A Tale of Edge Directionality in Graph Neural Networks

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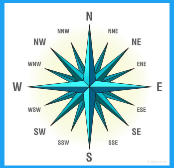
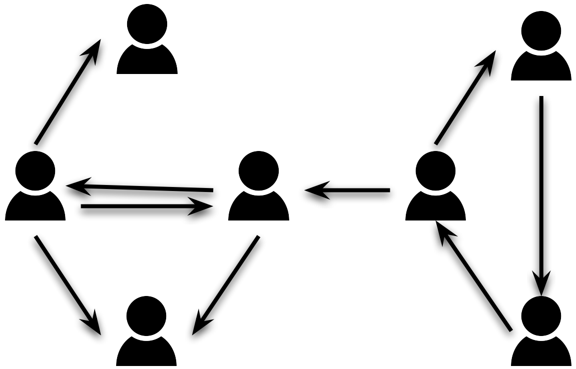


Graphs are Often Directed

Citation, social (interaction) and hyperlink networks among others



TGB Link Prediction Datasets

Scale	Name	Package	#Nodes	#Edges*	#Steps	Surprise	Metric
Small	tgbl-wiki-v2	0.1.2	9,227	157,474	152,757	0.108	MRR
Small	tgbl-review-v2	0.1.2	352,637	4,873,540	6,865	0.987	MRR
medium	tgbl-coin	0.1.2	638,486	22,809,486	1,295,720	0.120	MRR
large	tgbl-comment	0.1.2	994,790	44,314,507	30,998,030	0.823	MRR
large	tgbl-flight	0.1.2	18,143	67,169,570	1,385	0.024	MRR

Directed

The "Undirectedness" Assumption

Spectral GNNs [1] require an undirected graph to define convolution

$$\mathbf{y} = f_\theta(\mathbf{L})\mathbf{x}$$
$$= f_\theta(\mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top)\mathbf{x}$$
$$= \mathbf{U} f_\theta(\mathbf{\Lambda})\mathbf{U}^\top \mathbf{x}$$

Eigendecomposition requires a **symmetric Laplacian** → the graph has to be **undirected**

[1] M. Defferrard et al., "Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering", NeurIPS 2016

The “Undirectedness” Assumption

Spatial Methods (MPNNs) also fail to deal with directionality

in- and out-neighbors treated equally

$$\mathbf{m}_i^{(k)} = \mathrm{AGG}^{(k)}\left(\{\{\mathbf{x}_j^{(k-1)} : (i,j) \in E\}\}\right)$$
$$\mathbf{x}_i^{(k)} = \mathrm{COM}^{(k)}\left(\mathbf{x}_i^{(k-1)}, \mathbf{m}_i^{(k)}\right)$$

[2] J. Gilmer et al., “Neural Message Passing for Quantum Chemistry”, ICML 2017

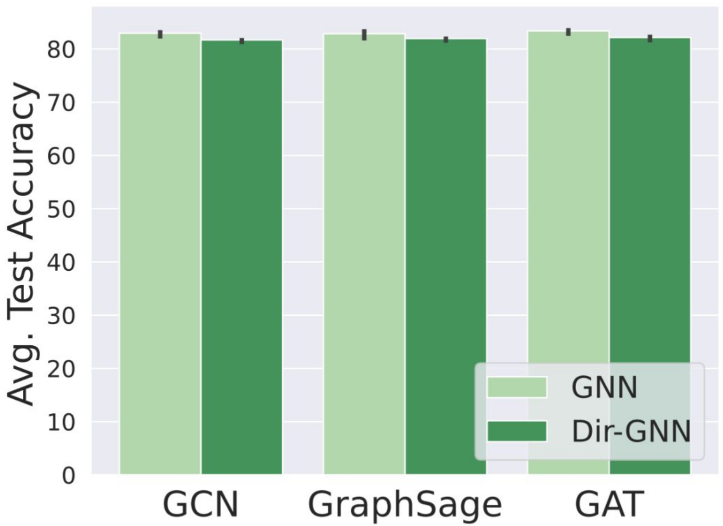
The “Undirectedness” Assumption

Making the graph undirected has become part of the standard preprocessing

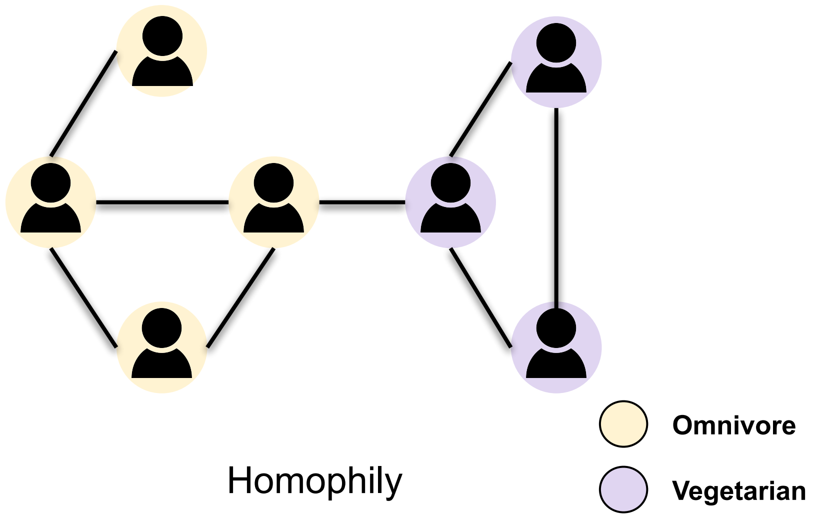
```python
def parse_npz(f):
    x = sp.csr_matrix((f['attr_data'], f['attr_indices'], f['attr_indptr']),
                      f['attr_shape']).todense()
    x = torch.from_numpy(x).to(torch.float)
    x[x > 0] = 1

    adj = sp.csr_matrix((f['adj_data'], f['adj_indices'], f['adj_indptr']),
                        f['adj_shape']).tocoo()
    row = torch.from_numpy(adj.row).to(torch.long)
    col = torch.from_numpy(adj.col).to(torch.long)
    edge_index = torch.stack([row, col], dim=0)
    edge_index, _ = remove_self_loops(edge_index)
    edge_index = to_undirected(edge_index, num_nodes=x.size(0))

    y = torch.from_numpy(f['labels']).to(torch.long)

    return Data(x=x, edge_index=edge_index, y=y)
```

The "Undirectedness" Assumption

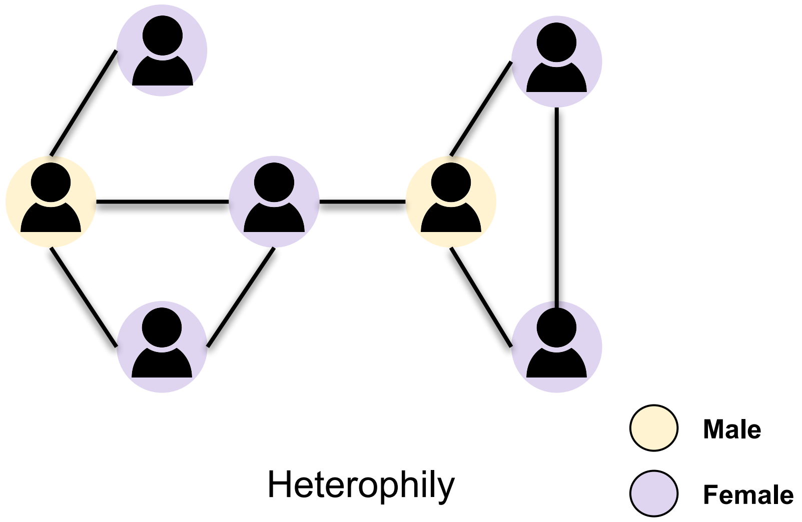
Undirected graphs perform equally well in common (homophilic) benchmarks



Homophily and Heterophily

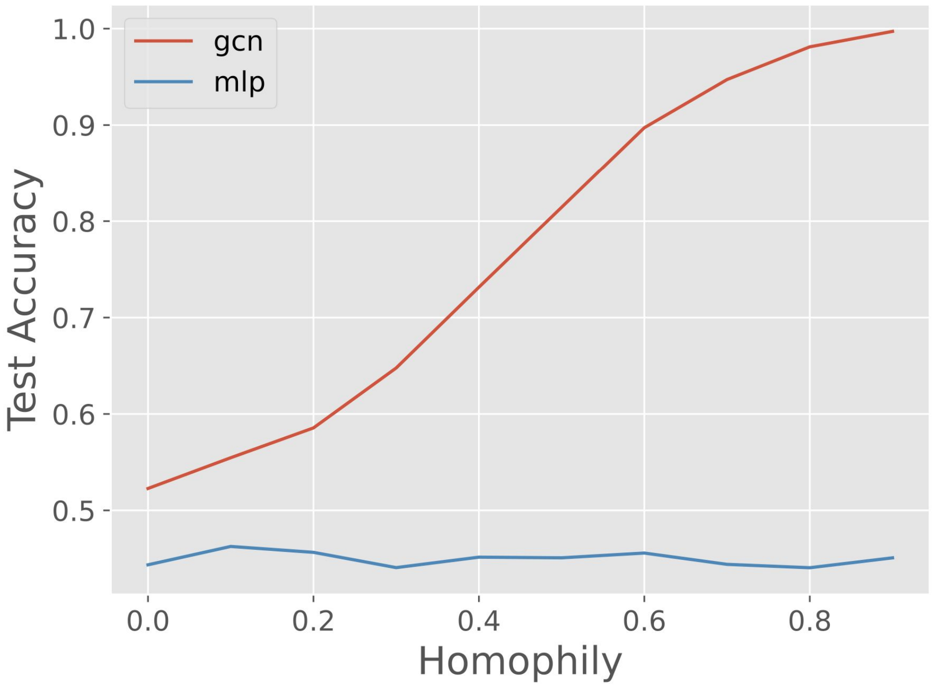


Homophily



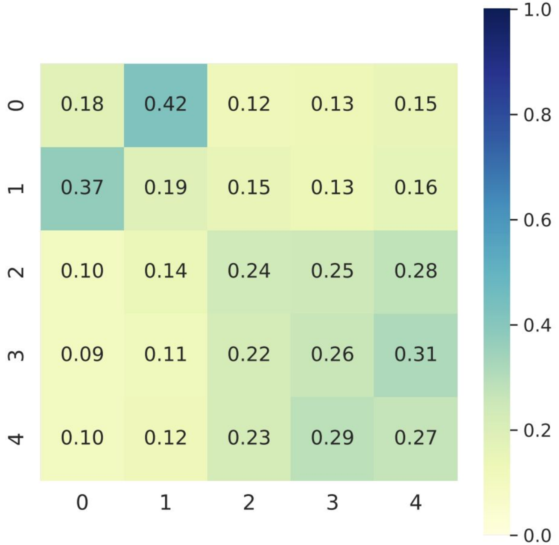
Heterophily

GNNs Struggle on Heterophilic Data



Measuring Homophily

Undirected Graphs



Class Compatibility Matrix

$$h = \frac{1}{|V|} \sum_{i \in V} \frac{\sum_{j \in \mathcal{N}(i)} I[y_i = y_j]}{d_i}$$

Node Homophily

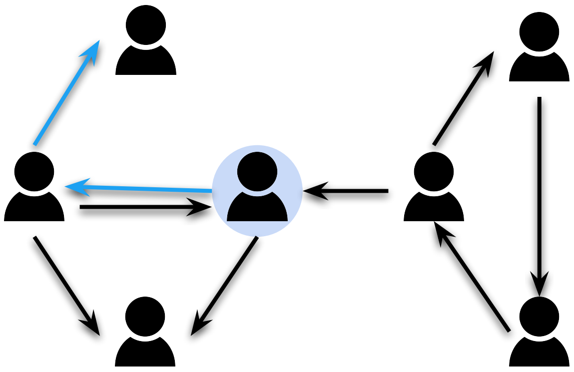
Measuring Homophily

Weighted directed graphs

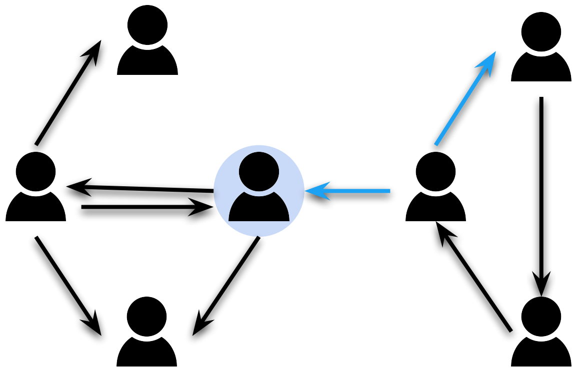
$$h(\mathbf{S}) = \frac{1}{|V|} \sum_{i \in V} \frac{\sum_{j \in \mathcal{N}(i)} s_{ij} I[y_i = y_j]}{\sum_{j \in \mathcal{N}(i)} s_{ij}}$$

Directed 2-hops

There are four different 2-hops for directed graphs



$\mathbf{A}^2$



$\mathbf{A}^\top \mathbf{A}$

Effective Homophily

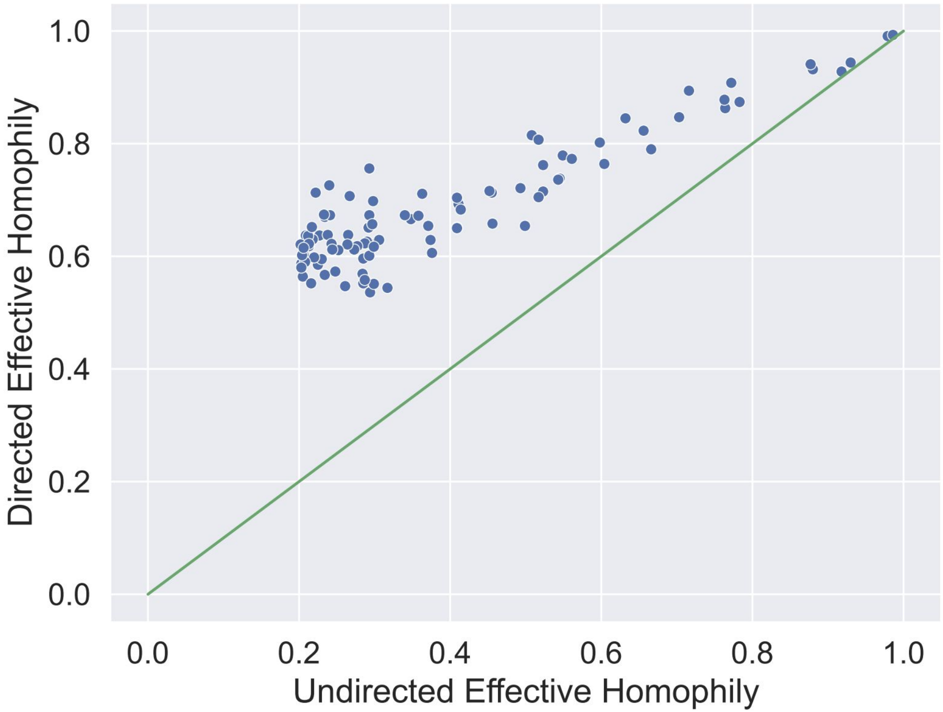
Going beyond the immediate neighbors

$$h^{(\mathrm{eff})} = \max_{k \geq 1} \max_{\mathbf{C} \in \mathcal{B}^k} h(\mathbf{C})$$

Higher-order hops

Directionality Enhances Effective Homophily

Synthetic graphs



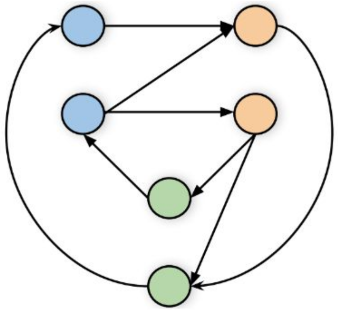
Directionality Enhances Effective Homophily

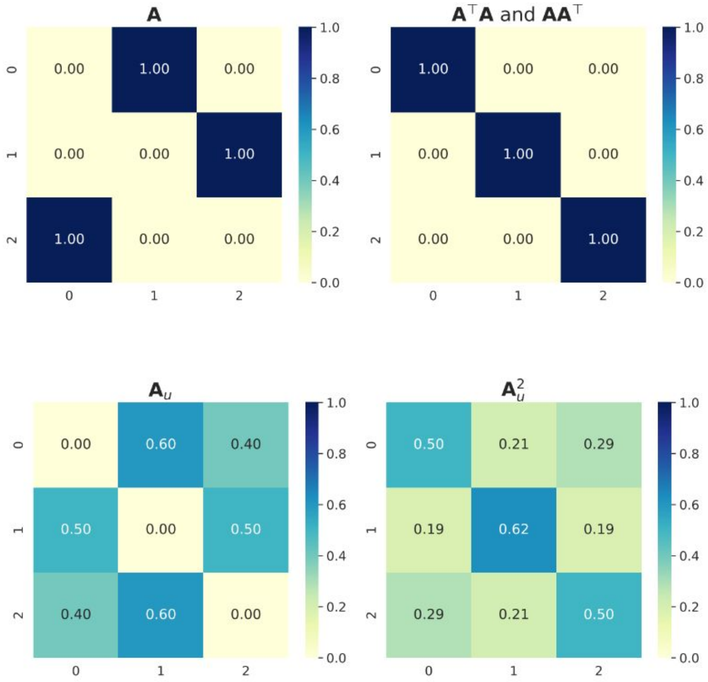
Real-world datasets

		$\mathbf{A}_u$	$\mathbf{A}_u^2$	$h_u^{(\text{eff})}$	$\mathbf{A}$	$\mathbf{A}^\top$	$\mathbf{A}^\top\mathbf{A}$	$\mathbf{A}\mathbf{A}^\top$	$h_d^{(\text{eff})}$	$h_{\text{gain}}^{(\text{eff})}$
Homophilic	CITESEER-FULL	0.958	0.951	0.958	0.954	0.959	0.971	0.951	0.971	1.36%
	CORA-ML	0.810	0.767	0.810	0.808	0.833	0.803	0.779	0.833	2.84%
	OGBN-ARXIV	0.635	0.548	0.635	0.632	0.675	0.658	0.556	0.675	6.3%
Heterophilic	CHAMELEON	0.248	0.331	0.331	0.249	0.274	0.383	0.335	0.383	15.71%
	SQUIRREL	0.218	0.252	0.252	0.219	0.210	0.257	0.258	0.258	2.38%
	ARXIV-YEAR	0.289	0.397	0.397	0.310	0.403	0.487	0.431	0.487	22.67%
	SNAP-PATENTS	0.221	0.372	0.372	0.266	0.271	0.478	0.522	0.522	40.32%
	ROMAN-EMPIRE	0.046	0.365	0.365	0.045	0.042	0.535	0.609	0.609	66.85%

Directionality Enhances Effective Homophily

An intuitive example





Dir-GNN

Aggregate from both in- and out-neighbors, but separately

$$\mathbf{m}_{i,\leftarrow}^{(k)} = \mathrm{AGG}_{\leftarrow}^{(k)}\left(\{\{\mathbf{x}_j^{(k-1)} : (j,i) \in E\}\}\right)$$
$$\mathbf{m}_{i,\rightarrow}^{(k)} = \mathrm{AGG}_{\rightarrow}^{(k)}\left(\{\{\mathbf{x}_j^{(k-1)} : (i,j) \in E\}\}\right)$$
$$\mathbf{x}_i^{(k)} = \mathrm{COM}^{(k)}\left(\mathbf{x}_i^{(k-1)}, \mathbf{m}_{i,\leftarrow}^{(k)}, \mathbf{m}_{i,\rightarrow}^{(k)}\right)$$

Separate aggregation
of in- and out-neighbors

From GCN to Dir-GCN

A general framework which can be used to extend any MPNN to directed graphs

$$\mathbf{X}^{(k)} = \sigma\left(\mathbf{A}_u \mathbf{X}^{(k-1)} \mathbf{W}^{(k)}\right)$$

$$\tilde{\mathbf{A}}_u = \mathbf{D}_u^{-1/2} \mathbf{A}_u \mathbf{D}_u^{-1/2}$$

$$\mathbf{X}^{(k)} = \sigma\left(\mathbf{A}_{\rightarrow} \mathbf{X}^{(k-1)} \mathbf{W}_{\rightarrow}^{(k)} + \mathbf{A}_{\rightarrow}^{\top} \mathbf{X}^{(k-1)} \mathbf{W}_{\leftarrow}^{(k)}\right)$$

$$\mathbf{A}_{\rightarrow} = \mathbf{D}_{\rightarrow}^{-1/2} \mathbf{A} \mathbf{D}_{\leftarrow}^{-1/2}$$

Dir-GNN Leads to More Homophilic Aggregations

It treats different 2-hops differently

$$\mathbf{X}^{(2)} = \mathbf{A}^2_{\rightarrow}\mathbf{X}^{(0)}\mathbf{W}^{(1)}_{\rightarrow}\mathbf{W}^{(2)}_{\rightarrow} + (\mathbf{A}^{\top}_{\rightarrow})^2\mathbf{X}^{(0)}\mathbf{W}^{(1)}_{\leftarrow}\mathbf{W}^{(2)}_{\leftarrow}$$
$$+ \boxed{\mathbf{A}_{\rightarrow}\mathbf{A}^{\top}_{\rightarrow}}\mathbf{X}^{(0)}\mathbf{W}^{(1)}_{\leftarrow}\mathbf{W}^{(2)}_{\rightarrow} + \boxed{\mathbf{A}^{\top}_{\rightarrow}\mathbf{A}_{\rightarrow}}\mathbf{X}^{(0)}\mathbf{W}^{(1)}_{\rightarrow}\mathbf{W}^{(2)}_{\leftarrow}$$

Expressivity Analysis

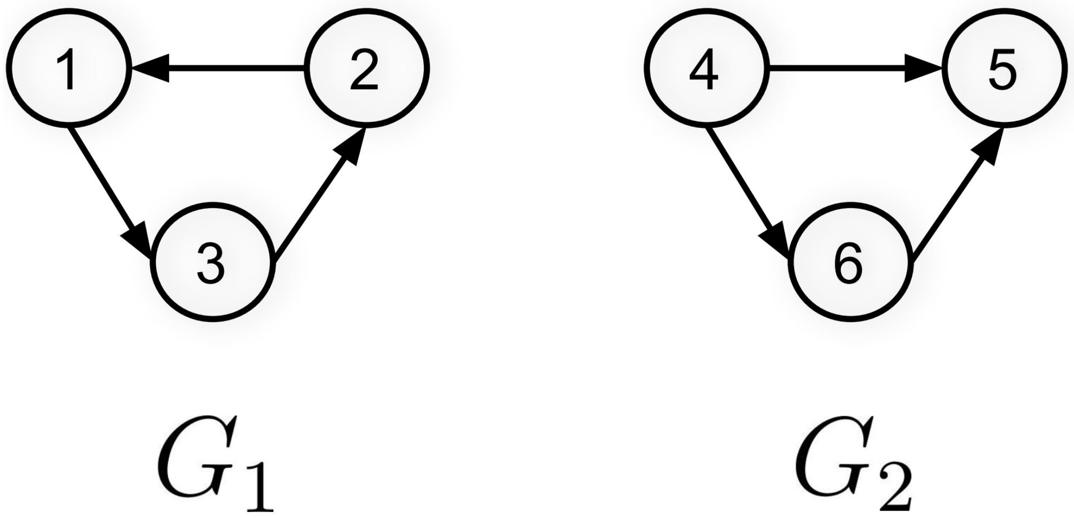
Dir-GNN is strictly more expressive than MPNNs

Theorem 4.1 (Informal). *Dir-GNN is as expressive as D-WL if* $\mathrm{AGG}_{\rightarrow}^{(k)}$, $\mathrm{AGG}_{\leftarrow}^{(k)}$, *and* $\mathrm{COM}^{(k)}$ *are injective for all* k.

Theorem 4.2 (Informal). *Dir-GNN is strictly more expressive than both MPNN-U and MPNN-D.*

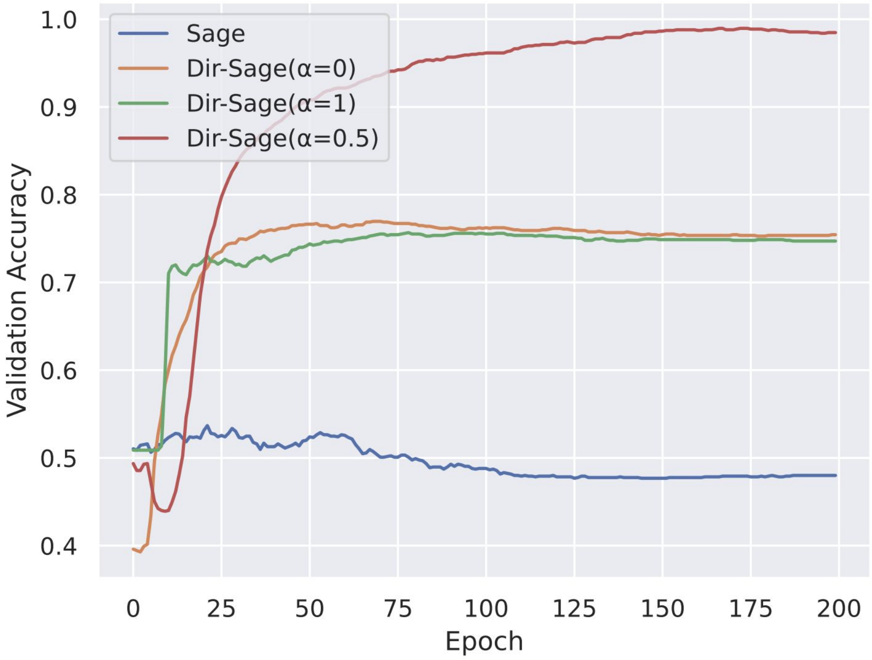
Dir-GNN $\sqsubseteq$ MPNN-U

MPNN-U fails to distinguish the two graphs below



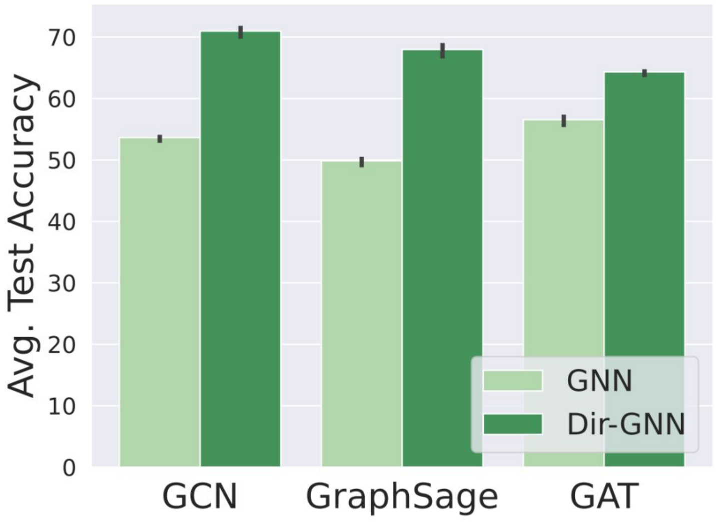
Empirical Results

Synthetic task where the label of a node depends both on in- and out-neighbors

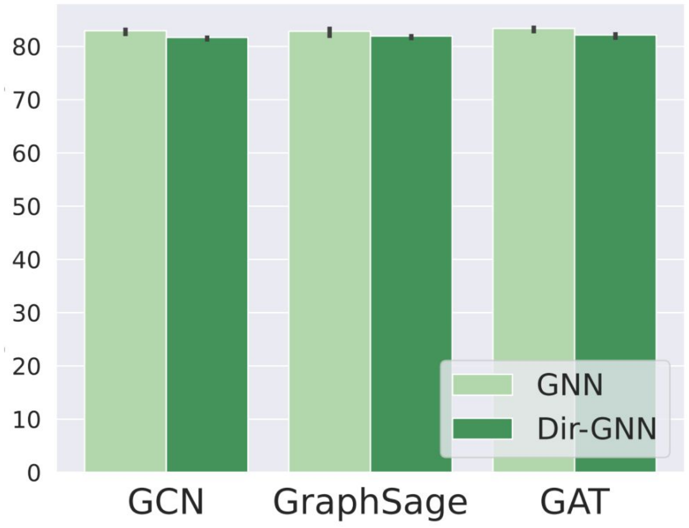


Empirical Results

Directionality leads to significant improvement on heterophilic datasets



(a) Heterophilic Graphs



(b) Homophilic Graphs

Empirical Results

Dir-GNN achieves state-of-the-art results on five heterophilic benchmarks

	Squirrel	Chameleon	Arxiv-year	Snap-patents	Roman-Empire
MLP	28.77 ± 1.56	46.21 ± 2.99	36.70 ± 0.21	31.34 ± 0.05	64.94 ± 0.62
GCN	53.43 ± 2.01	64.82 ± 2.24	46.02 ± 0.26	51.02 ± 0.06	73.69 ± 0.74
H_2GCN	37.90 ± 2.02	59.39 ± 1.98	49.09 ± 0.10	OOM	60.11 ± 0.52
GPR-GNN	54.35 ± 0.87	62.85 ± 2.90	45.07 ± 0.21	40.19 ± 0.03	64.85 ± 0.27
LINKX	61.81 ± 1.80	68.42 ± 1.38	56.00 ± 0.17	61.95 ± 0.12	37.55 ± 0.36
FSGNN	74.10 ± 1.89	78.27 ± 1.28	50.47 ± 0.21	65.07 ± 0.03	79.92 ± 0.56
ACM-GCN	67.40 ± 2.21	74.76 ± 2.20	47.37 ± 0.59	55.14 ± 0.16	69.66 ± 0.62
GloGNN	57.88 ± 1.76	71.21 ± 1.84	54.79 ± 0.25	62.09 ± 0.27	59.63 ± 0.69
Grad. Gating	64.26 ± 2.38	71.40 ± 2.38	63.30 ± 1.84	69.50 ± 0.39	82.16 ± 0.78
DiGCN	37.74 ± 1.54	52.24 ± 3.65	OOM	OOM	52.71 ± 0.32
MagNet	39.01 ± 1.93	58.22 ± 2.87	60.29 ± 0.27	OOM	88.07 ± 0.27
Dir-GNN	$\mathbf{75.31 \pm 1.92}$	$\mathbf{79.71 \pm 1.26}$	$\mathbf{64.08 \pm 0.26}$	$\mathbf{73.95 \pm 0.05}$	$\mathbf{91.23 \pm 0.32}$

Dir-GNN for Temporal Graphs

TGN [3] uses direction in message function, but discards it for the graph aggregation

Message Function

$$\mathbf{m}_u(t) = \mathrm{msg_s}\left(\mathbf{s}_u(t^-), \mathbf{s}_v(t^-), t, \mathbf{e}\right),$$
$$\mathbf{m}_v(t) = \mathrm{msg_d}\left(\mathbf{s}_v(t^-), \mathbf{s}_u(t^-), t, \mathbf{e}\right)$$

Direction-aware

Graph Aggregation

$$\mathbf{Z}(t) = \mathrm{GNN}(\mathbf{G}(t), \mathbf{E}(t), \mathbf{X}(t), \mathbf{S}(t))$$

Direction-unaware

[3] Rossi et al., “Temporal Graph Networks For Deep Learning On Dynamic Graphs”, ICML 2020 GRL Workshop;

Conclusion

Dir-GNN achieves state-of-the-art results on five heterophilic benchmarks

- Edge **directionality** has largely been **ignored** in GNNs
- Preserving directionality can make heterophilic datasets more **homophilic**
- We introduce **Dir-GNN**, a general framework for learning on directed graphs
- Dir-GNN is **more expressive** than MPNNs on directed graphs
- Dir-GNN leads to **large improvements** on **heterophilic** datasets
- Many temporal datasets are directed!

Questions?

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