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Artificial Intelligence for Future Agricultural Resilience, Management, and Sustainability

Augmentations in Hypergraph Contrastive Learning: Fabricated and Generative

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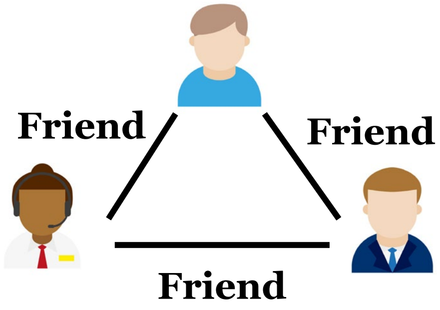
Background

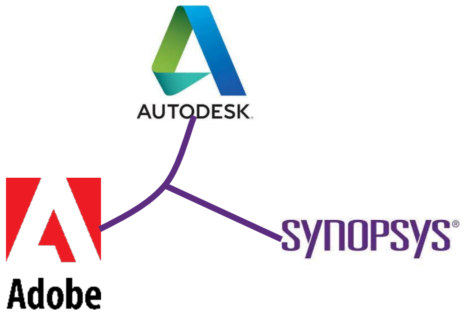
- **Hypergraphs** have raised a surge of interest in the research community

- Powerful tool to capture **higher-order relations** and model **complicated topological structures** in **broad applications**:

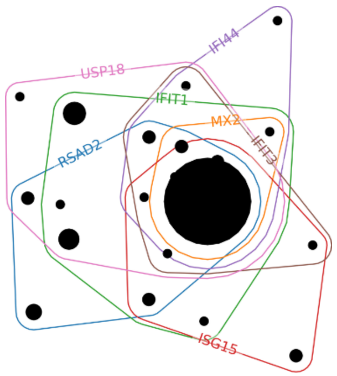
  - Recommender Systems: User Relations



  - Financial Analyses: Industry Groupings



  - Bioinformatics: Protein Complexes

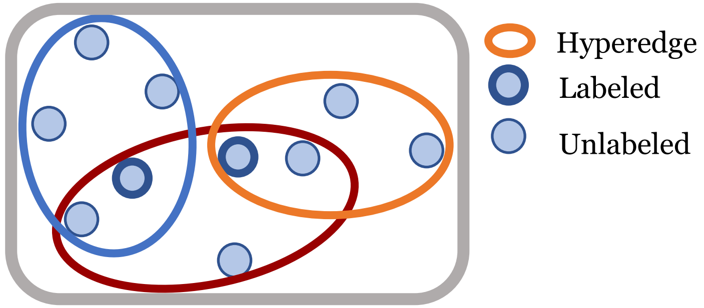


  - …

Song Feng, et al. "**Hypergraph models of biological networks to identify genes critical to pathogenic viral response**." *BMC Bioinformatics*. 2021.

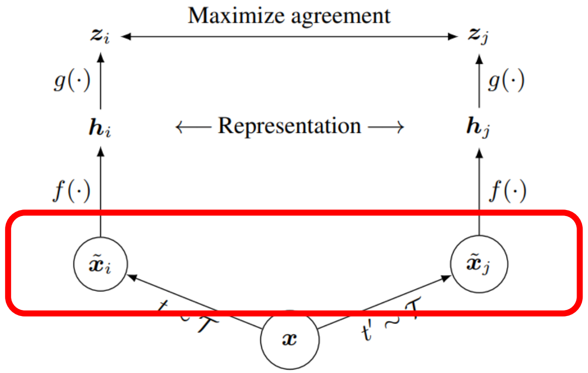
Problem

- **Label scarcity scenarios:** ubiquitous in real-world applications of hypergraphs



Restrict the **generalizability** of HyperGNNs!

- Inspired by emerging self-supervised learning on images/graphs → leverage **contrastive self-supervision** on hypergraphs

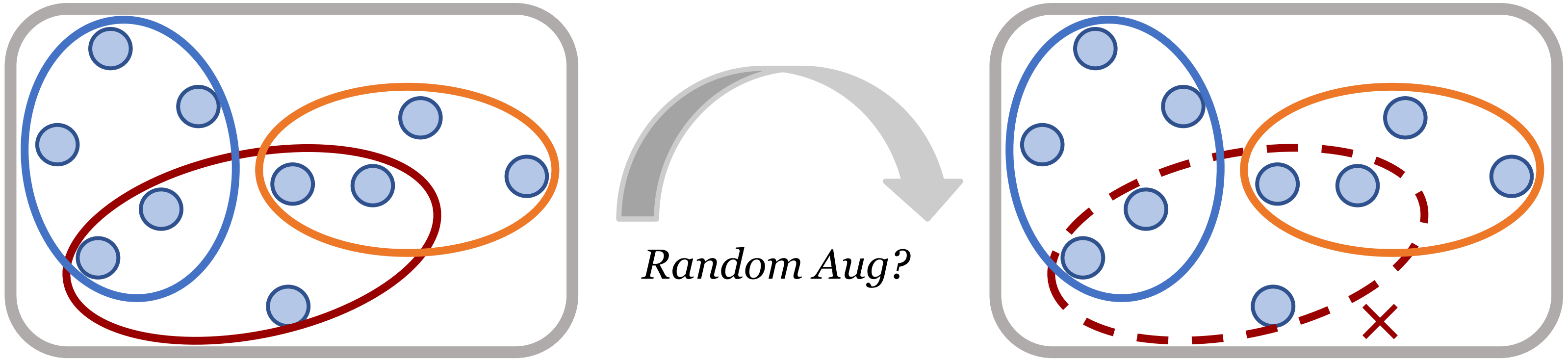


How to construct the **augmentations** on hypergraph?

Ting Chen, et al. "**A Simple Framework for Contrastive Learning of Visual Representations.**" *ICML*. 2020.

Augmentation in Hypergraphs

- **Bad view construction** would result in negative transfer



Doesn't perform well!

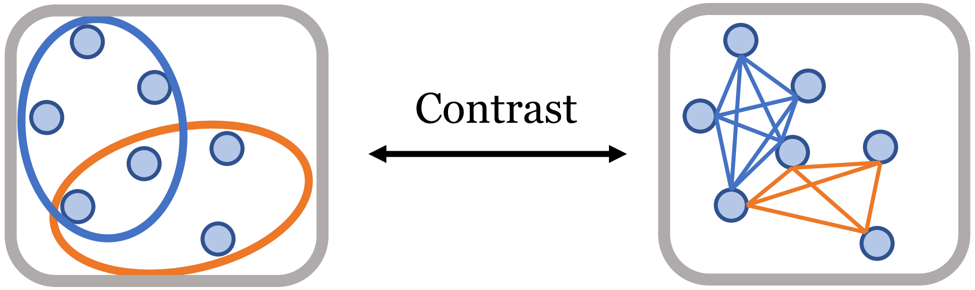
- **Non-trivial** to build hypergraph views due to their overly intricate topology
  - Overly intricate topology

$\sum_{e=1}^{N} \binom{N}{e}$ **possibilities** for one hyperedge on N vertices!

- Propose the first hypergraph generative augmentation in a data-driven manner
  - Parameterize the augmentation space in a learnable manner

Comparison with Existing Work

- Contrasting between the hypergraph and corresponding clique-expanded graph
  - Cause **information loss**



- Fabricated Augmentations on Graph
  - Can be applied to hypergraph
  - Rely on **domain knowledge**

- Our method generates better augmented views in a **data-driven manner**
  - Novel hypergraph generator → **parameterize** a certain **augmentation space** of hypergraphs
  - End-to-end pipeline → **jointly learn** hypergraph augmentations and model parameters

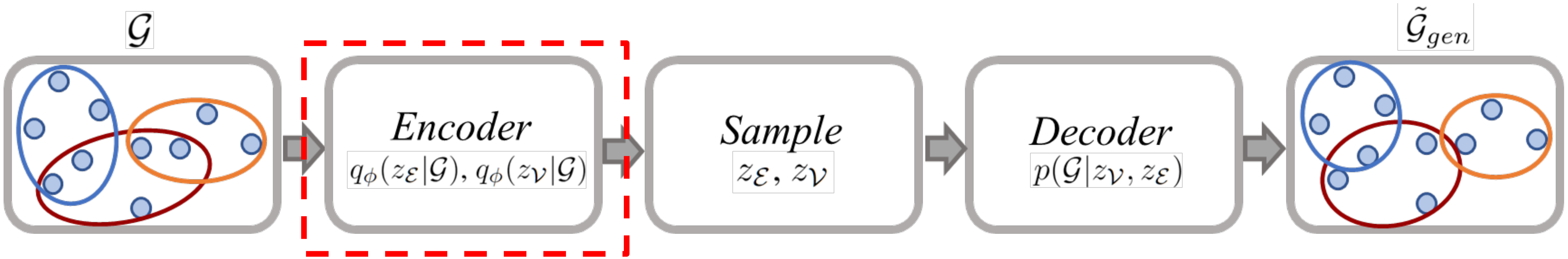
Matthias Hein, et al. "**The total variation on hypergraphs-learning on hypergraphs revisited.**" *NeurIPS 2013*.
Pan Li, et al. "**Submodular hypergraphs: p-laplacians, cheeger inequalities and spectral clustering.**" *ICML 2018*.

Method: Hypergraph Generative Models

- **Proposed method**: a novel variational hypergraph auto-encoder architecture (**VHGAE**) to parametrize the augmentation space of **edge perturbation**

- **Encoder**: embeds the **vertex** and **hyperedge** representation with **variational distribution**

$$\mu_{\mathcal{V}}, \mu_{\mathcal{E}} = h_1^{\mu}(\mathcal{G}), \qquad \log(\sigma_{\mathcal{V}}), \log(\sigma_{\mathcal{E}}) = h_1^{\sigma}(\mathcal{G}),$$



Method: Hypergraph Generative Models

- The sampled vertex and hyperedge representation $z_{\mathcal{E}}, z_{\mathcal{V}}$
- **Decoder** attempts to reconstruct the higher-order relations of hypergraph

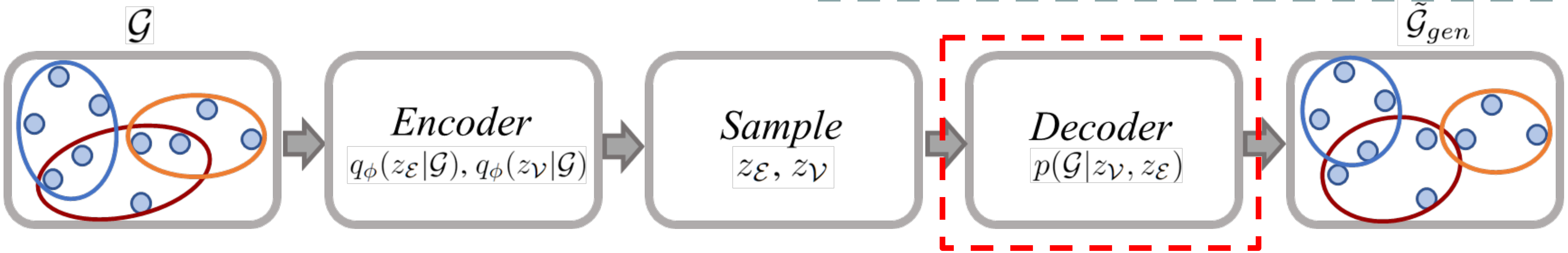
Relation Reconstruction

$$p(\tilde{\mathcal{G}}|z_{\mathcal{V}}, z_{\mathcal{E}}) = \prod_{e=1}^{|\mathcal{E}|}\prod_{v=1}^{|\mathcal{V}|} p(\tilde{\mathcal{E}}_{v,e}|z_v, z_e) = \prod_{e=1}^{|\mathcal{E}|}\prod_{v=1}^{|\mathcal{V}|} \mathrm{Sigmoid}\boxed{(z_v^T z_e)},$$

- Optimize the evidence lower bound (ELBO):

Variational Regularization

$$\mathrm{ELBO} = \mathbb{E}_{q_\phi(z_{\mathcal{E}}|\mathcal{G})}\mathbb{E}_{q_\phi(z_{\mathcal{V}}|\mathcal{G})}\left[\log p_\theta(\mathcal{G}|z_v, z_e)\right] - \boxed{\mathrm{KL}[q_\phi(z_{\mathcal{V}} \mid \mathcal{G}) \mid p(z_{\mathcal{V}})] - \mathrm{KL}[q_\phi(z_{\mathcal{E}} \mid \mathcal{G}) \mid p(z_{\mathcal{E}})]},$$



Method: Jointly Augmenting and Contrasting

- Main barrier: the **discrete sampling** of hyperedges which is **non-differentiable**
- To tackle it,

$$T(\mathcal{G}) = \boxed{\text{Gumbel-Softmax}}(p(\mathcal{G} \mid z_{\mathcal{V}}, z_{\mathcal{E}}))$$

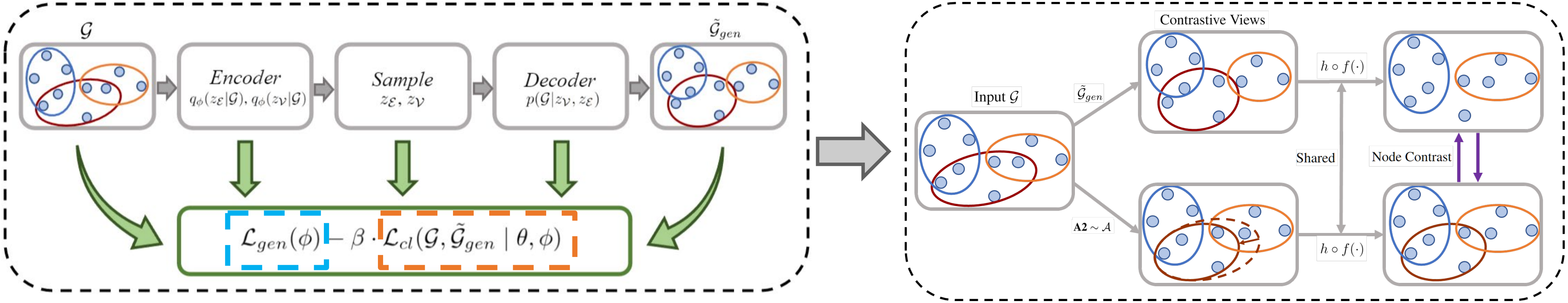
Differential Sampling

$$= \text{Sigmoid}((w_{\mathcal{V}\mathcal{E}} + \log(\delta) - \log(1-\delta))/\tau)$$

$$\tilde{\mathcal{G}}_{gen} = T(\mathcal{G}) \circ \mathcal{G},$$

VHGAE Optimization

HyperGNN Optimization



- Generator loss (-ELBO) to be minimized
- Maximizing CL loss in VHGAE to avoid capturing redundant information

Evaluation

- Data Sets
  - Vertex Classification

	Cora	Citeseer	Pubmed	Cora-CA	DBLP-CA	Zoo	20News	Mushroom	NTU2012	ModelNet40	Yelp	House	Walmart
$\lvert\mathcal{V}\rvert$	2708	3312	19717	2708	41302	101	16242	8124	2012	12311	50758	1290	88860
$\lvert\mathcal{E}\rvert$	1579	1079	7963	1072	22363	43	100	298	2012	12311	679302	341	69906
# feature	1433	3703	500	1433	1425	16	100	22	100	100	1862	100	100
# class	7	6	3	7	6	7	4	2	67	40	9	2	11
h_e	0.86	0.83	0.88	0.88	0.93	0.66	0.73	0.96	0.87	0.92	0.57	0.58	0.75
h_v	0.84	0.78	0.79	0.79	0.88	0.35	0.49	0.87	0.81	0.88	0.26	0.52	0.55

- Metrics
  - **Accuracy** (for generalization and robustness)
  - **Statistical Parity** and **Equalized Odds** (for fairness)

- Baselines
  - Fabricated Augmentation Operations
  - Existing self-supervised learning methods between hypergraph and clique-expanded graph

Augmentation Operations

Name	Operation
A0	Identity
A1	Naïve Hyperedge Perturbation
A2	Generalized Hyperedge Perturbation
A3	Vertex Dropping
A4	Attribute Masking
A5	Subgraph
A6	Generative Augmentation

Evaluation: Generalization

Group	Method	Cora	Citeseer	Pubmed	Cora-CA	DBLP-CA	Zoo	20Newsgroups	Mushroom
	SetGNN	67.93 ± 1.27	63.53 ± 1.32	84.33 ± 0.36	72.21 ± 1.51	89.51 ± 0.18	65.06 ± 12.82	79.37 ± 0.35	99.75 ± 0.11
Existing SS methods	Self	68.24 ± 1.12	62.49 ± 1.48	84.38 ± 0.38	72.74 ± 1.53	89.51 ± 0.23	57.35 ± 18.32	79.45 ± 0.32	95.83 ± 0.23
	Con	68.89 ± 1.80	62.82 ± 1.21	84.56 ± 0.34	73.22 ± 1.65	89.59 ± 0.13	61.05 ± 14.54	79.49 ± 0.45	95.85 ± 0.31
Fabricated Augmentations	A0	68.59 ± 1.33	62.25 ± 2.15	84.54 ± 0.42	71.85 ± 1.62	89.62 ± 0.24	62.57 ± 13.84	79.07 ± 0.46	99.77 ± 0.17
	A1	72.39 ± 1.34	66.28 ± 1.27	85.17 ± 0.37	75.45 ± 1.54	89.83 ± 0.21	65.80 ± 13.31	79.47 ± 0.32	99.80 ± 0.14
	A2	72.58 ± 1.09	66.40 ± 1.35	85.16 ± 0.38	75.62 ± 1.42	90.22 ± 0.23	66.35 ± 13.26	79.56 ± 0.42	99.80 ± 0.17
	A3	72.33 ± 1.23	65.79 ± 1.18	85.24 ± 0.28	75.34 ± 1.40	89.85 ± 0.16	65.79 ± 14.05	79.47 ± 0.34	99.81 ± 0.10
	A4	72.95 ± 1.19	66.22 ± 0.95	84.88 ± 0.38	75.29 ± 1.56	90.10 ± 0.18	62.59 ± 12.77	79.45 ± 0.48	99.80 ± 0.14
	A5	67.96 ± 0.99	63.21 ± 1.25	84.48 ± 0.40	72.61 ± 1.86	89.75 ± 0.24	62.47 ± 12.39	79.42 ± 0.52	99.79 ± 0.10
Our Generative Augmentation	A6	**73.12 ± 1.48**	**66.94 ± 1.00**	**85.72 ± 0.38**	**76.21 ± 1.26**	**90.28 ± 0.19**	**66.89 ± 12.44**	**79.78 ± 0.40**	**99.86 ± 0.10**

	NTU2012	ModelNet40	Yelp	House (0.6)	House (1.0)	Walmart (0.6)	Walmart (1.0)	Avg. Rank
SetGNN	73.86 ± 1.62	95.85 ± 0.38	28.78 ± 1.51	68.54 ± 1.89	58.34 ± 2.25	74.97 ± 0.22	59.13 ± 0.20	7.71
Self	73.41 ± 1.65	95.83 ± 0.23	23.49 ± 4.15	67.75 ± 3.29	58.54 ± 2.16	74.76 ± 0.20	58.83 ± 0.21	8.64
Con	73.27 ± 1.53	95.85 ± 0.31	26.14 ± 1.86	68.50 ± 2.52	58.56 ± 2.42	75.17 ± 0.21	59.39 ± 0.20	7.07
A0	73.54 ± 1.93	95.92 ± 0.18	29.43 ± 1.42	67.48 ± 3.21	57.39 ± 2.37	73.14 ± 0.21	56.49 ± 0.60	8.21
A1	74.71 ± 1.81	95.87 ± 0.27	27.18 ± 0.71	68.64 ± 2.99	58.10 ± 3.22	75.42 ± 0.13	60.09 ± 0.25	4.50
A2	74.88 ± 1.66	96.56 ± 0.34	31.39 ± 2.45	69.73 ± 2.60	58.90 ± 1.97	75.50 ± 0.18	60.19 ± 0.20	2.29
A3	74.68 ± 1.74	96.48 ± 0.29	27.57 ± 1.00	67.88 ± 2.90	58.51 ± 2.22	75.29 ± 0.23	60.19 ± 0.20	4.71
A4	74.83 ± 1.75	95.86 ± 0.28	29.64 ± 1.93	69.56 ± 2.89	58.91 ± 2.69	75.43 ± 0.18	59.90 ± 0.24	4.14
A5	74.41 ± 1.86	96.46 ± 0.33	29.24 ± 1.42	68.14 ± 2.97	57.70 ± 2.98	75.26 ± 0.18	59.81 ± 0.22	6.71
A6	**75.34 ± 1.91**	**96.93 ± 0.33**	**34.64 ± 0.39**	**70.96 ± 2.27**	**59.93 ± 1.99**	**75.62 ± 0.16**	**60.46 ± 0.20**	**1.00**

- Proposed generative augmentation (A6) achieves **substantial improvements**

Evaluation: Robustness & Fairness

Robustness

	Cora			Citeseer			ModelNet40		
	Random	Net	Minmax	Random	Net	Minmax	Random	Net	Minmax
SetGNN	66.87 ± 1.33	66.26 ± 1.54	66.58 ± 1.02	62.89 ± 1.57	62.81 ± 1.32	62.21 ± 1.64	95.74 ± 0.22	95.41 ± 0.28	93.33 ± 0.26
A2	71.90 ± 1.63	71.16 ± 0.92	70.86 ± 1.22	66.41 ± 1.08	65.38 ± 1.47	64.69 ± 0.98	96.09 ± 0.17	95.52 ± 0.24	93.64 ± 0.26
A4	72.11 ± 1.60	70.49 ± 1.29	70.52 ± 1.39	65.94 ± 1.24	65.15 ± 1.70	64.12 ± 1.19	95.79 ± 0.27	95.44 ± 0.25	93.35 ± 0.24
A6	**72.15 ± 1.70**	**71.94 ± 1.48**	**71.98 ± 1.36**	**66.60 ± 1.61**	**65.68 ± 1.09**	**65.51 ± 1.13**	**96.58 ± 0.24**	**96.23 ± 0.23**	**94.82 ± 0.33**
	NTU2012			House (0.6)			House (1.0)		
	Random	Net	Minmax	Random	Net	Minmax	Random	Net	Minmax
SetGNN	73.84 ± 2.18	73.38 ± 1.36	70.71 ± 1.89	67.16 ± 2.55	68.88 ± 2.68	64.78 ± 2.20	56.86 ± 1.93	59.95 ± 1.92	56.52 ± 2.52
A2	74.50 ± 2.03	73.86 ± 1.84	71.40 ± 1.64	67.71 ± 2.94	69.59 ± 2.32	65.23 ± 2.89	57.74 ± 2.70	60.73 ± 2.30	57.00 ± 1.94
A4	73.73 ± 1.59	73.72 ± 1.59	71.06 ± 1.53	67.55 ± 2.41	68.85 ± 1.38	64.97 ± 3.35	57.47 ± 2.72	60.10 ± 1.74	56.65 ± 2.26
A6	**75.06 ± 1.97**	**74.37 ± 1.99**	**72.09 ± 1.98**	**69.88 ± 3.27**	**73.14 ± 2.71**	**68.84 ± 2.71**	**60.06 ± 2.07**	**62.41 ± 1.77**	**58.76 ± 2.24**

Fairness

data set	Method	AUROC	F1	$\Delta_{SP}(\downarrow)$	$\Delta_{EO}(\downarrow)$
German Credit	SetGNN	59.16 ± 2.51	81.84 ± 0.93	2.65 ± 5.62	4.06 ± 6.76
	A2	59.81 ± 3.00	82.26 ± 0.13	**0.55 ± 0.95**	0.78 ± 0.70
	A4	59.66 ± 3.83	80.54 ± 3.52	3.03 ± 6.54	5.07 ± 7.81
	A6	**59.88 ± 3.04**	**82.36 ± 0.38**	0.95 ± 0.92	**0.47 ± 0.56**
Recidivism	SetGNN	96.51 ± 0.48	89.84 ± 0.97	8.63 ± 0.50	4.16 ± 0.51
	A2	96.34 ± 0.39	**90.09 ± 0.53**	8.53 ± 0.52	3.92 ± 0.68
	A4	96.45 ± 0.35	89.75 ± 0.68	**8.49 ± 0.27**	3.49 ± 0.66
	A6	**96.55 ± 0.54**	89.22 ± 0.55	8.51 ± 0.25	**3.13 ± 0.64**
Credit defaulter	SetGNN	73.46 ± 0.17	87.91 ± 0.27	2.79 ± 0.99	0.98 ± 0.69
	A2	73.43 ± 0.27	87.82 ± 0.24	2.64 ± 1.32	0.93 ± 0.87
	A4	73.58 ± 0.19	87.92 ± 0.25	2.84 ± 1.14	1.38 ± 0.32
	A6	**73.78 ± 0.16**	**88.03 ± 0.14**	**2.58 ± 0.91**	**0.81 ± 0.37**

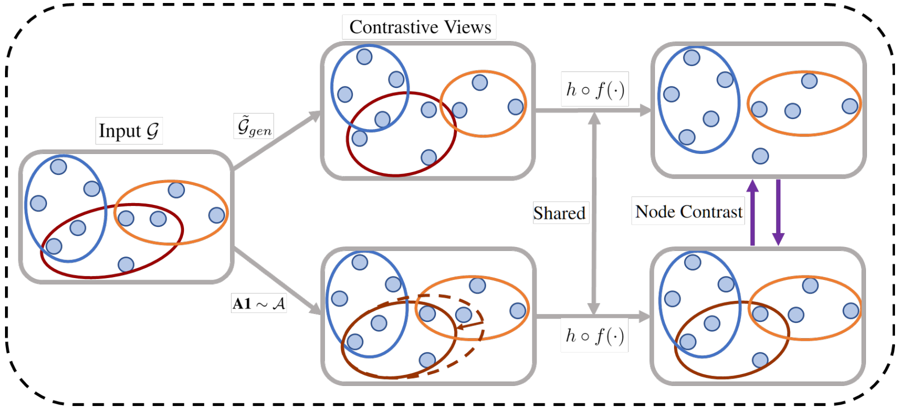
- First robustness and fairness evaluation for hypergraphs
- **Robust** against adversarial attacks
- **Fair** w.r.t. sensitive attributes

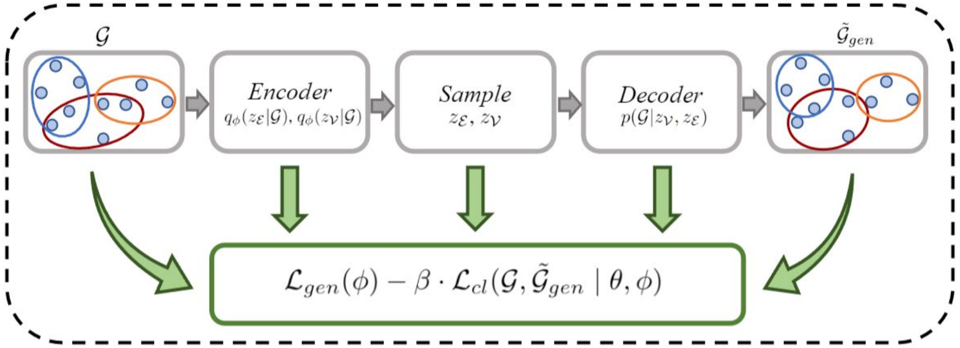
Conclusion

- **Problem**: Label scarcity scenarios of Hypergraph Application

- **Algorithms**: Generative Hypergraph Contrastive Learning (HyperGCL)
  - Parametrize the augmentation space
  - Jointly learn augmentation and model

- **Evaluation**: Effectiveness on generalization, robustness, and fairness
  - Vertex Classification





Our code is available at https://github.com/weitianxin/HyperGCL.

THANK YOU FOR LISTENING!

Contact: Tianxin Wei (Email: twei10@illinois.edu)

Code: https://github.com/weitianxin/HyperGCL