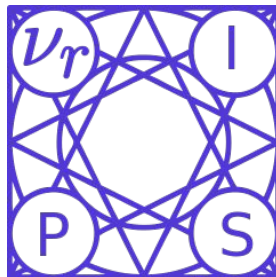


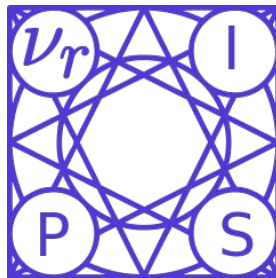
# HyperGraph Convolutional Network (HyperGCN)

To Appear as a Poster in Neural Information Processing Systems, 2019



# HyperGraph Convolutional Network (HyperGCN)

To Appear as a Poster in Neural Information Processing Systems, 2019



Madhav



Prateek



Vikram



Prof. Anand Louis

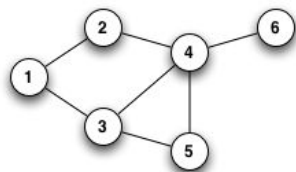


Prof. Partha Talukdar

Joint work with

# Motivation

**networks have complex relationships**



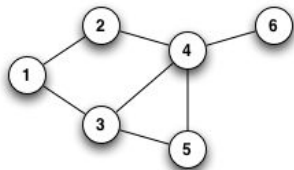
**simple graphs do not capture such relationships**

# Motivation

networks have complex relationships



co-authorship



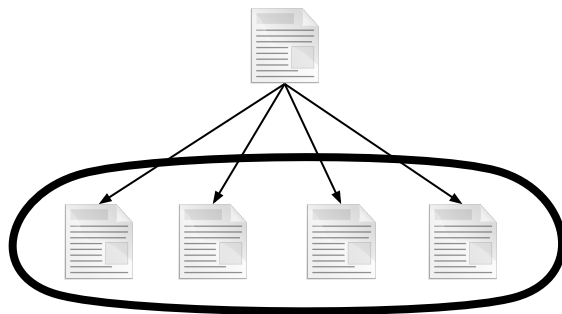
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# Motivation

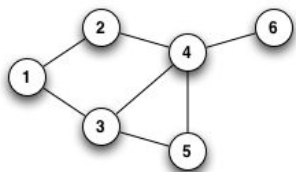
networks have complex relationships



co-authorship



co-citation



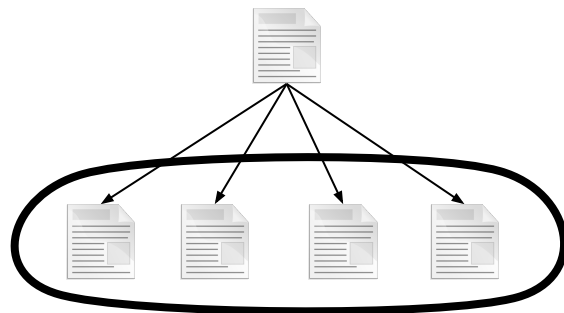
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# Motivation

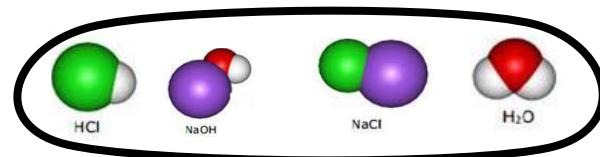
networks have complex relationships



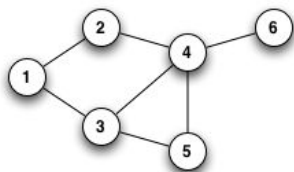
co-authorship



co-citation

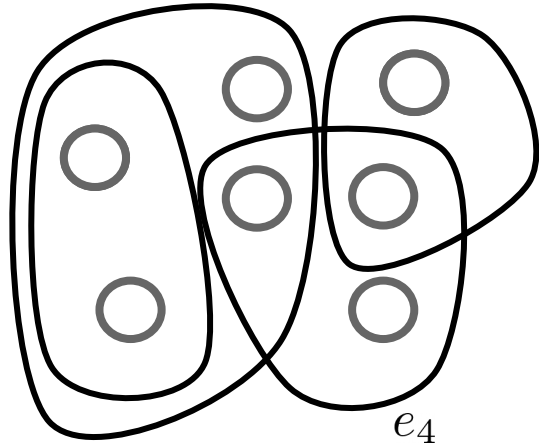


chemical reaction



simple graphs do not capture such relationships

# Hypergraph

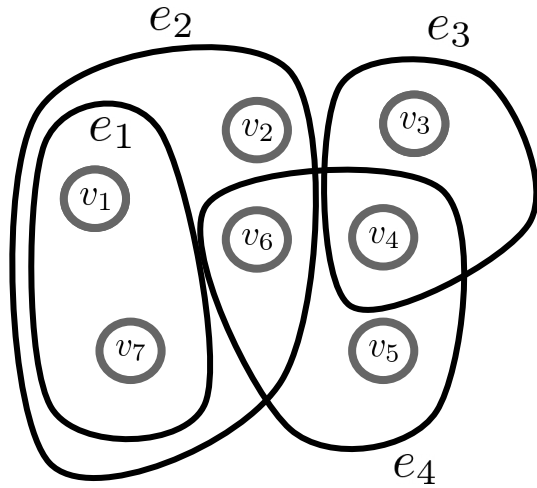


**an edge can connect any number of vertices**

$$\mathcal{H} = (V, E)$$

$$E \subseteq 2^V$$

# Hypergraph



**an edge can connect any number of vertices**

$$V = \{v_1, v_2, v_3, v_4, v_5, v_6, v_7\}$$

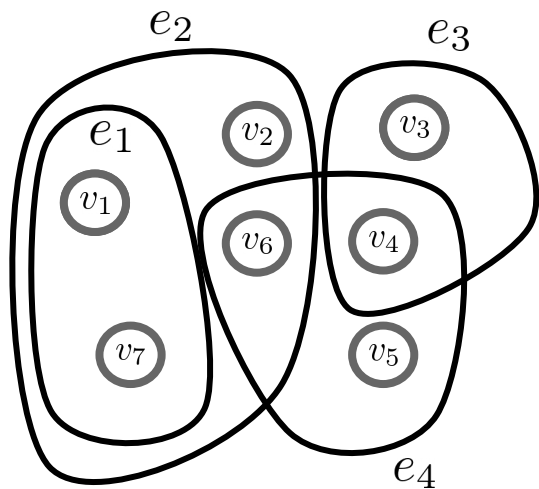
$$E = \{e_1, e_2, e_3, e_4\}$$

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# Hypergraph



$$\mathcal{H} = (V, E)$$

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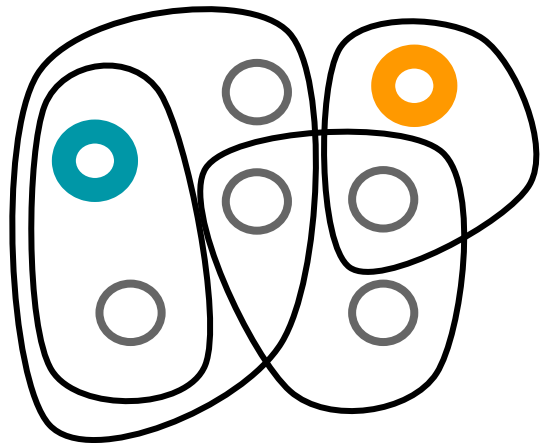
$$e_1 = \{v_1, v_7\}$$

$$e_2 = \{v_1, v_2, v_6, v_7\}$$

$$e_3 = \{v_3, v_4\}$$

$$e_4 = \{v_4, v_5, v_6\}$$

# Hypergraph-based Semi-Supervised Learning (SSL)

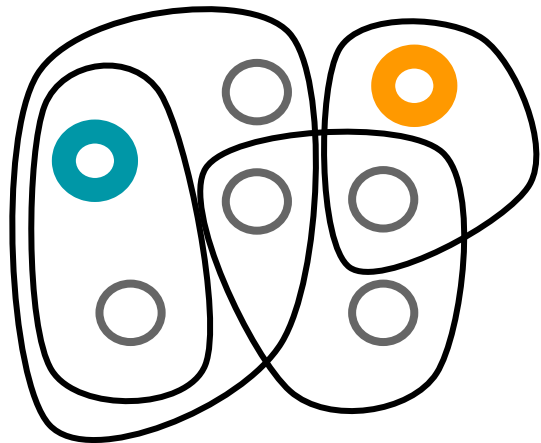


**use labelled and unlabelled data for training**

$$\mathcal{H} = (V, E)$$

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# Hypergraph-based Semi-Supervised Learning (SSL)



use labelled and unlabelled data for training

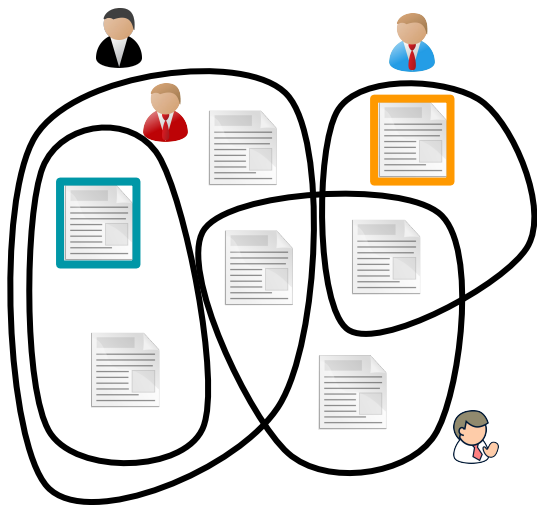
expensive

cheap

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# Hypergraph-based Semi-Supervised Learning (SSL)



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**expensive**

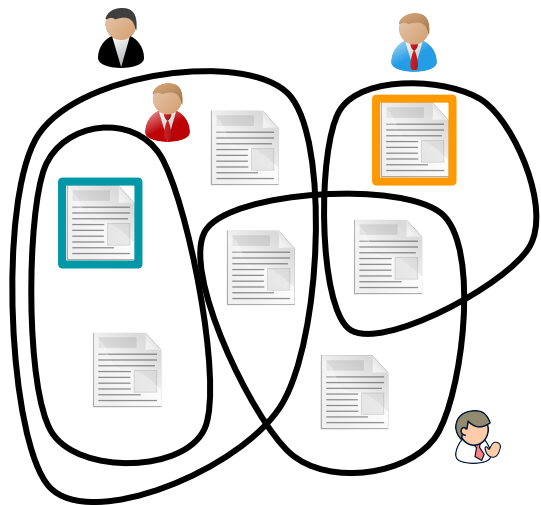
**cheap**

e.g. document classification in co-authorship

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**expensive**

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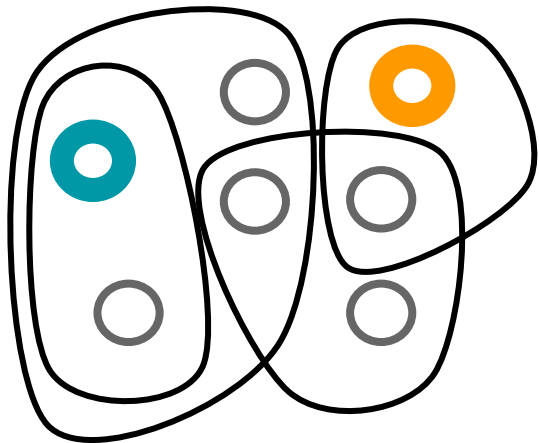
e.g. document classification in co-authorship

$$\text{Learn } f : \{x_1, \dots, x_n\} \rightarrow \{y_1, \dots, y_c\}$$

$$\mathcal{H} = (V, E)$$

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# Related Work



$$\mathcal{H} = (V, E)$$

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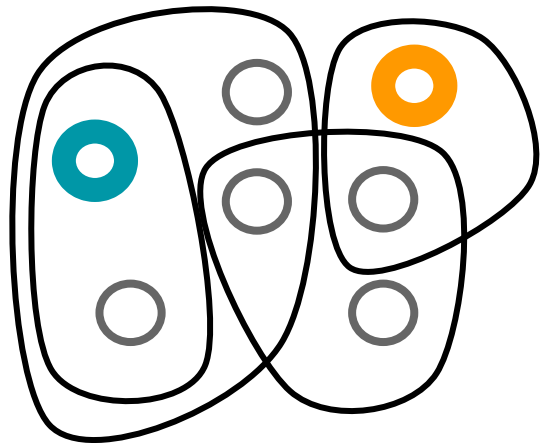
explicit regularisation

$$\mathcal{L} = \underbrace{\mathcal{L}_S}_{\text{supervised}} + \underbrace{\lambda \cdot Q(\mathcal{H}, f)}_{\text{unsupervised}}$$

- Zhou et al. NIPS'06
- Hein et al. NIPS'13
- Anand Louis. STOC'15
- Chan and Liang. COCOON'18

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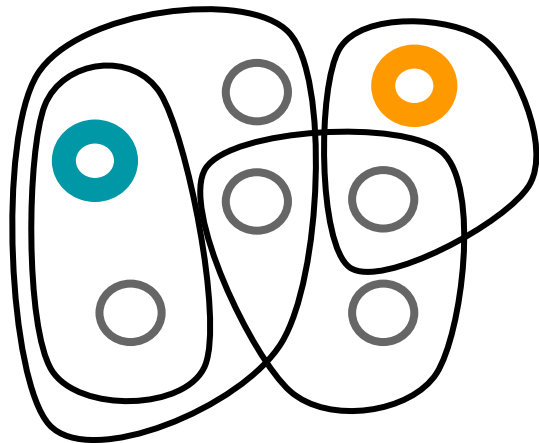
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**✗ hyperedges encode similarity**

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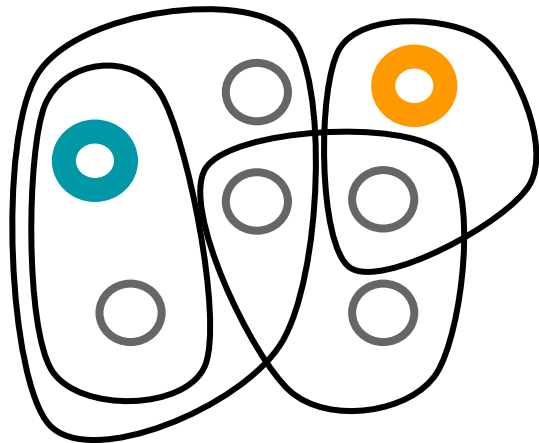
## Our focus: Implicit regularisation

$$f_{\text{Neural}}(\mathcal{H}, X) = ?$$

$$\mathcal{L} = \mathcal{L}_S$$



# Related Work



$$\mathcal{H} = (V, E)$$

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## explicit regularisation

$$\mathcal{L} = \underbrace{\mathcal{L}_S}_{\text{supervised}} + \underbrace{\lambda \cdot Q(\mathcal{H}, f)}_{\text{unsupervised}}$$

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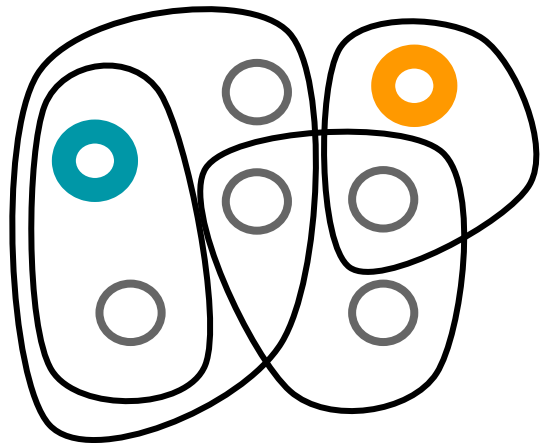
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**✓ hyperedges need not encode similarity**

# Related Work



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**hyperedges need not encode similarity**

e.g.



# Hypergraph total variation [ Hein et al. NeurIPS'13 ]

$$\mathcal{L} = \mathcal{L}_S + \lambda \cdot Q(\mathcal{H}, f)$$

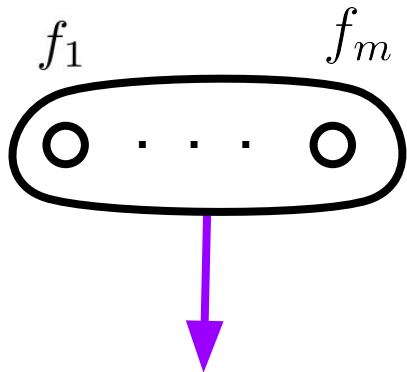
graphs:  $Q(\mathcal{G}, f) = \sum_{\{u,v\} \in E} (f_u - f_v)^2$

# Hypergraph total variation [ Hein et al. NeurIPS'13 ]

$$\mathcal{L} = \mathcal{L}_S + \lambda \cdot Q(\mathcal{H}, f)$$

hypergraphs:  $Q(\mathcal{H}, f) = \sum_{e \in E} \left( \max_{s \in e} f_s - \min_{i \in e} f_i \right)^2$

# Hypergraph total variation [ Hein et al. NeurIPS'13 ]



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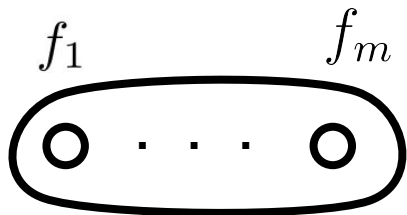
$$\text{hypergraphs: } Q(\mathcal{H}, f) = \sum_{e \in E} \left( \max_{s \in e} f_s - \min_{i \in e} f_i \right)^2$$

$\arg \max_{s \in e} f_s$



$\arg \min_{i \in e} f_i$

# Hypergraph total variation [ Hein et al. NIPS 13 ]

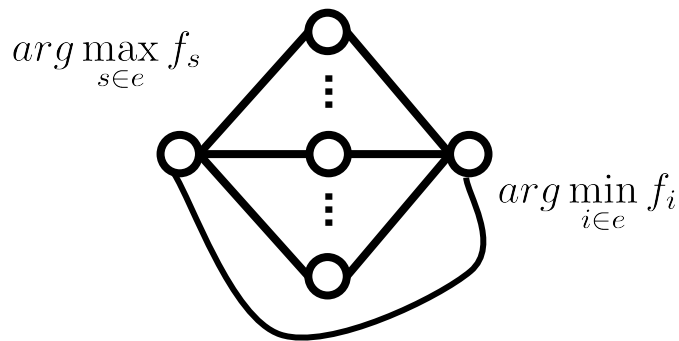


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hypergraphs:  $Q(\mathcal{H}, f) = \sum_{e \in E} \left( \max_{s \in e} f_s - \min_{i \in e} f_i \right)^2$

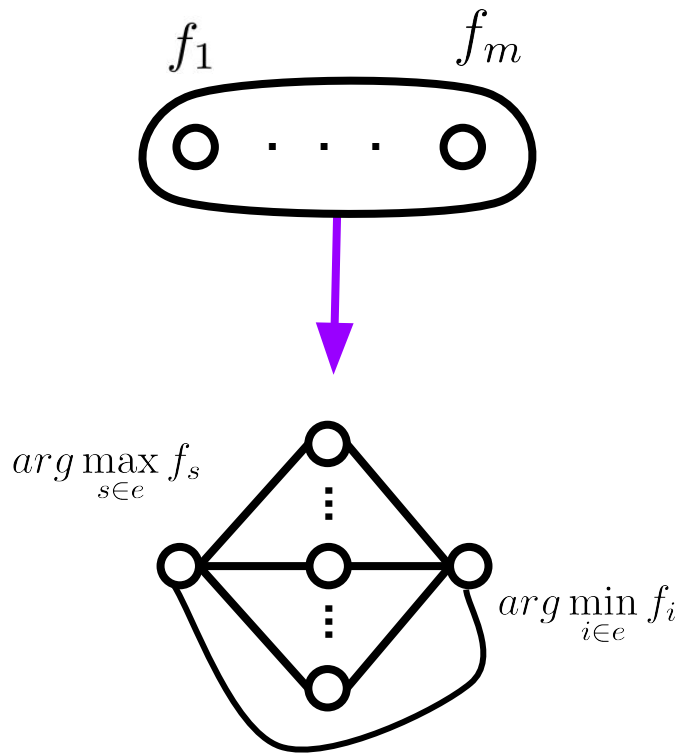
$$+ \sum_{e \in E} \sum_{m \in e} \left[ \left( \max_{s \in e} f_s - f_m \right)^2 + \left( f_m - \min_{i \in e} f_i \right)^2 \right]$$

[ Chan and Liang, COCOON 18 ]



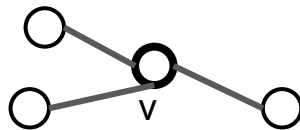
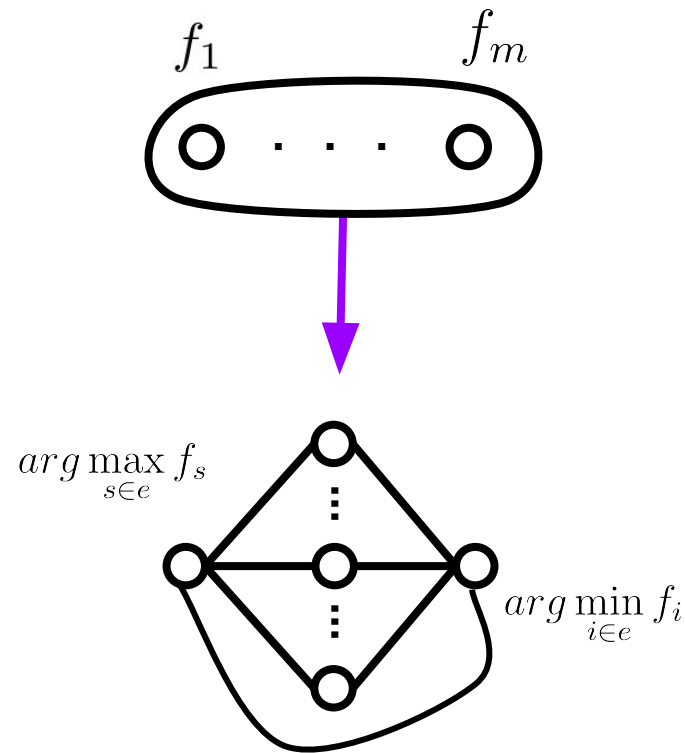
# Graph-based Hypergraph Modelling

Graph neural network [[Kipf and Welling, ICLR'16](#)]



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Graph neural network [Kipf and Welling, ICLR'16]

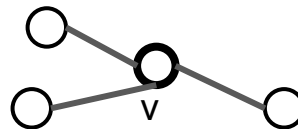
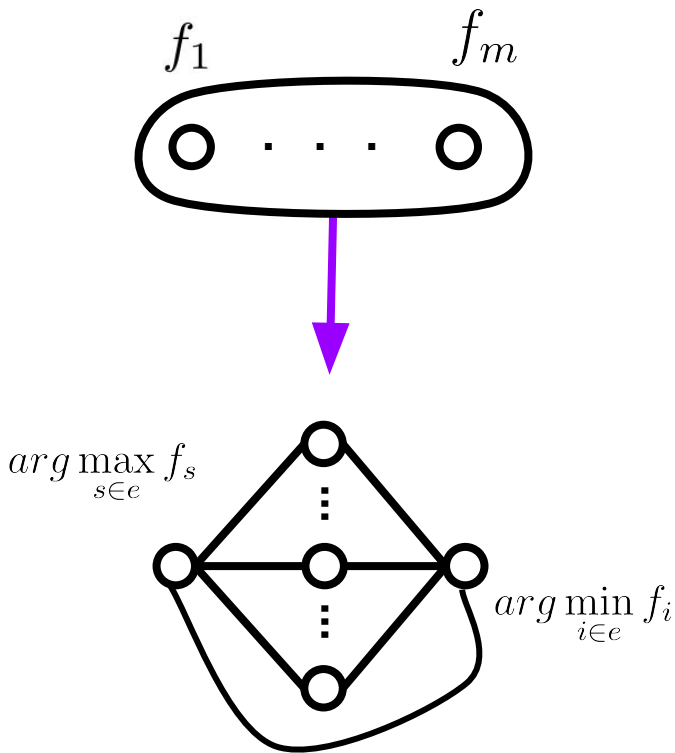


$$h_v^{\{l\}} = \sigma \left( \frac{W^{\{l\}}}{|\mathcal{N}_v|} \sum_{\{u,v\} \in \mathcal{N}_v} h_u^{\{l-1\}} + b \right)$$



# Graph-based Hypergraph Modelling

Graph neural network [Kipf and Welling, ICLR'16]



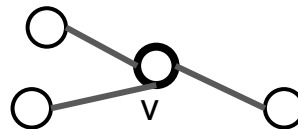
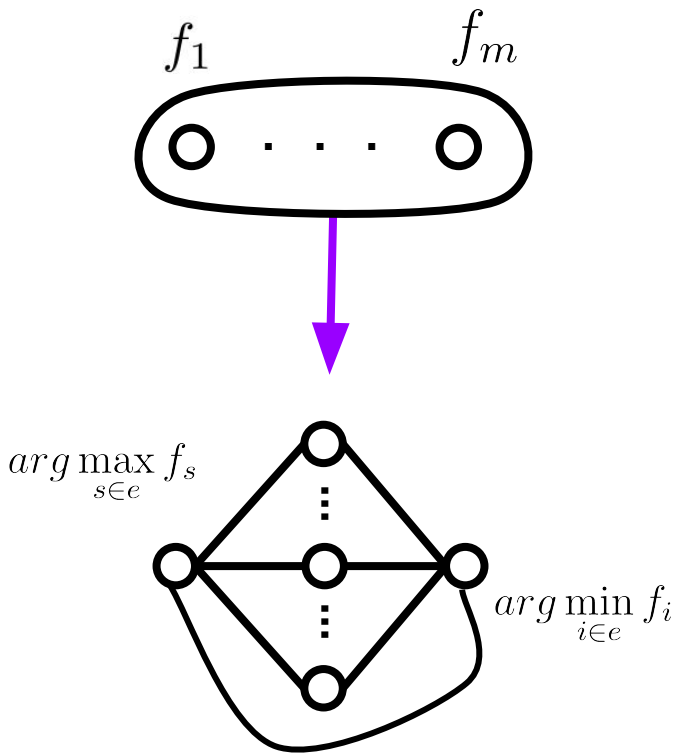
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representation in current layer

representation in previous layer

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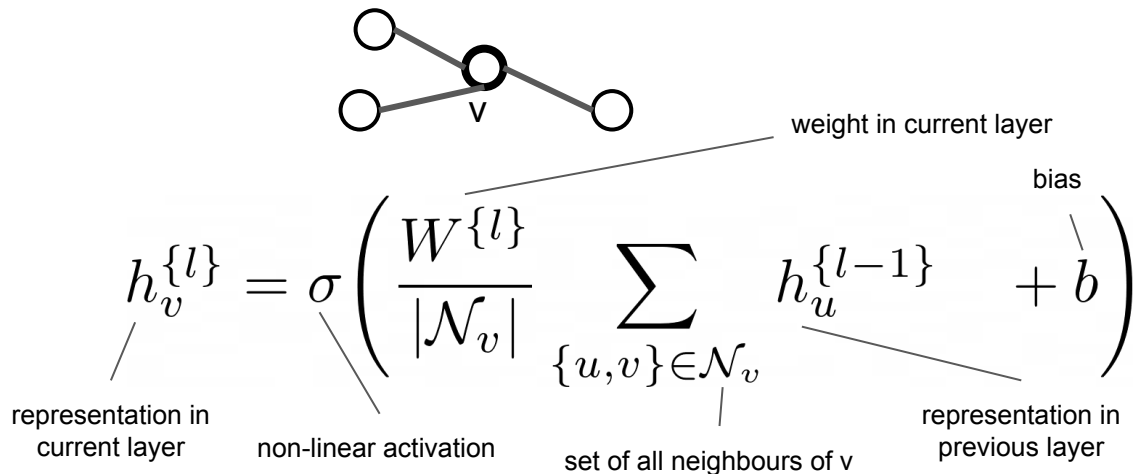
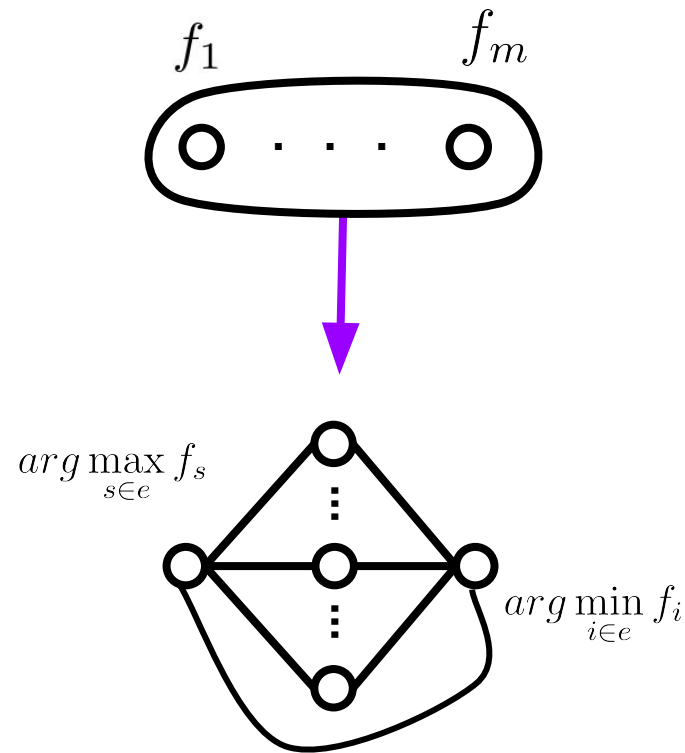


$$h_v^{\{l\}} = \sigma \left( \frac{W^{\{l\}}}{|\mathcal{N}_v|} \sum_{\{u,v\} \in \mathcal{N}_v} h_u^{\{l-1\}} + b \right)$$

$h_v^{\{l\}}$ : representation in current layer  
 $\sigma$ : non-linear activation  
 $\{u,v\} \in \mathcal{N}_v$ : set of all neighbours of  $v$   
 $h_u^{\{l-1\}}$ : representation in previous layer

# Graph-based Hypergraph Modelling

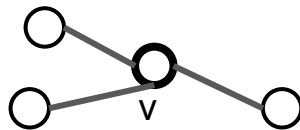
Graph neural network [Kipf and Welling, ICLR'16]



# Graph-based Hypergraph Modelling

Graph neural network [Kipf and Welling, ICLR'16]

$$H^{\{l\}} = \sigma \left( A \cdot H^{\{l-1\}} \cdot W^{\{l\}} \right)$$



weight in current layer

$$h_v^{\{l\}} = \sigma \left( \frac{W^{\{l\}}}{|\mathcal{N}_v|} \sum_{\{u,v\} \in \mathcal{N}_v} h_u^{\{l-1\}} + b \right)$$

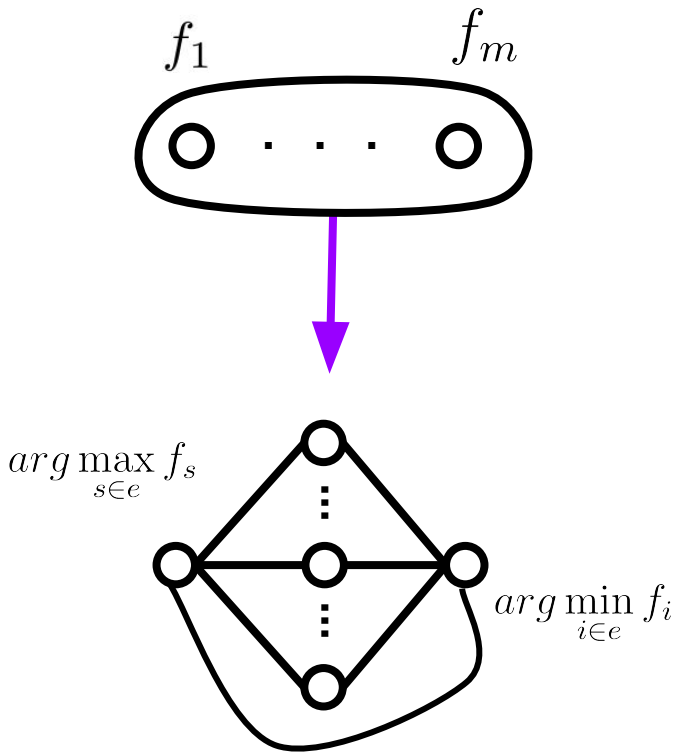
representation in  
current layer

non-linear activation

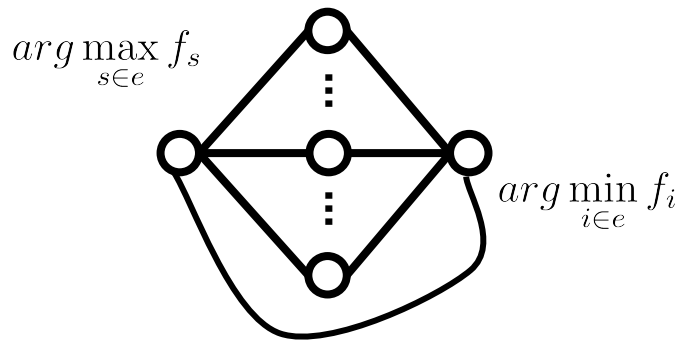
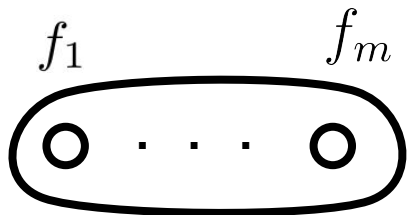
set of all neighbours of v

representation in  
previous layer

bias



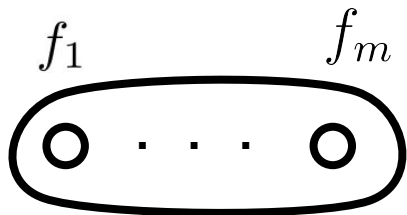
# Hypergraph Convolutional Network



$$H^{\{l\}} = \sigma \left( A \cdot H^{\{l-1\}} \cdot W^{\{l\}} \right)$$

$$\text{Set } f = H^{\{l-1\}} \cdot W^{\{l\}}$$

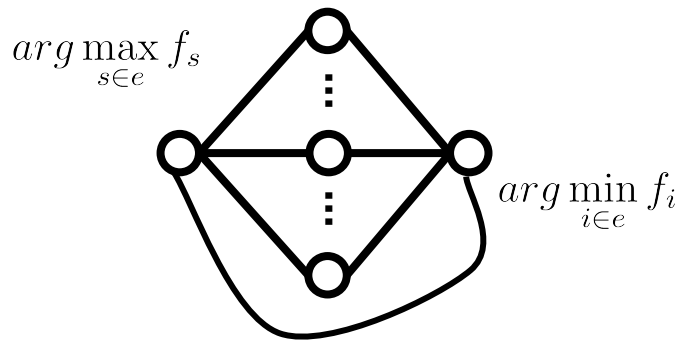
# Hypergraph Convolutional Network



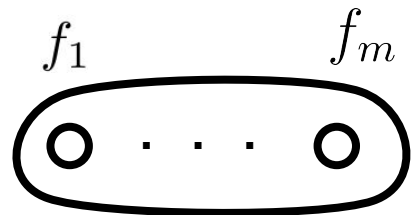
$$H^{\{l\}} = \sigma \left( \begin{matrix} A & H^{\{l-1\}} & W^{\{l\}} \\ n \times n & n \times d_{l-1} & d_{l-1} \times d_l \end{matrix} \right)$$

Set  $f = H^{\{l-1\}} \cdot W^{\{l\}}$

**parameters shared across input**



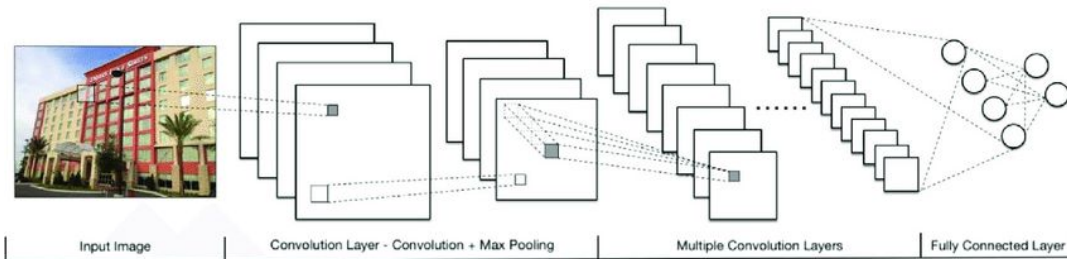
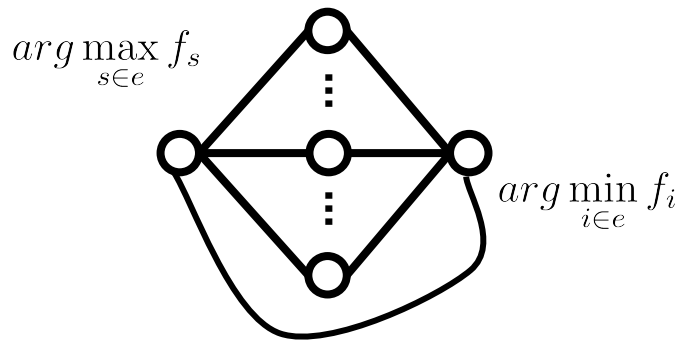
# Hypergraph Convolutional Network



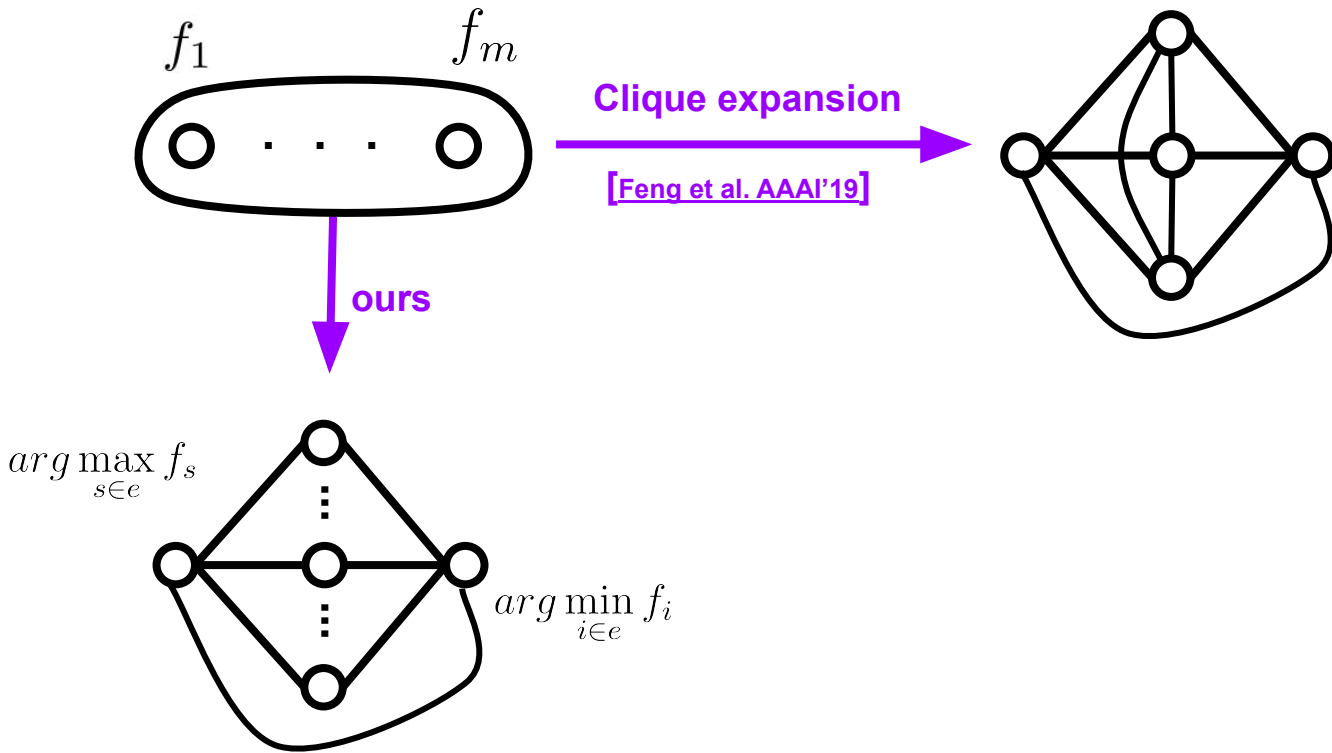
$$H^{\{l\}} = \sigma \left( \underset{n \times n}{A} \cdot \underset{n \times d_{l-1}}{H^{\{l-1\}}} \cdot \underset{d_{l-1} \times d_l}{W^{\{l\}}} \right)$$

Set  $f = H^{\{l-1\}} \cdot W^{\{l\}}$

**parameters shared across input**

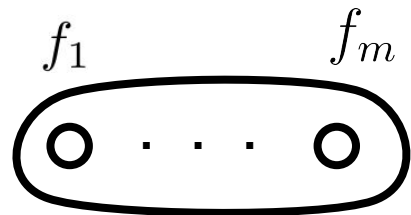


# A simple, strong baseline



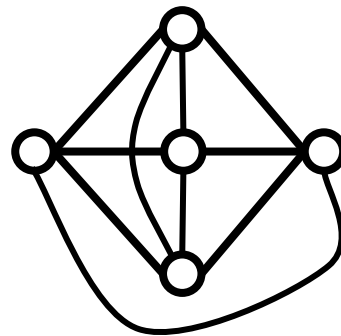


# A simple, strong baseline



Clique expansion

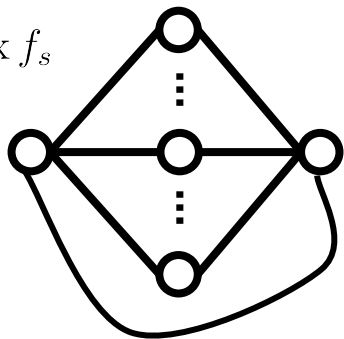
[Feng et al. AAAI'19]



Graph is fixed

ours

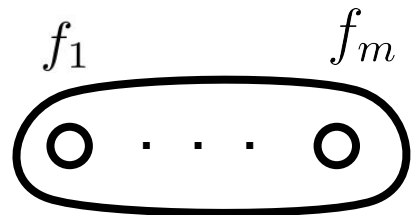
$\arg \max_{s \in e} f_s$



Graph depends on  
representation

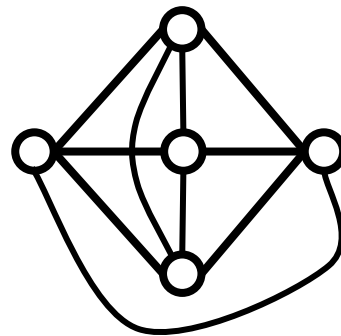
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# A simple, strong baseline



Clique expansion

[Feng et al. AAAI'19]

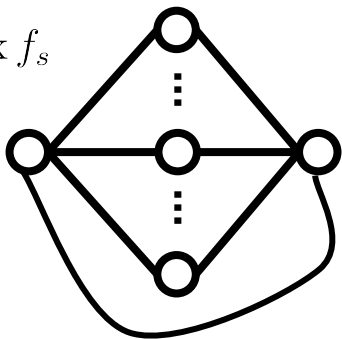


Graph is fixed

number of edges is  $\binom{m}{2}$

ours

$\arg \max_{s \in e} f_s$

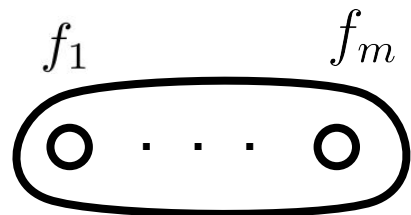


Graph depends on  
representation

$\arg \min_{i \in e} f_i$

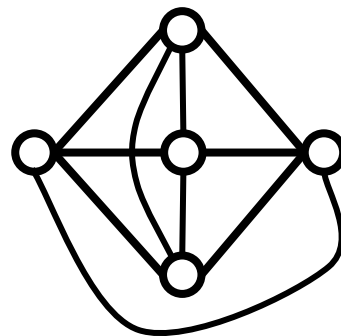
number of edges is  $2m-3$

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Clique expansion

[Feng et al. AAAI'19]

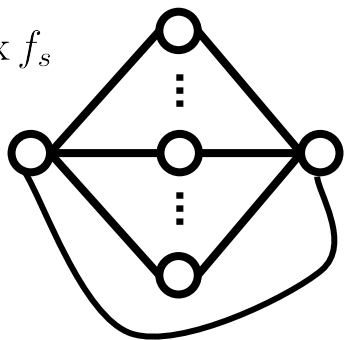


**Graph is fixed**

number of edges is  $mC_2$

ours

$\arg \max_{s \in e} f_s$



**Graph depends on representation**

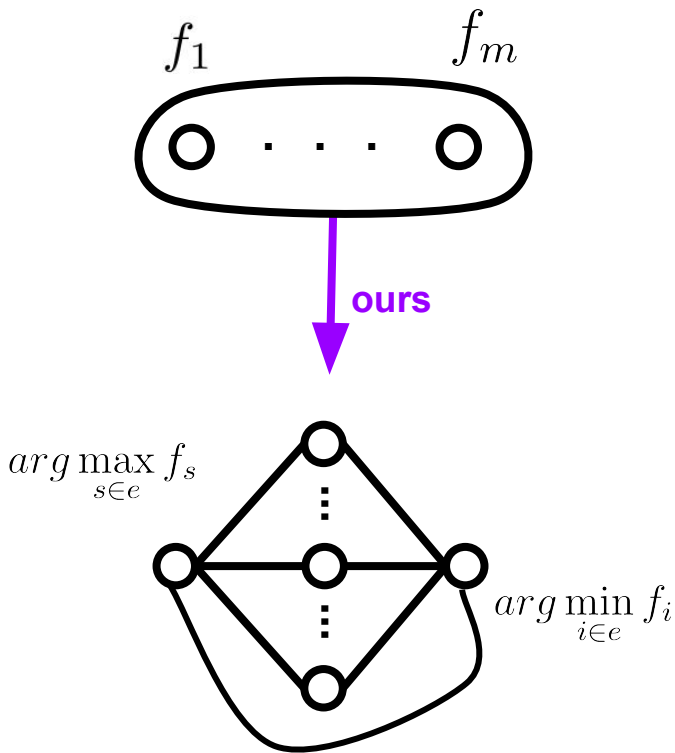
$\arg \min_{i \in e} f_i$

number of edges is  $2m-3$

document classification on co-citation networks

	Cora	Citeseer
Avg. Hyperedge size	$3.0 \pm 1.1$	$3.2 \pm 2.0$
GCN on Clique Expansion	$32.41 \pm 1.8$	$37.40 \pm 1.6$
HyperGCN	$32.37 \pm 1.7$	$37.35 \pm 1.6$

# FastHyperGCN



$$H^{\{l\}} = \sigma \left( \begin{matrix} A & H^{\{l-1\}} & W^{\{l\}} \\ n \times n & n \times d_{l-1} & d_{l-1} \times d_l \end{matrix} \right)$$

## HyperGCN

Set  $f = H^{\{l-1\}} \cdot W^{\{l\}}$

## FastHyperGCN

Set  $f = H^{\{0\}} = X$

# Experiments on large noisy hypergraphs

Test accuracy (lower is better) on co-authorship and co-citation datasets

	DBLP
Avg. Hyperedge size	$8.5 \pm 8.8$
GCN on Clique Expansion	$45.27 \pm 2.4$
HyperGCN	<b><math>41.64 \pm 2.6</math></b>
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Test accuracy (lower is better) on co-authorship and co-citation datasets

	DBLP	Pubmed	Cora
Avg. Hyperedge size	$8.5 \pm 8.8$	$4.3 \pm 5.7$	$4.2 \pm 4.1$
GCN on Clique Expansion	$45.27 \pm 2.4$	$29.41 \pm 1.5$	$31.90 \pm 1.9$
HyperGCN	<b><math>41.64 \pm 2.6</math></b>	<b><math>25.56 \pm 1.6</math></b>	<b><math>30.08 \pm 1.8</math></b>
FastHyperGCN	$41.78 \pm 2.8$	$29.48 \pm 1.6$	$32.54 \pm 1.8$

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Average training time (lower is better) of an epoch

	DBLP	Pubmed
GCN on Clique Expansion	0.115s	0.019s
FastHyperGCN	<b>0.035s</b>	<b>0.016s</b>

# What NeurIPS reviewers liked in the paper

- Bridges different fields  
Spectral hypergraph theory + graph neural networks

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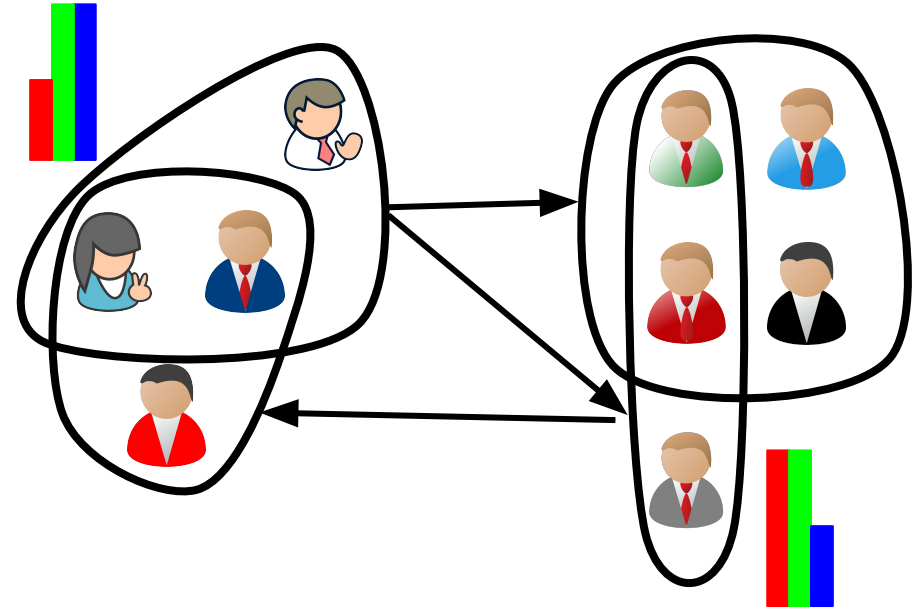
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- Bridges different fields  
Spectral hypergraph theory + graph neural networks
- Reduces complexity from quadratic to linear  
 $mC_2$  to  $2m-3$
- Improves performance on large noisy hypergraphs  
lower error and training time

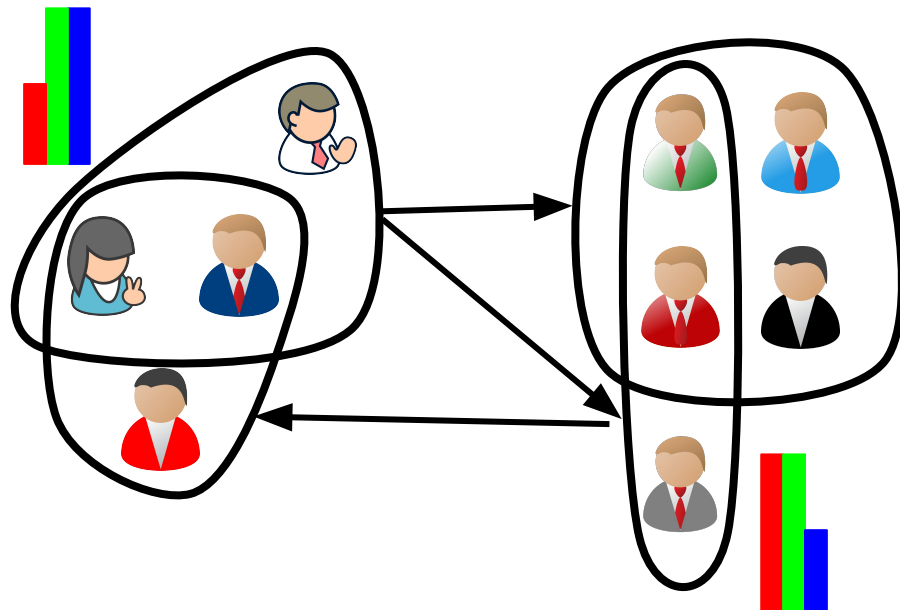
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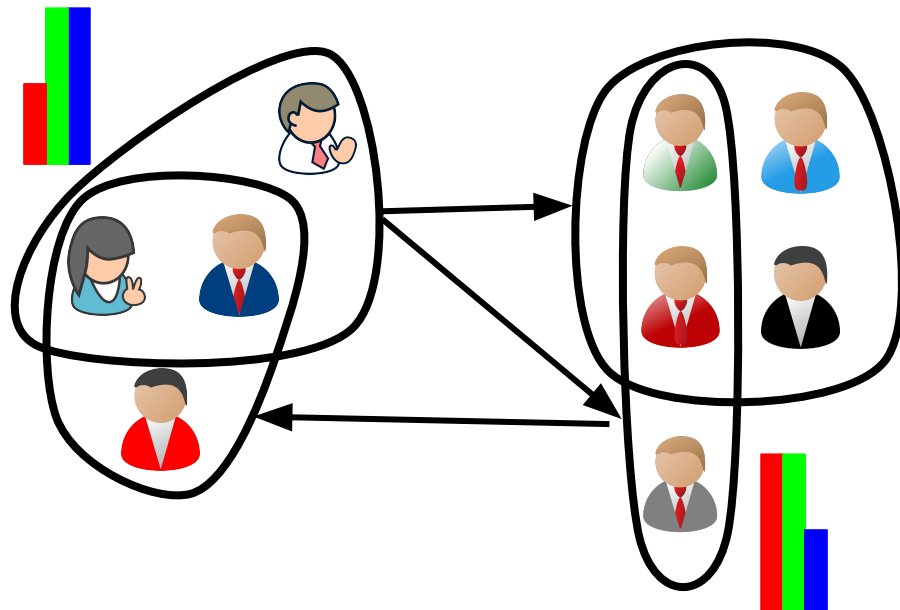


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- **Soft Semi-supervised learning** (submitted to ICLR 2020)

- **Unsupervised learning**

**✗ Inherently transductive**  
cannot handle unseen vertices at test time



# Q & A

