5</u>	58.0	57.7	13.0	13.8	OOM		00	Μ	79.6	61.7	85.0	73.7	3.1
<b>GRACE</b> *	44.4	45.6	33.3	45.7	16.7	41.9	37.9	43.3	16.7	41.9	7.3	29.4	00	Μ	OOM		74.6	47.5	79.4	59.9	4.9
S <sup>2</sup> -HHGR	51.0	56.8	<u>41.1</u>	<u>53.1</u>	27.7	<u>53.2</u>	<u>45.4</u>	52.3	60.3	<u>62.7</u>	<u>90.9</u>	91.1	39.0	58.7	<u>18.6</u>	60.6	82.7	<u>71.2</u>	<u>91.0</u>	<u>90.6</u>	<u>2.1</u>
TriCL	<u>54.5</u>	60.6	44.1	57.4	<u>30.0</u>	51.7	49.8	56.7	63.1	63.0	91.2	<u>89.3</u>	<u>35.6</u>	<u>54.2</u>	3.8	<u>65.1</u>	83.2	71.5	95.7	94.7	1.6

#### **Qualitative Analysis**

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



#### **Road Map**

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## Conclusion

- We proposed <u>TriCL</u>, 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: <u>https://github.com/wooner49/TriCL</u>* 









#### The 37<sup>TH</sup> AAAI Conference (AAAI 2023)

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



Dongjin Lee



Kijung Shin