Breaking the Heterophily Mixing Barrier in Graph Learning: A Mixed-Curvature Product Manifold Approach

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Introduction

1 Challenge — GNNs Fail under Heterophily.
Their message passing mechanism assumes similar neighbors, but this breaks down when connected nodes belong to different classes.

2 Core Issue — Heterophily Mixing.
Messages from dissimilar classes become entangled during aggregation, diluting class-discriminative info.

3 Limitation — Existing Fixes Are Coarse.
Spectral filters, signed messages & rewiring lack class-awareness and fail to adapt to local heterophily patterns.

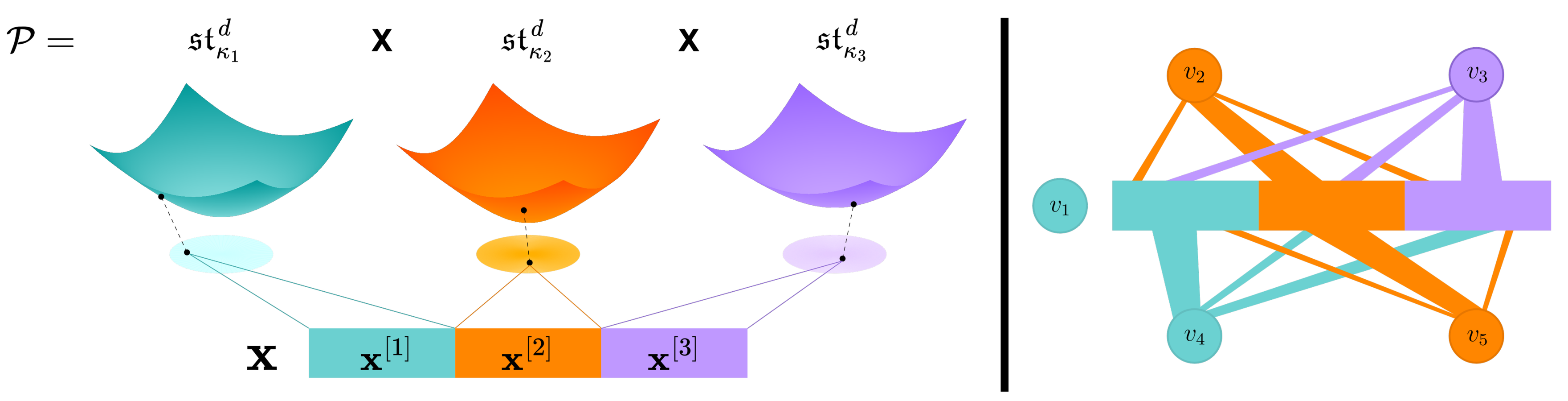
4 Key Insight — Route Messages by Class.
Information should propagate along class-specific tracks to prevent semantic interference.

5 Our Solution — XMan-GNN Disentangles Mixing.
We model nodes on a *mixed-curvature product manifold*, guiding message flow into class-aligned submanifolds.

Proposed Method: XMan-GNN

Basic Idea

- XMan-GNN assumes that *nodes of different classes lie on distinct geometric manifolds*.
- During message passing, information is constrained to flow *within class-specific submanifolds*, preventing semantic interference from heterogeneous neighbors.



Key Steps

Step 1: Attention-based Soft Label Assignment

- We employ attention scores to estimate the likelihood of two nodes belonging to the same class, which dynamically guide message routing toward the correct submanifolds.

$$\mathbf{s}_{i,j}^{(l)} = \mathrm{Softmax}\left(\frac{\mathbf{W}_{att}^{(l)}\sigma(\mathbf{h}_i^{(l)}+\mathbf{h}_j^{(l)})}{\sqrt{C}}\right)$$

Step 2: Manifold-aware Message Aggregation

- Messages are assembled and aggregated separately on each submanifold using Möbius gyromidpoint as the aggregator, weighted by their attention scores.

$$\mathbf{m}_{i,j}^{(l)}[r] = \mathbf{s}_{i,j}^{(l)}[r] \otimes_{\kappa} \exp_{\mathbf{0}}^{\kappa_r}(\mathbf{h}_j^{(l)})$$

$$\mathbf{z}_i^{(l)}[r] = \bigodot_{v_j\in\mathcal{N}(v_i)} [\mathbf{m}_{i,j}^{(l)}[r], 1]_{\kappa_r} = \frac{1}{2} \otimes_{\kappa_r} \left(\frac{\sum_{v_j\in\mathcal{N}(v_i)} \lambda^{\kappa_r}_{\mathbf{m}_{i,j}^{(l)}[r]} \mathbf{m}_{i,j}^{(l)}[r]}{\sum_{v_j\in\mathcal{N}(v_i)} (\lambda^{\kappa_r}_{\mathbf{m}_{i,j}^{(l)}[r]} - 1)}\right)$$

Step 3: Initial Residual Connections

- To preserve the node's intrinsic features, we introduce initial residual connections using the Möbius gyromidpoint.

$$\mathbf{x}_i^{(l)} = \frac{1}{2} \otimes_{\mathcal{K}} \left(\frac{\alpha\lambda^{\mathcal{K}}_{\mathbf{z}_i^{(l)}}\mathbf{z}_i^{(l)} + (1-\alpha)\lambda^{\mathcal{K}}_{\mathbf{x}_i^{(0)}}\mathbf{x}_i^{(0)}}{\alpha\lambda^{\mathcal{K}}_{\mathbf{z}_i^{(l)}} + (1-\alpha)\lambda^{\mathcal{K}}_{\mathbf{x}_i^{(0)}} - 1}\right)$$

Results

- **Performance on *heterophilic* graphs**

	Texas	Wisconsin	Cornell	Actor	Squirrel	Chameleon	Amazon-Ratings	BlogCatalog	Avg. Rank
MLP	78.65±4.75	84.31±3.28	74.86±4.84	34.64±0.98	34.11±1.80	52.08±2.13	46.73±0.85	93.07±0.30	9.8
GCN	48.11±6.82	48.82±5.51	38.92±7.27	27.32±0.98	27.12±1.13	40.46±2.27	47.97±0.64	77.81±0.89	18.4
GAT	46.22±7.78	49.41±5.02	45.95±5.92	28.38±1.32	29.93±1.36	44.28±2.19	46.74±0.92	63.72±5.15	17.9
HGCN	64.59±10.22	64.31±5.17	52.16±4.84	24.71±0.70	57.53±1.91	67.36±1.14	44.35±0.59	79.34±1.46	13.1
HyboNet	61.08±6.96	59.41±4.48	49.73±8.82	25.29±0.96	53.49±1.93	70.39±2.32	43.25±0.25	74.20±1.02	14.5
HypFormer	80.27±4.69	84.12±4.59	72.16±6.29	33.40±0.82	33.57±1.93	47.37±1.90	**51.93**±0.60	94.59±0.93	9.6
SGFormer	60.54±4.22	63.33±7.34	52.16±4.99	33.05±1.74	32.19±2.58	41.58±2.50	42.99±0.50	96.57±0.41	14.6
GOAT	54.32±6.33	56.08±5.05	46.22±6.45	30.00±3.35	33.85±1.21	38.73±7.23	50.28±2.15	92.26±0.87	16.0
PolyFormer	60.54±6.30	60.20±6.39	57.30±5.77	32.69±2.63	42.96±1.65	58.36±1.70	40.84±3.69	92.15±1.68	14.4
Polynormer	76.76±8.73	77.65±3.64	71.08±3.43	35.29±1.44	38.14±1.27	50.33±1.15	43.99±0.44	96.59±0.42	9.5
H2GCN	80.81±5.05	76.47±5.26	69.19±5.57	32.99±1.03	33.29±1.64	56.07±2.05	43.17±0.50	96.03±0.67	11.1
GPR-GNN	74.59±4.55	77.65±4.57	71.62±7.18	34.85±0.78	31.60±0.84	40.70±1.74	43.44±0.27	95.24±0.44	12.4
FAGCN	67.30±4.90	64.51±3.77	60.27±4.84	35.89±0.94	35.75±1.54	50.88±1.80	42.21±0.41	93.72±0.91	12.4
GloGNN	75.95±5.60	83.92±5.60	72.97±5.41	35.45±1.17	57.54±1.39	71.32±2.38	44.63±0.52	92.17±0.56	8.4
ACM-GCN	87.84±4.40	88.43±3.22	80.34±5.89	35.82±1.09	54.40±1.88	66.93±1.85	38.52±0.43	94.98±0.68	6.9
GOAL	83.62±6.72	86.98±4.46	80.68±6.29	35.96±1.04	60.53±1.65	71.65±1.68	37.94±0.33	95.12±0.53	6.1
AERO-GNN	75.95±5.98	68.04±12.34	65.95±3.67	35.74±1.59	36.00±1.15	52.59±2.24	37.47±0.27	95.78±0.73	11.4
Ordered GNN	83.78±5.27	86.47±4.42	75.68±3.20	36.09±0.81	37.32±1.27	50.61±2.09	51.02±0.82	95.27±0.38	6.0
PCNet	60.81±7.28	81.37±3.19	70.27±4.83	35.70±0.84	30.63±1.93	43.73±4.52	38.11±0.74	93.82±1.01	13.9
M2M-GNN	86.22±4.09	88.82±4.21	77.57±3.64	35.91±1.15	**63.20**±1.71	75.37±1.68	50.19±0.69	**96.92**±0.48	2.8
XMan-GNN	**90.27**±3.46	**90.59**±3.31	**84.86**±2.16	**37.07**±0.58	62.46±1.39	**76.63**±0.76	50.89±0.65	96.89±0.37	**1.5**

- **Performance on *homophilic* graphs**

	Cora	CiteSeer	PubMed	Deezer-Europe	Photo	Physics	Avg. Rank
MLP	73.98±1.89	72.51±1.60	86.81±0.37	65.69±0.56	92.25±0.78	96.01±0.26	15.8
GCN	85.69±0.89	75.27±1.75	87.41±0.44	62.70±0.57	94.57±0.56	96.38±0.19	14.0
GAT	85.84±1.15	74.51±1.47	86.57±0.45	60.85±0.85	93.88±1.07	96.10±0.27	16.2
HGCN	82.90±1.36	71.83±1.68	81.80±0.77	56.32±0.68	92.51±0.76	95.62±0.16	20.0
HyboNet	85.33±1.21	72.31±1.62	84.39±0.60	61.44±0.46	93.25±0.66	95.94±0.15	18.7
HypFormer	87.65±0.96	76.25±1.34	88.80±0.36	65.29±0.77	95.23±0.26	96.72±0.19	6.8
SGFormer	85.47±1.28	73.94±1.75	86.61±0.46	65.69±0.83	94.97±0.45	96.42±0.24	12.7
GOAT	80.56±1.59	67.21±1.71	88.49±0.46	65.57±0.71	94.52±0.50	96.63±0.24	13.7
PolyFormer	86.00±0.92	74.69±1.72	89.10±0.43	64.22±3.03	93.83±0.97	96.76±0.14	12.5
Polynormer	86.68±0.82	74.97±1.30	89.27±0.30	66.06±0.71	95.55±0.44	96.85±0.13	6.2
H2GCN	87.00±0.88	75.28±1.43	89.31±0.41	65.07±0.55	95.53±0.53	96.85±0.23	6.2
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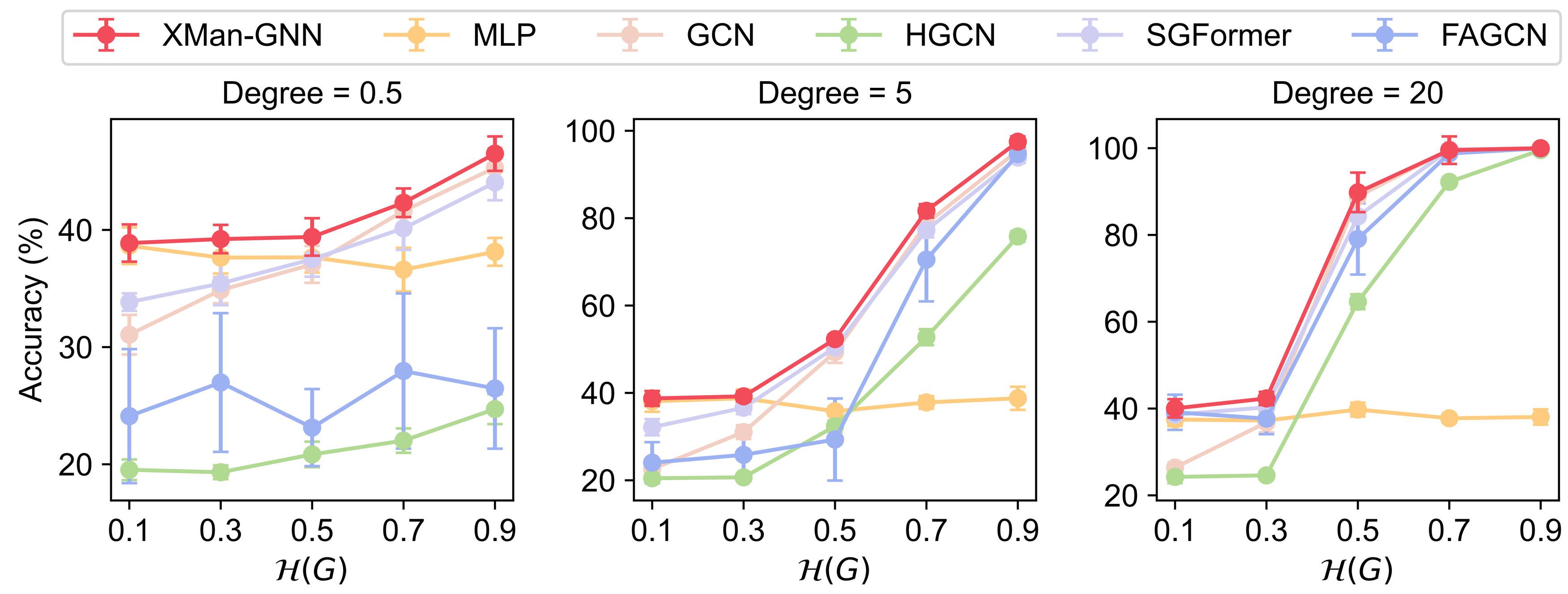
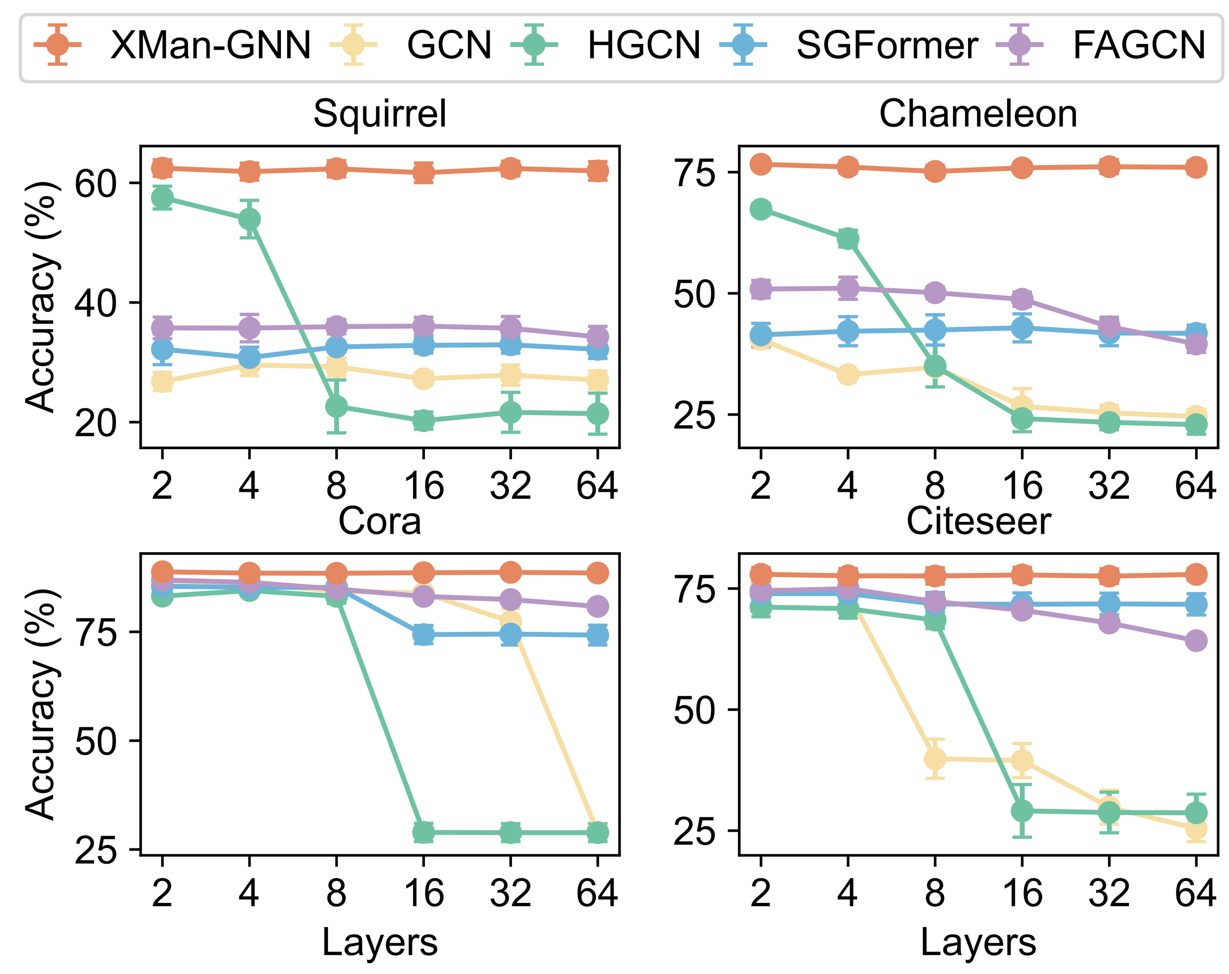
GOAL	87.47±0.88	76.24±1.39	89.25±0.54	64.92±0.62	95.32±0.53	96.72±0.12	7.3
AERO-GNN	86.74±1.29	75.62±1.59	85.28±0.54	64.58±0.43	93.48±0.67	96.54±0.23	13.7
Ordered GNN	87.53±1.18	76.37±1.83	89.74±0.40	66.07±0.49	95.47±0.75	96.82±0.14	3.3
PCNet	86.82±1.00	76.44±1.32	85.64±0.52	64.51±0.58	93.22±0.41	95.41±0.16	14.2
M2M-GNN	87.38±0.97	76.31±1.06	90.04±0.32	64.63±0.44	95.22±0.58	96.82±0.19	6.3
XMan-GNN	**88.79**±1.05	**77.90**±1.42	**90.11**±0.39	**66.82**±0.42	**96.05**±0.45	**97.11**±0.16	**1.0**

- **Evaluation on Synthetic Benchmarks**



- **Over-smoothing Analysis**



- **Conclusion**: XMan-GNN disentangles heterophily mixing by routing messages on class-specific manifolds in mixed-curvature space, achieving state-of-the-art performance on diverse graphs.

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