Hierarchical Graph Representation Learning with Differentiable Pooling

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Speaker: Ziyuan Ye

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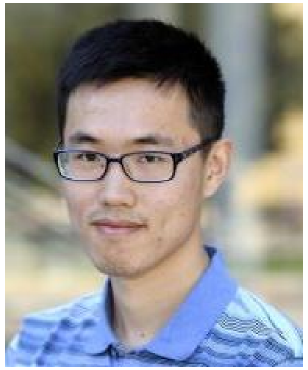
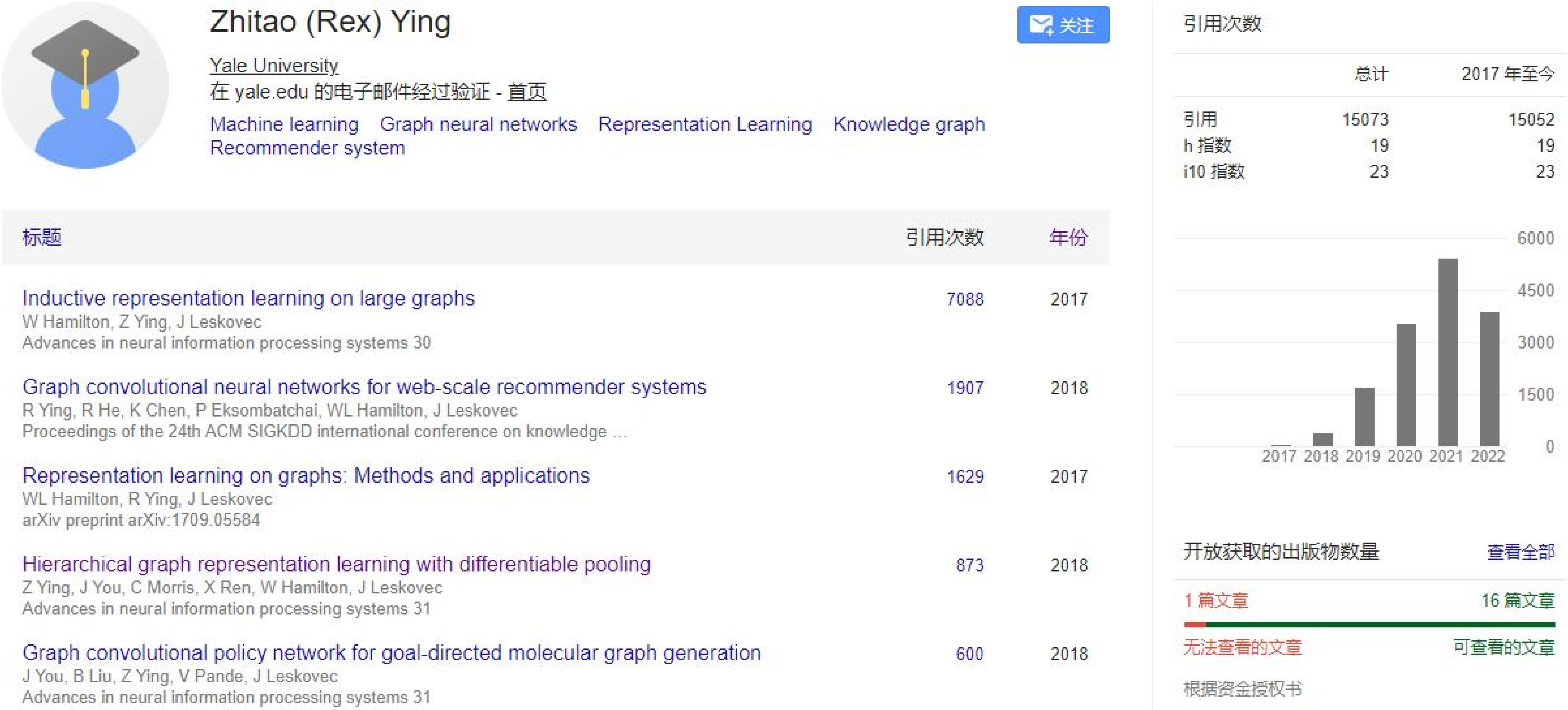
Ying, Z., You, J., Morris, C., Ren, X., Hamilton, W., & Leskovec, J. (2018). Hierarchical graph representation learning with differentiable pooling. Advances in neural information processing systems (NeurIPS), 31.

About the authors



Representative Work:

- ✓ GraphSAGE
- ✓ GNNExplainer
- ✓ DIFFPOOL



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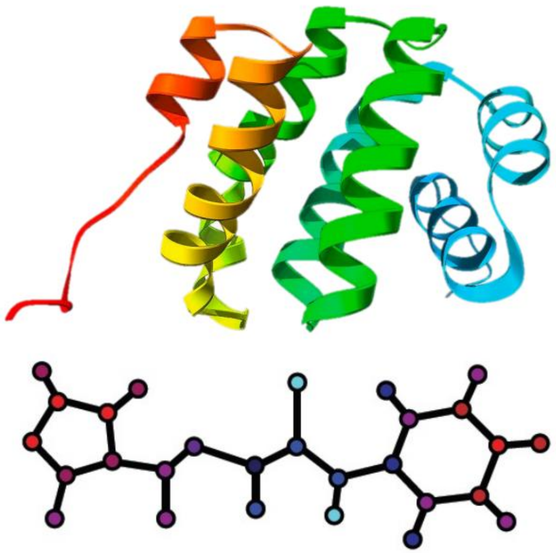
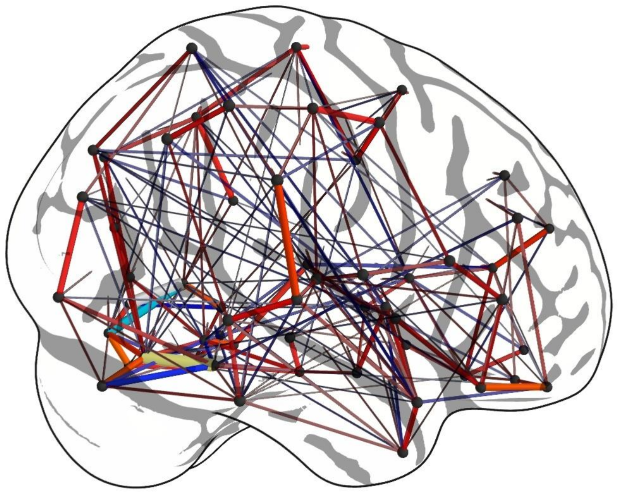
Content

Graphs = System of Relations and Interactions



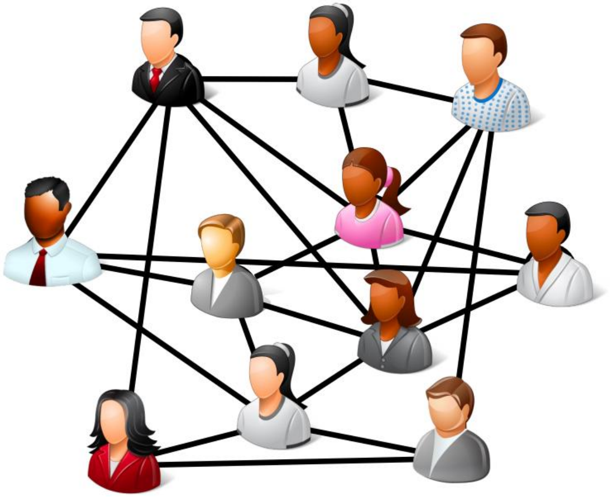
Molecules



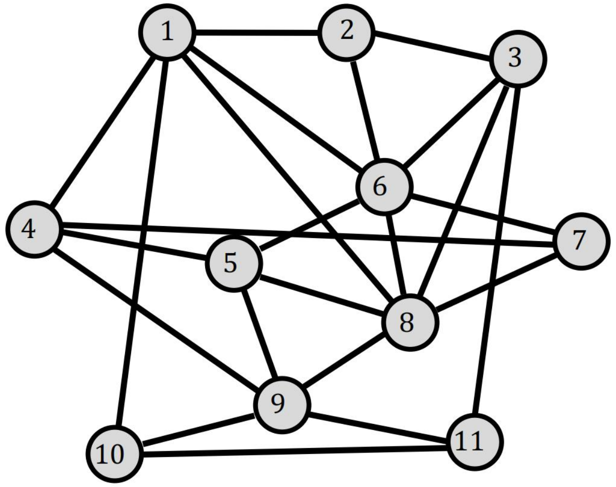
Brain connectivity

Social Network

Graph Classification via Graph Neural Networks (GNNs)

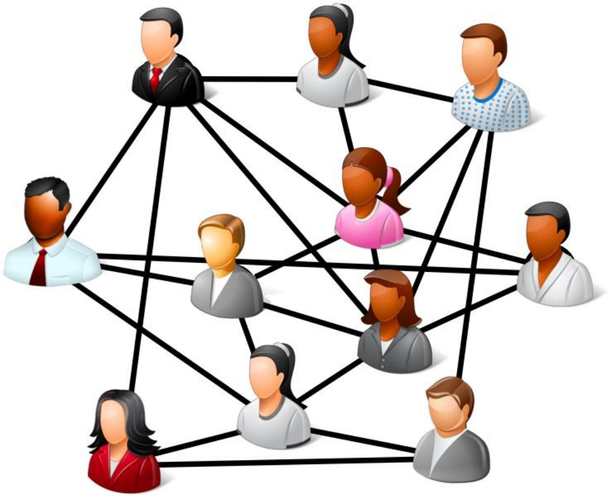


Social network

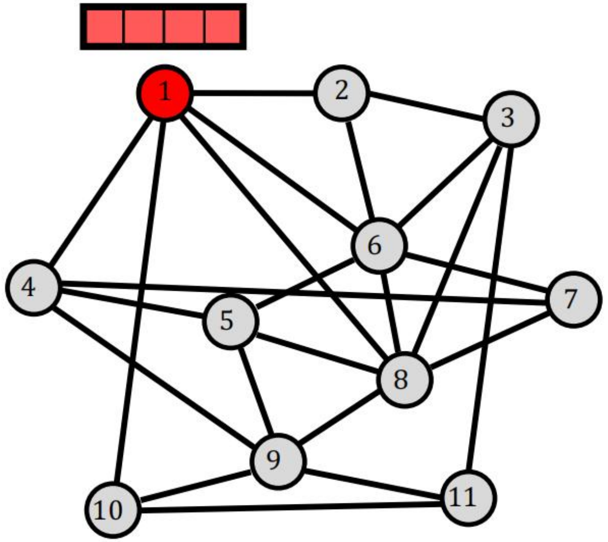


Graph

Graph Classification via GNNs

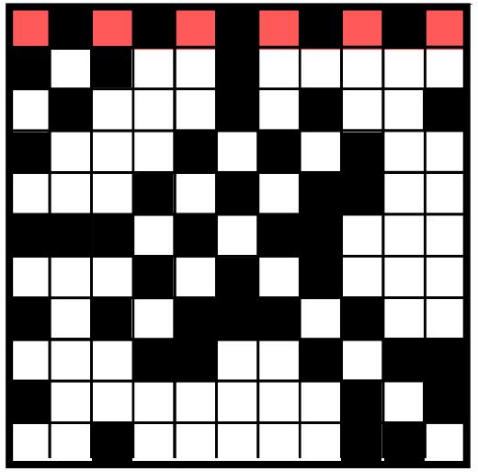


Social network



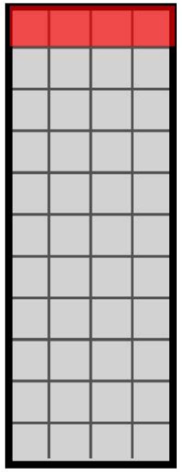
Graph

Adjacency matrix $n \times n$



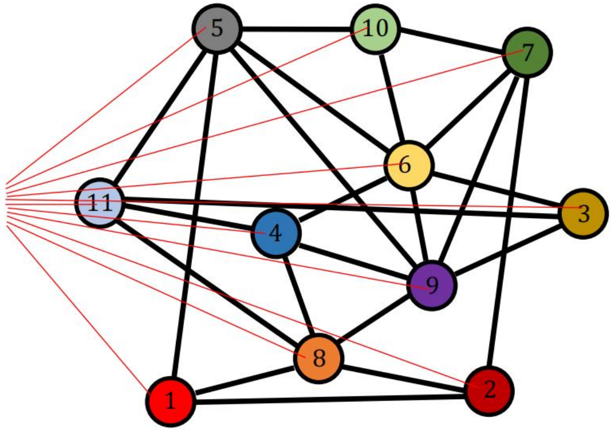
A

Feature matrix $n \times d$

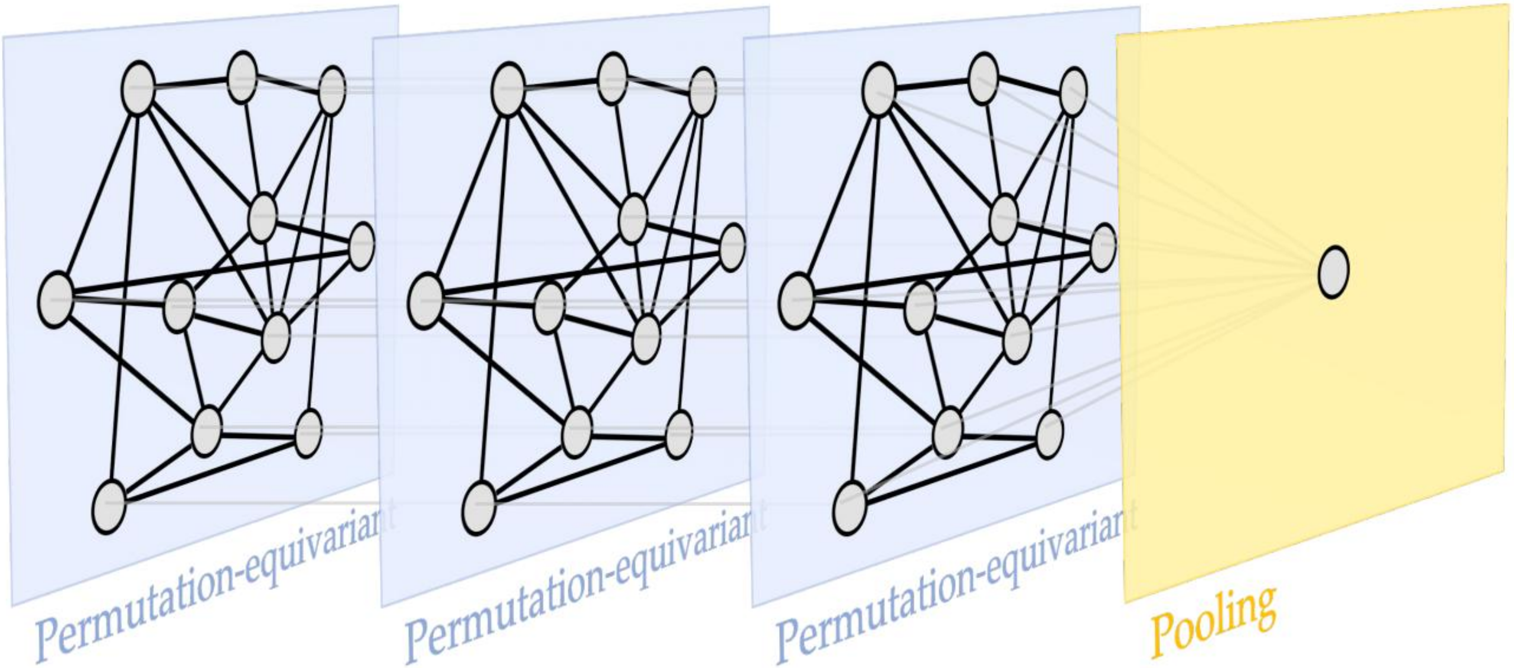


X

Graph function $f(\boldsymbol{X}, \boldsymbol{A})$

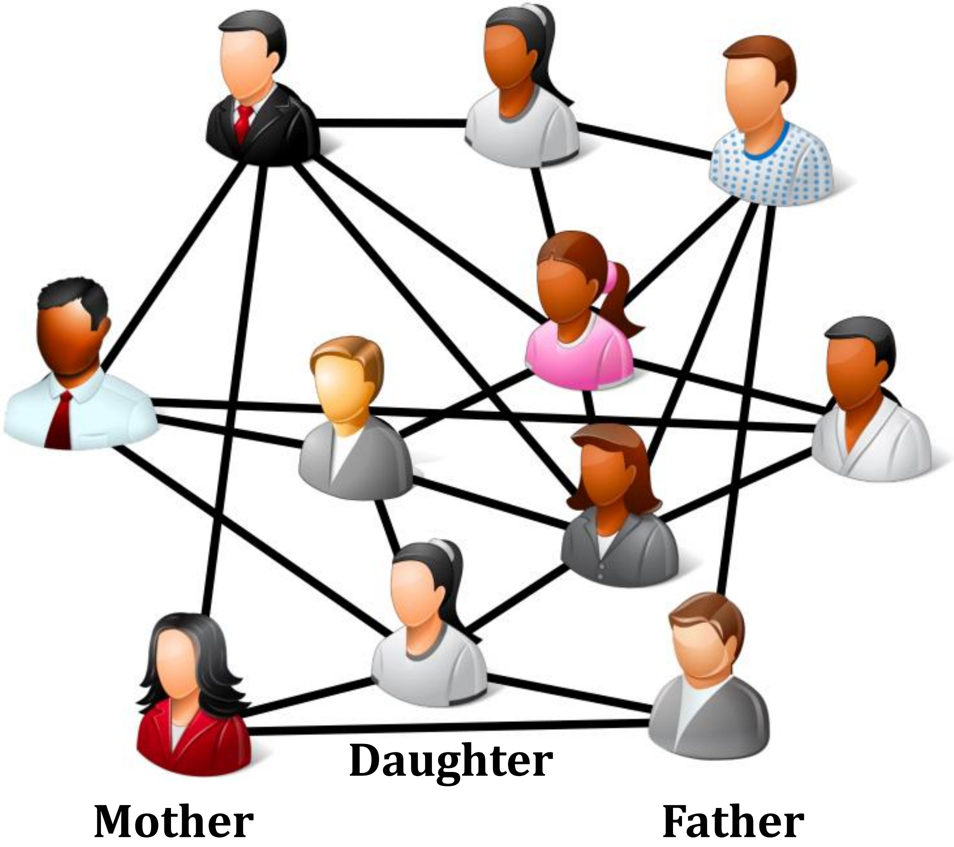


Graph pooling in GNNs

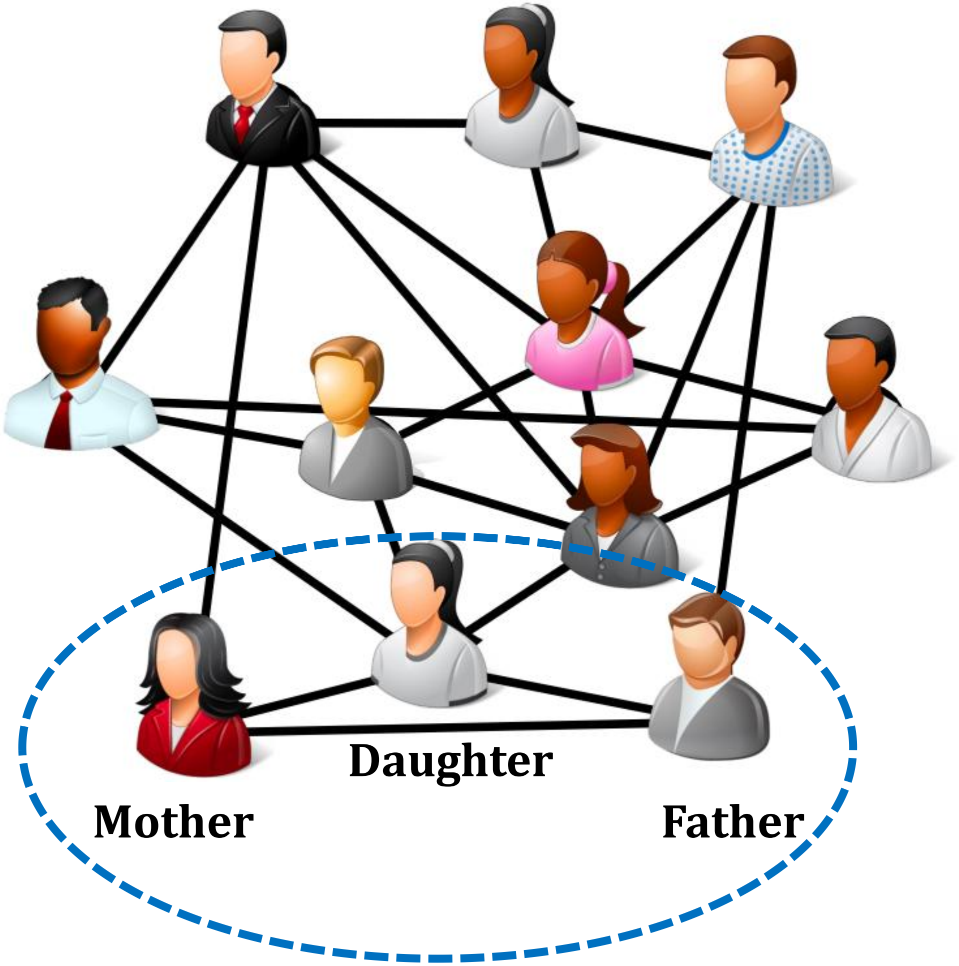


Ignoring any hierarchical structure that might be present in the graph

Graph pooling in GNNs



Graph pooling in GNNs



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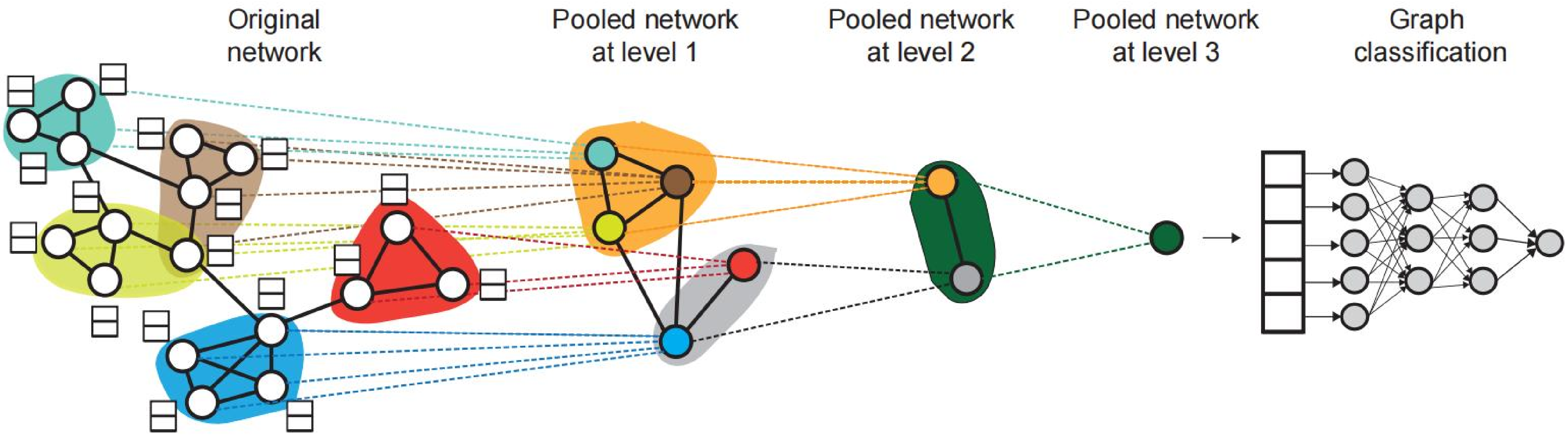
Notation

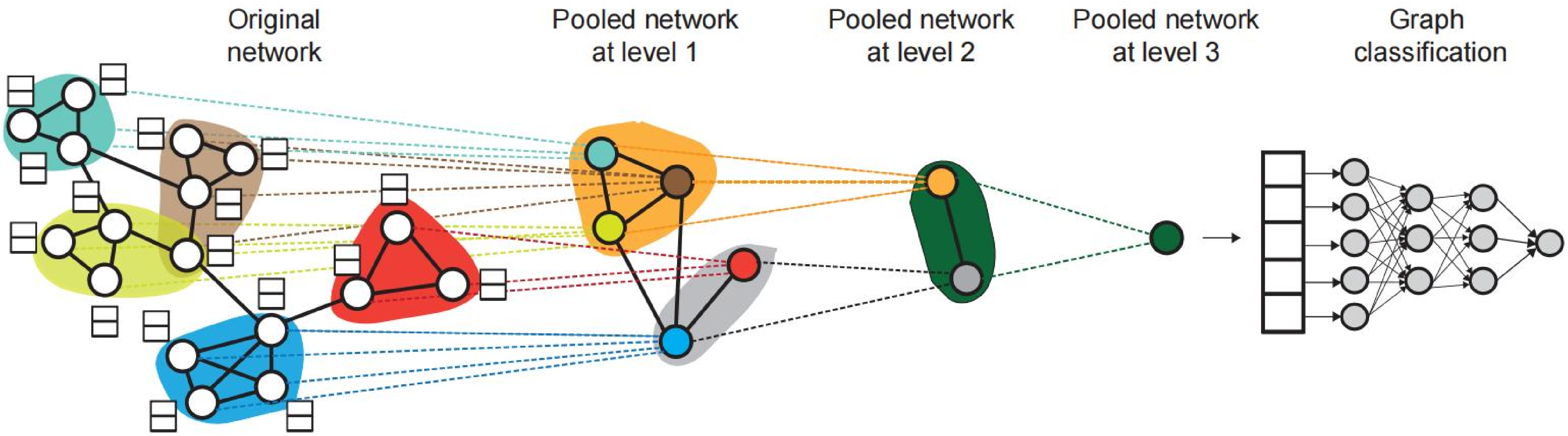
Adjacency matrix	$A \in \{0,1\}^{n \times n}$
Feature matrix	$F \in \mathbb{R}^{n \times d}$
Graph	G as (A, F)
Node embeddings computed after k steps of GNN	$H^{(k)} \in \mathbb{R}^{n \times d}$
Node embeddings of coarsened graph	$Z^{(k)} \in \mathbb{R}^{m \times d}$, $m < n$
Dataset	$\mathcal{D} = \{(G_1, y_1), (G_2, y_2), ...\}$, $y_i \in \mathcal{Y}$
Learnable cluster assignment matrix	$S^{(l)} \in \mathbb{R}^{n_l \times n_{l+1}}$
Goal of graph classification	$f : \mathcal{G} \to \mathcal{Y}$

DIFFPOOL



Graph coarsening and classification via DIFFPOOL

DIFFPOOL

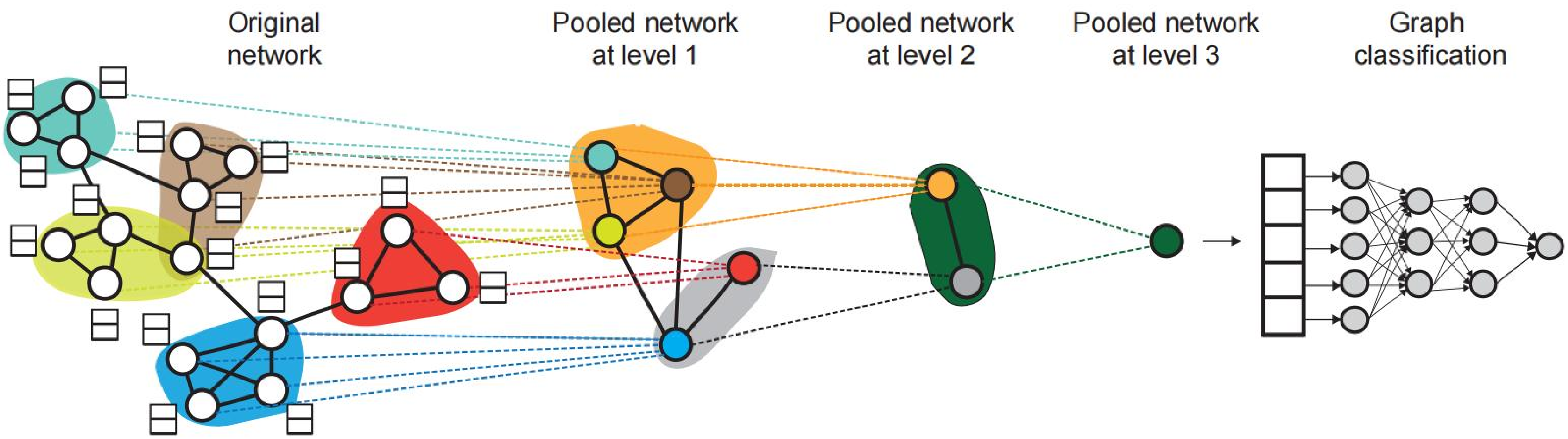


Graph coarsening and classification via DIFFPOOL

Learning cluster assignment matrix

$$S^{(l)} = \text{softmax}\left(\text{GNN}_{l,\text{pool}}(A^{(l)}, X^{(l)})\right)$$

DIFFPOOL



Graph coarsening and classification via DIFFPOOL

Learning cluster assignment matrix

$$S^{(l)} = \text{softmax}\left(\text{GNN}_{l,\text{pool}}(A^{(l)}, X^{(l)})\right)$$

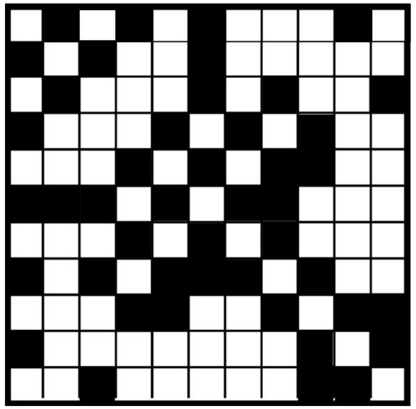
Updating embeddings and adjacency matrix

$$Z^{(l)} = \text{GNN}_{l,\text{embed}}(A^{(l)}, X^{(l)})$$

$$X^{(l+1)} = {S^{(l)}}^T Z^{(l)} \in \mathbb{R}^{n_{l+1} \times d},$$

$$A^{(l+1)} = {S^{(l)}}^T A^{(l)} S^{(l)} \in \mathbb{R}^{n_{l+1} \times n_{l+1}}$$

DIFFPOOL: Regularization terms

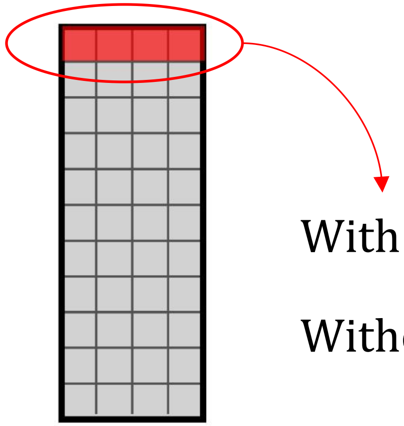


Adjacency matrix $n \times n$

Entropy Regularization

$$L_{\mathrm{E}} = \frac{1}{n} \sum_{i=1}^{n} H(S_i)$$

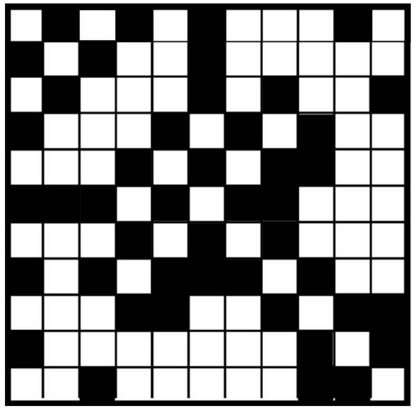
Assignment matrix $n \times m$



With: [0.95, 0.01, 0.02, 0.02]

Without: [0.33, 0.34, 0.20, 0.13]

DIFFPOOL: Regularization terms



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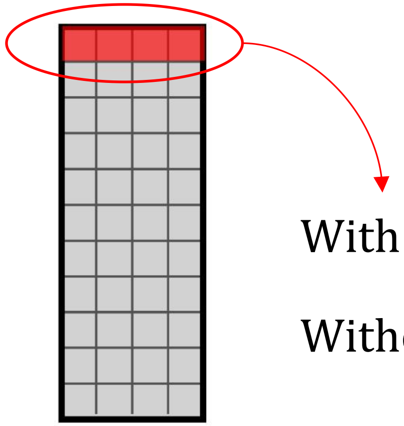
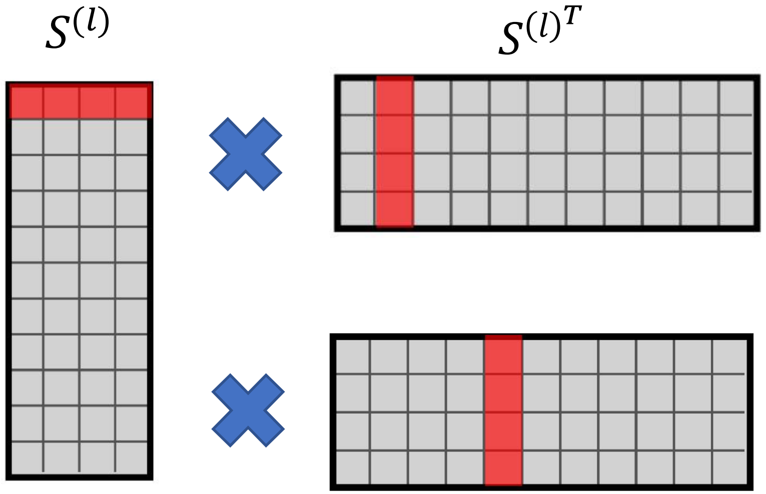


With: [0.95, 0.01, 0.02, 0.02]

Without: [0.33, 0.34, 0.20, 0.13]

Auxiliary Link Prediction Objective

$$L_{\mathrm{LP}} = ||A^{(l)}, S^{(l)} S^{(l)^T} ||_F$$



The higher the better

The lower the better

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Experimental results

	Method	Data Set					
		ENZYMES	D&D	REDDIT-MULTI-12K	COLLAB	PROTEINS	Gain
Kernel	GRAPHLET	41.03	74.85	21.73	64.66	72.91	
	SHORTEST-PATH	42.32	78.86	36.93	59.10	76.43	
	1-WL	53.43	74.02	39.03	78.61	73.76	
	WL-OA	60.13	79.04	44.38	80.74	75.26	
GNN	PATCHYSAN	–	76.27	41.32	72.60	75.00	4.17
	GRAPHSAGE	54.25	75.42	42.24	68.25	70.48	–
	ECC	53.50	74.10	41.73	67.79	72.65	0.11
	SET2SET	60.15	78.12	43.49	71.75	74.29	3.32
	SORTPOOL	57.12	79.37	41.82	73.76	75.54	3.39
	DIFFPOOL-DET	58.33	75.47	46.18	**82.13**	75.62	5.42
	DIFFPOOL-NOLP	61.95	79.98	46.65	75.58	76.22	5.95
	DIFFPOOL	**62.53**	**80.64**	**47.08**	75.48	**76.25**	**6.27**

Content

Take-home Message

- **Motivation:**
  - ➢ Original GNN architectures are unable to infer and aggregate the information in a hierarchical way.
- **Challenge:**
  - ➢ Graphs contain no natural notion of spatial locality, i.e., one cannot simply pool together all nodes in a "m × m patch" on a graph.
- **Main contributions:**
  - ➢ Propose DIFFPOOL that can generate hierarchical representations of graphs;
  - ➢ DIFFPOOL can be combined with various graph neural network architectures in an end-to-end fashion;

Thanks for your attention!