MaxCutPool: Differentiable Feature-Aware MAXCUT for Pooling in Graph Neural Networks

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CODE

ICLR

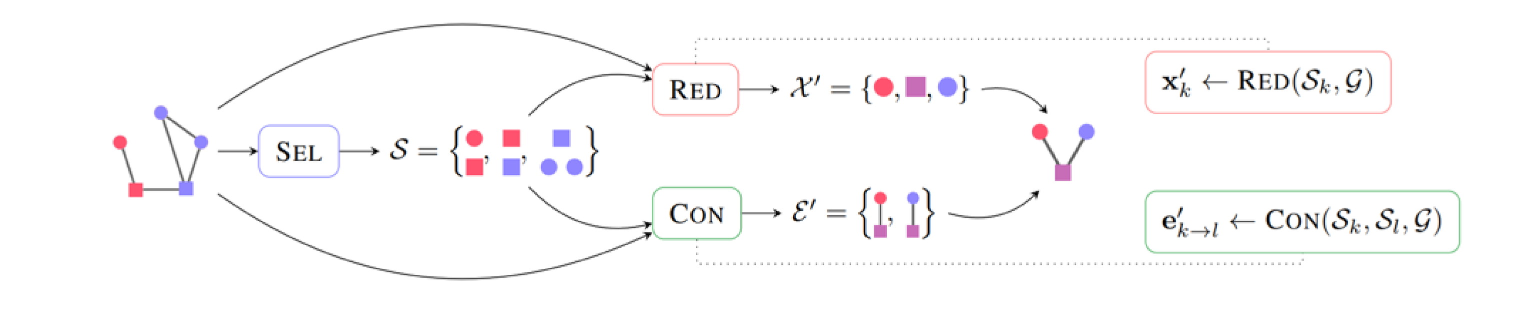
MAIN IDEA

- Adjacent nodes in a graph contain redundant information due to smoothing effects of message passing (MP)
- MAXCUT finds complementary groups of nodes by maximizing dissimilarity between connected nodes
- Pruning redundant nodes preserves information while reducing graph size

KEY CONTRIBUTIONS

- MAXCUT computation for attributed graphs
- New hierarchical pooling layer especially effective for heterophilic graphs
- General scheme for node-to-supernode assignment
- First heterophilic dataset for graph classification

SELECT-REDUCE-CONNECT (SRC) [1]



HETEROPHILIC MESSAGE PASSING

Consider the MP operator $\boldsymbol{X}' = \sigma(\boldsymbol{P}\boldsymbol{X}\boldsymbol{\Theta})$.

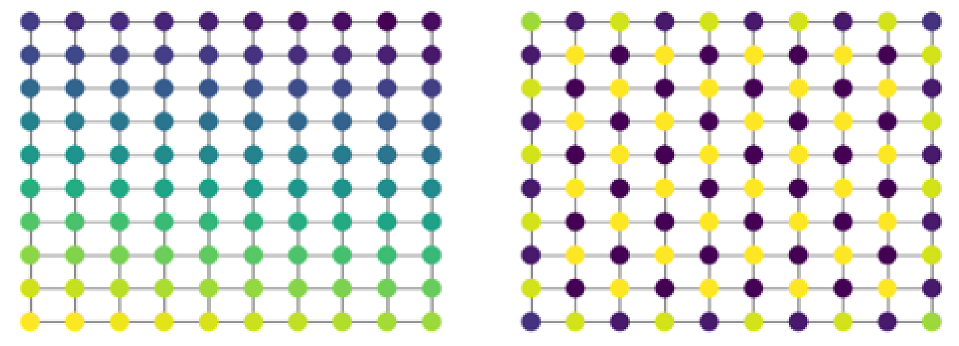
- Standard MP:

$$\boldsymbol{P} = \hat{\boldsymbol{D}}^{-\frac{1}{2}}\hat{\boldsymbol{A}}\hat{\boldsymbol{D}}^{-\frac{1}{2}}$$

- Heterophilic MP (HetMP):

$$\boldsymbol{P} = \boldsymbol{I} - \delta \boldsymbol{L}^{\text{sym}}, \delta > 1$$

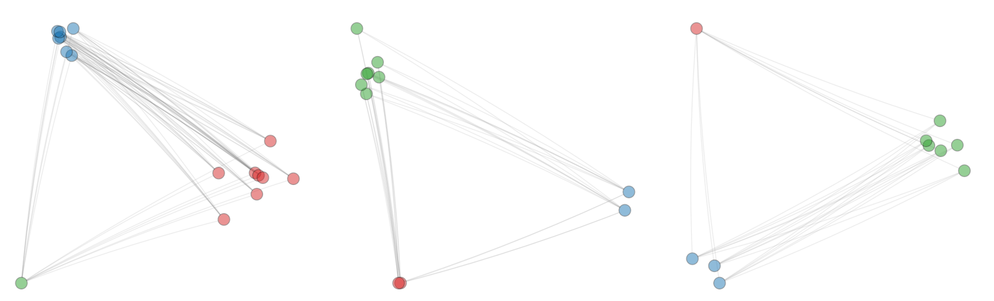
- HetMP can learn non-smooth graph signals



Left: standard MP; right: HetMP

MULTIPARTITE DATASET

- First heterophilic benchmark for graph classification
- Complete C-partite graphs
- Nodes only connect to different-colored clusters
- Class determined by rightmost cluster color
- Structure independent from the label
- Tests GNNs to distinguish between relevant (node features) and irrelevant (connectivity) information



3-partite graphs

REFERENCES

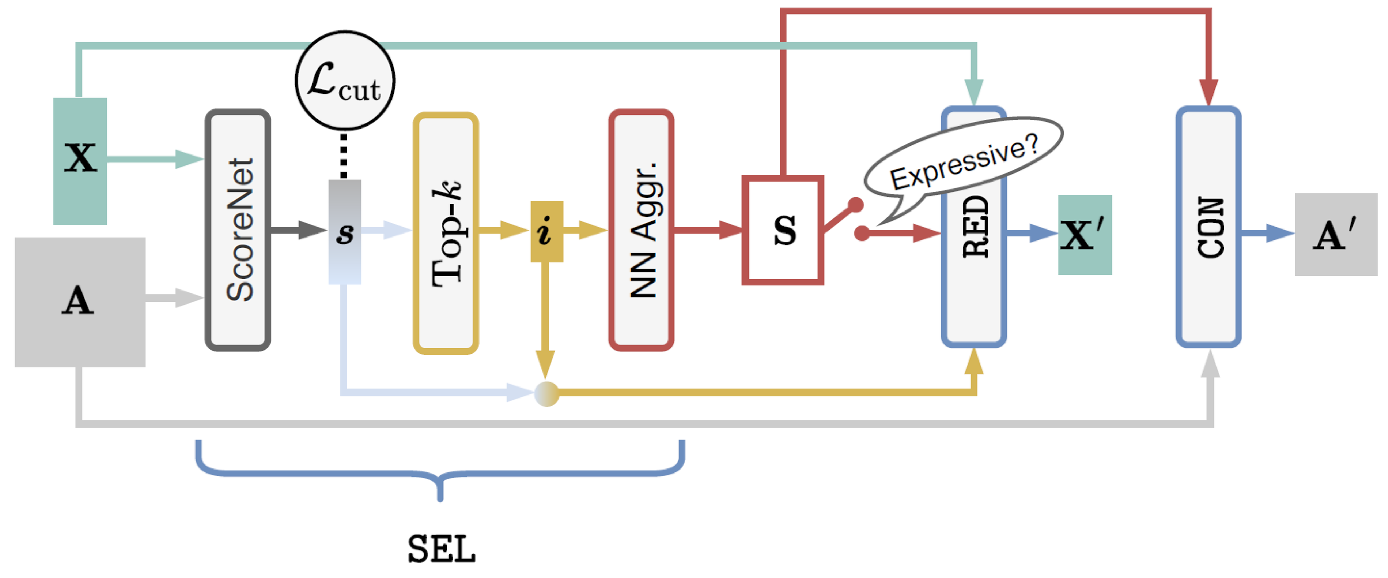
1. D. Grattarola et al., "Understanding Pooling in Graph Neural Networks," *IEEE TNNLS*, 2024

MAXCUTPOOL STRUCTURE

We introduce an auxiliary loss function defined as

$$\mathcal{L}_{\text{cut}} = \frac{\boldsymbol{s}^\top \boldsymbol{A}\boldsymbol{s}}{|\mathcal{E}|}$$

where $\boldsymbol{s} \in [-1, 1]^N$ is the score vector, $\boldsymbol{A}$ is the adjacency matrix and $|\mathcal{E}|$ is the total edge weight.



- Optimizes partition to maximize cut edges
- Connected nodes have opposite scores
- Enables end-to-end differentiable training
- Integrates with task-specific objectives

SELECT

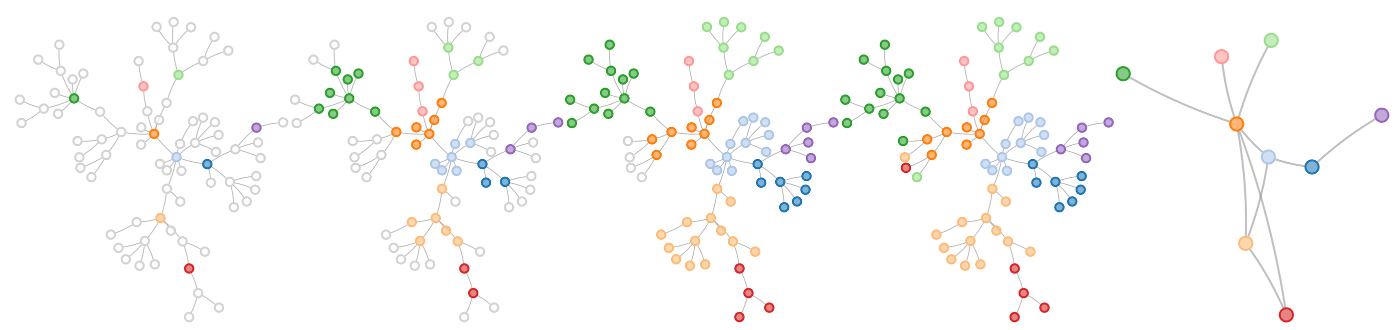
- A ScoreNet with HetMP layers generates a score vector $\boldsymbol{s}$
- Top-K scores identify supernodes: $\boldsymbol{i} = \text{top}_K(\boldsymbol{s})$
- Builds assignment matrix $\boldsymbol{S}$ via breadth-first propagation
- Each node is assigned to the closest supernode

REDUCE

- MaxCutPool: $[\boldsymbol{X}']_{i:} = s_i \odot [\boldsymbol{X}]_{i:}$
- MaxCutPool-E: $\boldsymbol{X}' = \boldsymbol{s} \odot \boldsymbol{S}^\top \boldsymbol{X}$

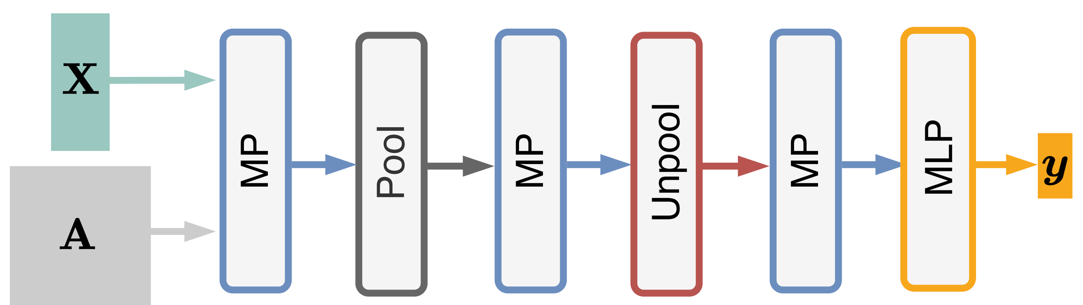
CONNECT

- Pooled adjacency: $\boldsymbol{A}' = \boldsymbol{S}^\top \boldsymbol{A}\boldsymbol{S}$

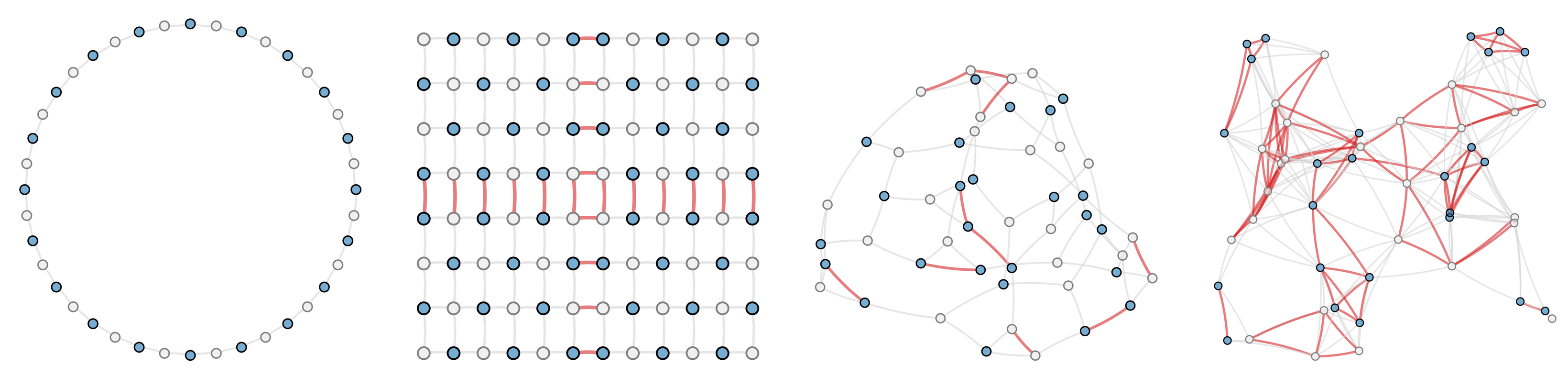


NODE CLASSIFICATION

Pooler	Roman-e.	Amazon-r.	Minesw.	Tolokers	Questions	Score
Top-k	26±7	46±4	94±1	89±5	64±3	1
k-MIS	23±3	48±2	75±2	84±2	83±1	1
NDP	22±5	53±2	98±0	88±6	68±4	3
MaxCutPool	56±3	53±1	96±1	87±3	82±4	4
MaxCutPool-E	60±4	53±2	97±1	91±2	85±5	**5**



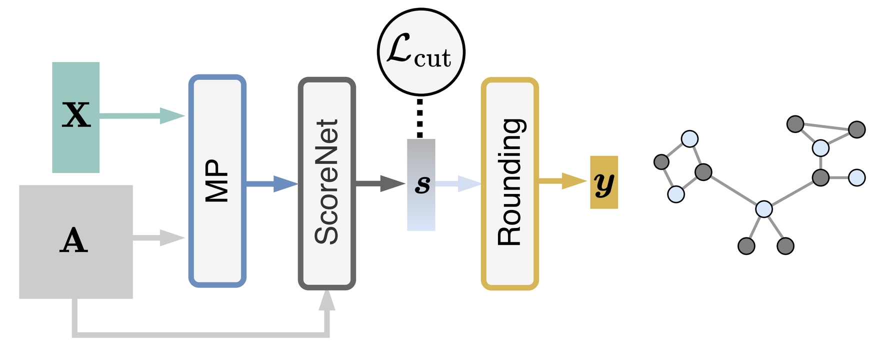
MAXCUT EVALUATION



Maxcut partitions. Red edges are not cut.

Dataset	GW	NDP	GCN	MaxCutPool
BarabasiAlbert	0.6875	0.6589	0.7240	0.7292
Community	0.6767	0.6429	0.6805	0.6814
ErdősRenyi	0.6920	0.6858	0.6797	0.7105
Grid (10×10)	1.0000	1.0000	0.9222	1.0000
Grid (60×40)	-	0.9787	0.1862	0.9815
Minnesota	-	0.9104	0.8904	0.9130
RandRegular	0.4827	0.8760	0.8733	0.9040
Ring	1.0000	1.0000	0.4200	1.0000
Sensor	0.6000	0.5719	0.6281	0.6406

- It serves as an initial assessment
- Our method was compared to traditional algorithms and standard GCN
- Thanks to HetMP we are always able to find good cuts



GRAPH CLASSIFICATION

Pooler	GCB-H	COLLAB	EXPWL1	Mult.	Mutag.	NCI1	REDDIT-B	Score
DiffPool	51±8	70±2	69±3	9±1	78±2	75±2	90±2	1
DMoN	74±3	68±2	73±3	52±2	80±2	77±2	88±2	3
EdgePool	75±4	72±3	90±2	55±3	80±2	77±3	91±2	4
Graclus	75±3	72±3	90±2	25±18	80±2	77±2	90±3	4
k-MIS	75±4	71±2	99±1	58±2	79±2	75±3	90±2	4
MinCutPool	75±5	70±2	71±3	56±3	78±3	73±3	87±2	1
Top-k	56±5	72±2	73±2	43±3	75±3	73±2	77±2	0
MaxCutPool	73±3	77±2	100±0	90±2	77±2	75±2	89±3	5
MaxCutPool-E	74±3	77±2	100±0	87±5	79±1	76±2	89±2	**7**
MaxCutPool-NL	61±6	77±3	100±0	91±1	76±3	74±2	86±3	3