Polynomial Sheaf Diffusion and Equivariant Sheaf Neural Networks

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8 November 2025, Podgorica, Montenegro

EEML Workshops — MMLW 2025

Introduction & Background

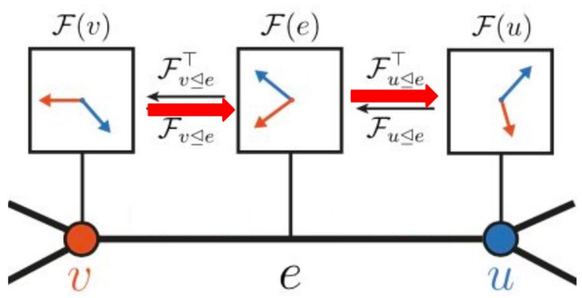
PROBLEM

Most of GNNs present an accuracy degradation in heterophilic cases and when adding too many layers:

- Rely on the **Homophilic Assumption**.
- Suffer from **Oversmoothing Effect**.

SOLUTION → SHEAF NEURAL NETWORKS

- **False Assumption**: Graph Nodes live in the same global feature space.
- Assign a vector space (**stalk**) to each node and edge and learn **restriction maps** (transport maps) among them.



How to move a vector x from v to u?

Moving $\mathbf{x} \in \mathcal{F}(v) \rightarrow \mathcal{F}(u)$ is done via maps composition!

$$\mathcal{F}^{\top}_{u \trianglelefteq e} \mathcal{F}_{v \trianglelefteq e} \mathbf{x} \in \mathcal{F}(u)$$

Sheaf Laplacian

Q: Can we measure the **total disagreement** at each node?

- ▶ Space of 0-Cochains: $C^0(\mathcal{G}, \mathcal{F}) := \bigoplus_{u \in \mathcal{V}} \mathcal{F}(u)$
- ▶ Space of 1-Cochains: $C^1(\mathcal{G}, \mathcal{F}) := \bigoplus_{e \in \mathcal{E}} \mathcal{F}(e)$
- ▶ Co-boundary Map: $\delta : C^0(\mathcal{G}, \mathcal{F}) \rightarrow C^1(\mathcal{G}, \mathcal{F})$
  - ↳ Measures the nodes disagreement

A: Build the **Sheaf Laplacian** $L_{\mathcal{F}} := \delta^{\top}\delta$

$$L_{\mathcal{F}}(\mathbf{x})_u = \sum_{u, v \trianglelefteq e} \mathcal{F}^{\mathsf{T}}_{u \trianglelefteq e}(\mathcal{F}_{u \trianglelefteq e}\mathbf{x}_u - \mathcal{F}_{v \trianglelefteq e}\mathbf{x}_v)$$

Polynomial Sheaf Diffusion

Optimise Sheaf Diffusion process

- Replaces the ”one-step” diffusion with the action of a polynomial over the Sheaf Laplacian.

Double Interpretation:

- **Spectral**: Frequency–selective filter on the sheaf signal.
- **Spatial**: The degree K determines the receptive field, mixing information across all paths of length up to K in a single pass.

Since the spectral response is always $0 \leq p(\lambda) \leq 1$ on the L spectrum, the Dirichlet Energy cannot increase.

Spectrum Upper Bound $\lambda_{\max}$:

- For $\Delta_{\mathcal{F}}$ (Normalized Case), we have $\lambda_{\max} = 2$ since the spectrum is bounded, i.e., $\sigma(\Delta_{\mathcal{F}}) \subset [0, 2]$.
- For $L_{\mathcal{F}}$ (Unnormalized Case), we have 2 options:
  - *Analytic Bound* $\lambda_{\max} \leq 2 \max_v \deg(v)$
  - *Iterative Power Estimate*:

$$\hat{\lambda}_{\max} = \frac{\mathbf{z}^{\top} L_{\mathcal{F}} \mathbf{z}}{\mathbf{z}^{\top}\mathbf{z}}, \quad \mathbf{z} \leftarrow \frac{L_{\mathcal{F}}\mathbf{z}}{\|L_{\mathcal{F}}\mathbf{z}\|}, \text{ for a few steps } N_{steps}$$

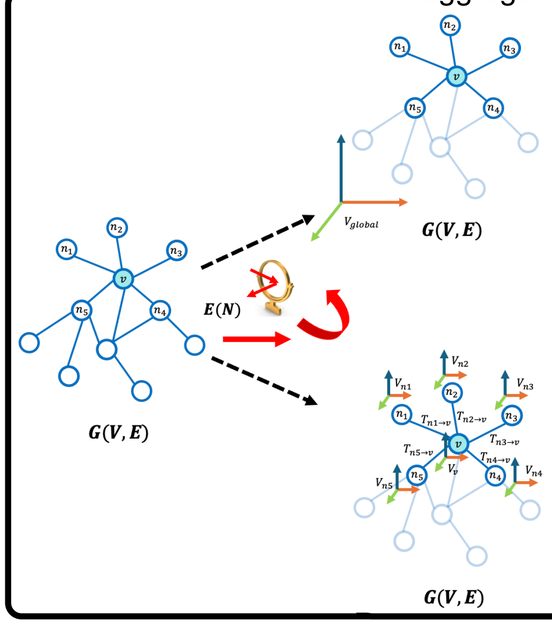
Research Questions

- **Can we optimise Sheaf Diffusion process?**
- **Can we extend SNN to GDL?**

Equivariant Sheaf NNs

Extends SNNs with geometry-aware diffusion layers

- Start from Coordinate-free Message Passing EGNN model.
- Based on Euclidean Invariants (pairwise angles/distances).
- Learn Sheaf Transports $T_{i \rightarrow v}$ per edge, before Invariances aggregation, to align neighbours' vector into node v local gauge (feature space).



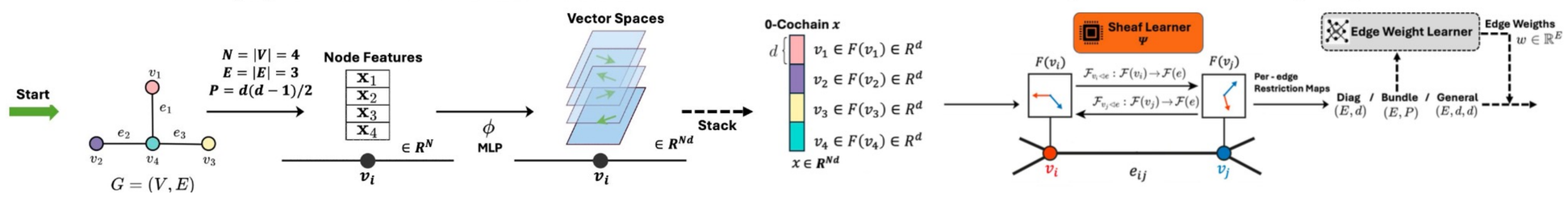
$$m_{ij}^{\text{vec}} = \phi_{\text{vec}}(T_{ij}v_j - v_i,\ r_{ij},\ h_i, h_j), \qquad m_{ij}^{\text{sca}} = \phi_{\text{sca}}(r_{ij}, h_i, h_j),$$

learned sheaf transport — node i vector features — Euclidean invariants — scalar node i and j features — MLP — MLP

$$h_i' = \psi_{\text{sca}}\Big(h_i, \sum_j m_{ij}^{\text{sca}}\Big) \qquad v_i' = v_i + \sum_j \psi_{\text{vec}}(m_{ij}^{\text{vec}})$$

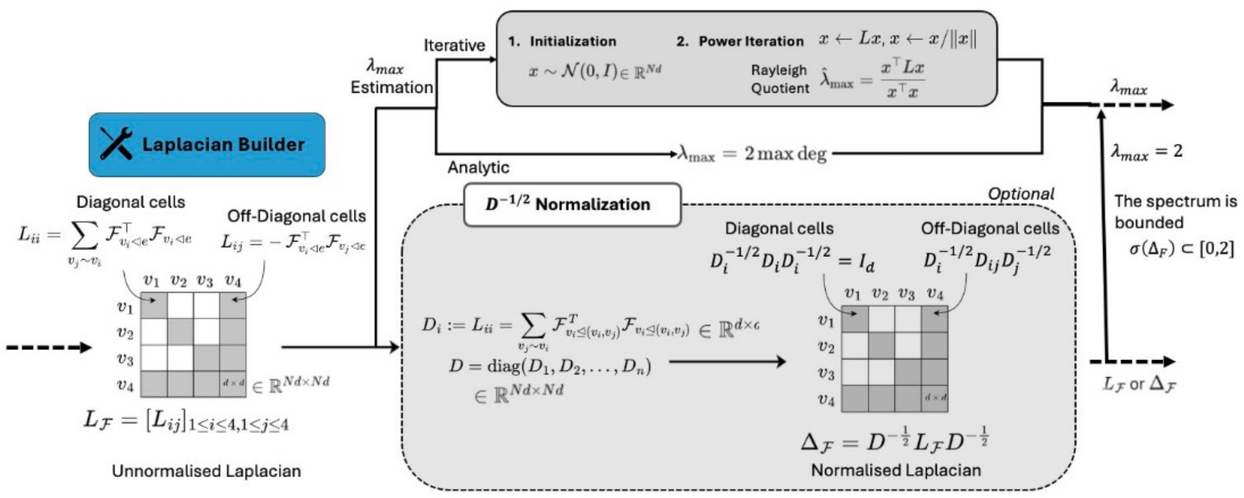
Aggregation — Aggregation

1) Augment Node Features to Stalk width Dimensionality d

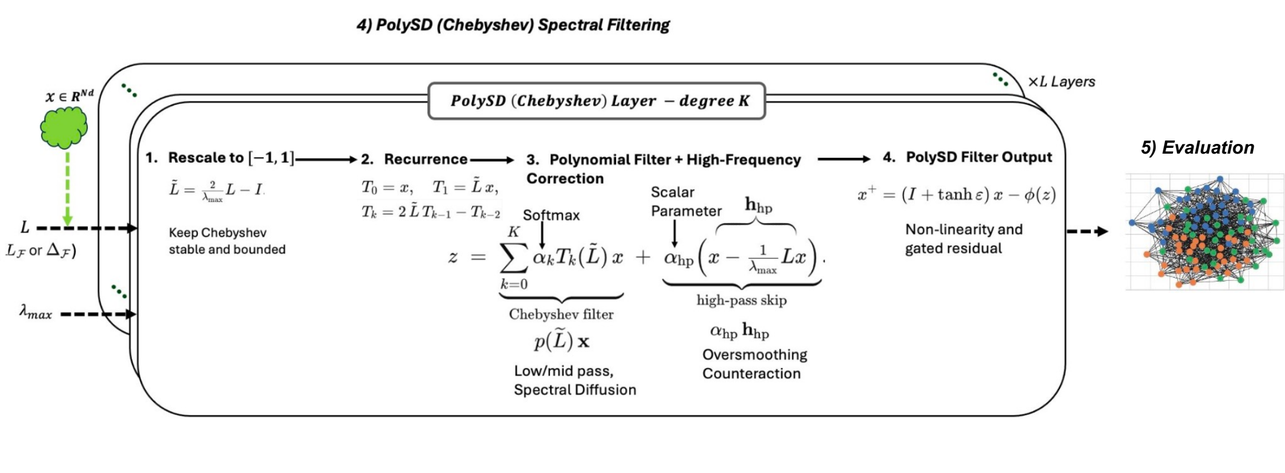


2) Learn the d×d Restriction Maps using Sheaf Learners

3) Build a Sheaf Laplacian from the Learned d×d Restriction Maps



4) PolySD (Chebyshev) Spectral Filtering



5) Evaluation

Experiments & Results

Real-World Benchmark

	Texas	Wisconsin	Film	Squirrel	Chameleon	Cornell	Citeseer	Pubmed	Cora
Homophily level	**0.11**	**0.21**	**0.22**	**0.22**	**0.23**	**0.30**	**0.74**	**0.80**	**0.81**
#Nodes	183	251	7,600	5,201	2,277	183	3,327	18,717	2,708
#Edges	295	466	26,752	198,493	31,421	280	4,676	44,327	5,278
#Classes	5	5	5	5	5	5	7	3	6
DiagChebySD	**88.68±3.12**	87.84±4.45	37.14±1.26	**56.61±2.06**	**70.41±2.47**	**86.49±5.54**	**77.74±1.26**	89.67±0.34	**88.67±1.29**
BundleChebySD	**89.74±5.32**	87.65±3.29	37.47±0.86	54.33±2.67	**69.29±1.88**	85.40±7.94	**77.57±1.55**	**89.75±0.34**	88.12±1.35
GeneralChebySD	**88.94±4.53**	88.23±4.56	37.20±0.77	53.88±1.65	67.34±2.45	**86.49±5.80**	77.10±1.30	89.73±0.41	**88.47±1.19**
RiSNN - NoT	87.89±4.28	88.04±2.39	*N/A*	51.24±1.71	66.58±1.81	82.97±6.17	75.07±1.56	87.91±0.55	85.86±1.31
RiSNN	86.84±3.72	87.84±2.60	*N/A*	53.30±3.30	65.15±2.40	85.95±6.14	76.23±1.81	88.00±0.42	85.27±1.11
JdSNN - NoW	87.30±4.53	88.43±2.83	*N/A*	51.28±1.80	66.45±3.46	84.59±6.95	75.93±1.41	88.09±0.49	84.39±1.47
JdSNN	87.37±5.10	**89.22±3.42**	*N/A*	49.89±1.71	66.40±2.33	85.41±4.55	73.27±1.86	88.19±0.55	85.43±1.73
Conn - NSD	86.16±2.24	88.73±4.47	37.91±1.28	45.19±1.57	65.21±2.04	85.95±7.72	75.61±1.93	89.28±0.38	83.74±2.19
SAN	84.05±5.33	86.47±3.87	37.09±1.18	50.96±1.40	67.46±1.90	84.32±5.64	72.57±1.50	87.12±0.30	85.90±1.85
ANSD	85.68±4.69	87.45±3.19	37.66±1.40	54.39±1.76	68.38±2.14	84.59±5.93	76.81±1.82	89.21±0.37	87.20±1.03
Diag - NSD	85.67±6.95	88.63±2.75	**37.79±1.01**	54.78±1.81	68.68±1.73	**86.49±7.35**	77.14±1.85	89.42±0.43	87.14±1.06
O(d) - NSD	85.95±5.51	**89.41±4.74**	**37.81±1.15**	**56.34±1.32**	68.04±1.58	84.86±4.71	76.70±1.57	89.49±0.40	86.90±1.13
Gen - NSD	82.97±5.13	**89.21±3.84**	**37.80±1.22**	53.17±1.31	67.93±1.58	85.68±6.51	76.32±1.65	89.33±0.35	87.30±1.15
GGCN	84.86±4.55	86.86±3.29	37.54±1.56	**55.17±1.58**	**71.14±1.84**	85.68±6.63	77.14±1.45	89.15±0.37	87.95±1.05
H2GCN	84.86±7.23	87.65±4.98	35.70±1.00	36.48±1.86	60.11±2.15	82.70±5.28	77.11±1.57	89.49±0.38	87.87±1.20
GPRGNN	78.38±4.36	82.94±4.21	34.63±1.22	31.61±1.24	46.58±1.71	80.27±8.11	77.13±1.67	87.54±0.38	87.95±1.18
FAGCN	82.43±6.89	82.94±7.95	34.87±1.25	42.59±0.79	55.22±3.19	79.19±9.79	*N/A*	*N/A*	*N/A*
MixHop	77.84±7.73	75.88±4.90	32.22±2.34	48.30±1.48	60.50±2.53	73.51±6.34	76.26±1.33	85.31±0.61	87.61±0.85
GCNII	77.57±3.83	80.39±3.40	37.44±1.30	38.47±1.58	63.86±3.04	77.86±3.79	77.33±1.48	**90.15±0.43**	**88.37±1.25**
Geom - GCN	66.76±2.72	64.51±3.66	31.59±1.15	38.15±0.92	60.00±2.81	60.54±3.67	**78.02±1.15**	**89.95±0.47**	85.35±1.57
PairNorm	60.27±4.34	48.43±6.14	27.40±1.24	50.44±2.04	62.74±2.82	58.92±3.15	73.59±1.47	87.53±0.44	85.79±1.01
GraphSAGE	82.43±6.14	81.18±5.56	34.23±0.99	41.61±0.74	58.73±1.68	75.95±5.01	76.04±1.30	88.45±0.50	86.90±1.04
GCN	55.14±5.16	51.76±3.06	27.32±1.10	53.43±2.01	64.82±2.24	60.54±5.30	76.50±1.36	88.42±0.50	86.98±1.27
GAT	52.16±6.63	49.41±4.09	27.44±0.89	40.72±1.55	60.26±2.50	61.89±5.05	76.55±1.23	87.30±1.10	86.33±0.48
MLP	80.81±4.75	85.29±3.31	36.53±0.70	28.77±1.56	46.21±2.99	81.89±6.40	74.02±1.90	75.69±2.00	87.16±0.37

▶ New s.o.t.a. results on heterophilic and homophilic datasets.
▶ Diag models invert NSD* trend → Implicit performances speed-up.
▶ Stalk dimension has not big impact as it was for NSD.
▶ No Oversmoothing → PolySD mantains highest results when L increases.

*Cristian Bodnar, Francesco Di Giovanni, Benjamin Chamberlain, Pietro Lio, and Michael Bronstein. Neural sheaf diffusion: A topological perspective on heterophily and oversmoothing in gnns. *Advances in Neural Information Processing Systems*, 35:18527–18541, 2022.

PolySD VS NSD – #Layers Ablation

Layers	2	4	8	16	32	Best	PolySD Improvement
PubMed (h=0.80, $\#N = 18{,}707$, $\#E = 44{,}327$, $\#C = 3$)							
DiagChebySD: 88.18±0.40 (K=8), #params=48,665							
BundleChebySD: 87.91±0.32 (K=4), #params=49,621							
GeneralChebySD: 87.87±0.49 (K=8), #params=52,505							
Diag-NSD	87.82±0.55	**87.92±0.51**	87.92±0.52	65.92±20.39	39.49±1.60	4	**+0.26%**
#params	48,655	50,507	54,211	61,619	76,435	50,507	**-3,65% (-1,842)**
Bundle-NSD	87.70±0.56	87.85±0.42	**87.94±0.36**	87.63±0.47	37.03±4.72	8	**-0.03%**
#params	49,615	52,427	58,051	69,299	91,795	58,051	**-14,52%(-8,430)**
General-NSD	87.48±0.64	87.62±0.36	**87.72±0.68**	39.94±1.03	39.33±2.25	8	**+0.15%**
#params	52,495	58,187	69,571	92,339	137,875	69,571	**-24,53%(-17,066)**
Chameleon (h=0.23, $\#N = 2{,}277$, $\#E = 31{,}421$, $\#C = 5$)							
DiagChebySD: 70.57±1.32 (K=16), #params=194,835							
BundleChebySD: 66.64±2.35 (K=8), #params=195,787							
GeneralChebySD: 67.39±2.50 (K=16), #params=198,675							
Diag-NSD	**64.43±2.06**	61.27±5.14	57.34±6.10	22.92±1.42	22.89±2.59	2	**+6.15%**
#params	194,817	196,669	200,373	207,781	222,597	194,817	**+0.009%(+18)**
Bundle-NSD	47.10±10.14	**54.08±6.30**	50.57±3.53	24.91±2.87	23.05±2.46	4	**+12.56%**
#params	195,777	198,589	204,213	215,461	237,957	198,589	**-1,41%(-2,802)**
General-NSD	**59.60±4.53**	58.18±3.56	26.05±3.41	23.79±3.41	20.07±3.74	2	**+7.79%**
#params	198,657	204,349	215,733	238,501	284,037	198,657	**+0%(+0)**
Squirrel (h=0.22, $\#N = 5{,}201$, $\#E = 198{,}493$, $\#C = 5$)							
DiagChebySD: 47.72±1.20 (K=16), #params=174,675							
BundleChebySD: 44.48±3.22 (K=16), #params=176,913							
GeneralChebySD: 42.02±2.50 (K=6), #params=179,785							
Diag-NSD	41.98±1.17	**42.60±1.83**	42.05±1.54	20.80±1.33	OOM	4	**+5.12%**
#params	175,937	177,789	181,493	188,901	N/A	177,789	**-1,75%(-3,114)**
Bundle-NSD	**42.46±1.45**	42.30±1.83	37.99±2.61	22.86±3.03	OOM	2	**+2.02%**
#params	176,897	179,709	185,333	196,581	N/A	176,897	**+0.009%(+16)**
General-NSD	39.11±1.96	**39.96±1.76**	33.69±1.32	OOM	OOM	4	**+2.06%**
#params	179,777	185,469	196,853	N/A	N/A	185,469	**-3.06%(-5,684)**

▶ Pick best K for the three models and run #layers and #channels ablation.
▶ PolySD needs low K for homophilic and higher K for heterophilic datasets.
▶ Despite more layers and more hidden channels, PolySD performs better than NSD → Parameter Savings

N-Body System

Method	MSE
ESNN-Diag	0.0248
ESNN-DiagVel	0.0678
ESNN-ChebyDiag	0.0185
ESNN-ChebyDiagVel	0.0124
ESNN-Bundle	0.0238
ESNN-BundleVel	0.0226
ESNN-ChebyBundle	0.0275
ESNN-ChebyBundleVel	0.0268
ESNN-General	0.0190
ESNN-GeneralVel	0.0177
ESNN-ChebyGeneral	0.0216
ESNN-ChebyGeneralVel	0.0348
Linear	0.0819
SE(3) Transformer	0.0244
Tensor Field Network	0.0155
Graph Neural Network	0.0107
Radial Field	0.0104
EGNN	0.0071

QM9 Benchmark

Method	G	$\varepsilon_{\text{LUMO}}$
ESNN-Diag	6.91	29.89
ESNN-ChebyDiag	2.50	19.76
ESNN-Bundle	8.12	39.68
ESNN-ChebyBundle	4.04	25.65
ESNN-General	5.39	32.54
ESNN-ChebyGeneral	4.39	17.32
NMP	20	38
SchNet	19	34
Cormorant	21	38
L1Net	14	35
LieConv	19	25
DimeNet++*	6	20
TFN	–	38
SE(3)-Tr.	–	33
EGNN	12	25