Deep Learning on Topological Spaces

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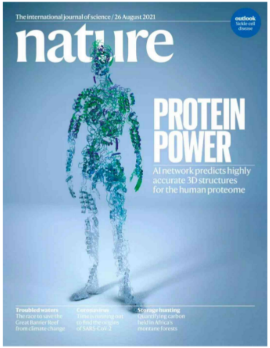
Based on works with F. Frasca, F. di Giovanni, Y.G. Wang, G. Montufar, N. Otter, B. Chamberlain, M. Bronstein, and P. Liò

Deep Exploration of non-Euclidean Data with Geometric and Topological Representation Learning
Kelowna, Canada
July 14, 2022

Geometric Deep Learning

Data often resides on structured domains: molecules, maps, social networks, . . .



Graph Machine Learning

Data is a graph G with n nodes and a node feature matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$.

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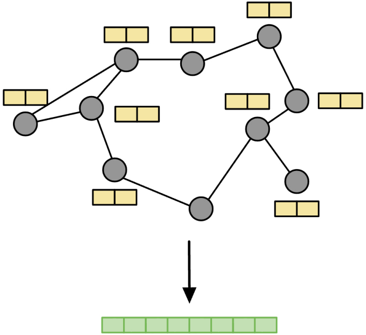
Graph-Level Tasks



e.g. predicting solubility of molecules

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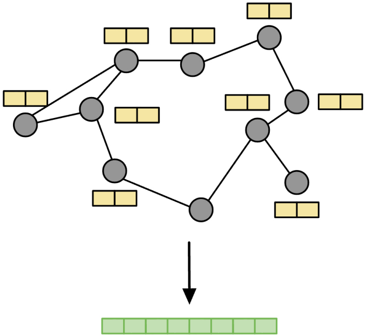

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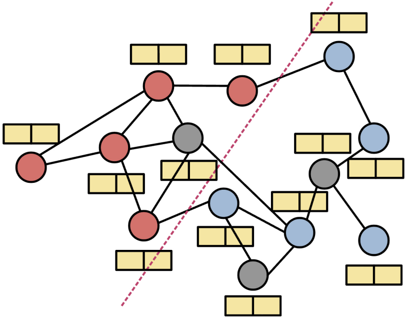
Node-level Tasks

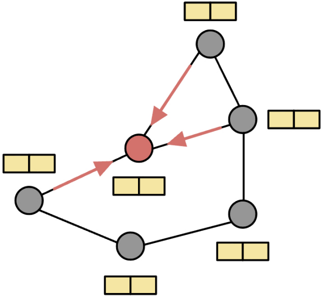


e.g. fraud detection

Message Passing Neural Networks

Most Graph Neural Networks (GNNs) can be understood as message passing:

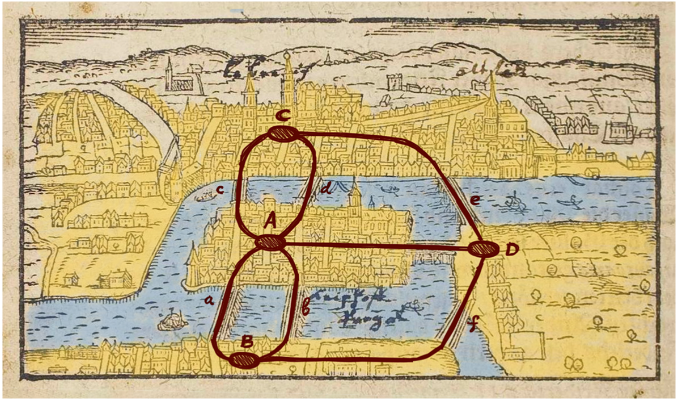
$$m_v^k := \mathrm{AGGREGATE}\left(\left\{h_u^{k-1} \mid u \in \mathcal{N}(v)\right\}\right) \qquad h_v^k := \mathrm{COMBINE}\left(h_v^{k-1}, m_v^k\right)$$



How to design AGGREGATE and COMBINE is a very active area of research.

Graphs and Topology

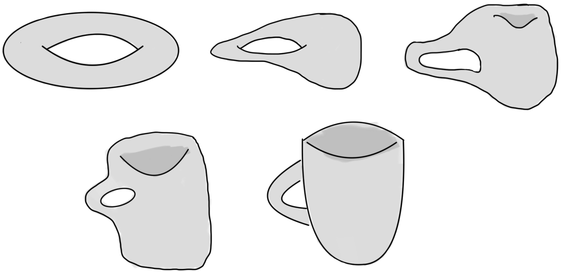
Graph Theory and Topology share a common history: Leonard Euler's paper *geometria situs* ("geometry of location")



Source: Wikipedia

So what is Topology?

It's a branch of mathematics studying objects under continuous deformations. To a topologist, a mug and a donut are the same.



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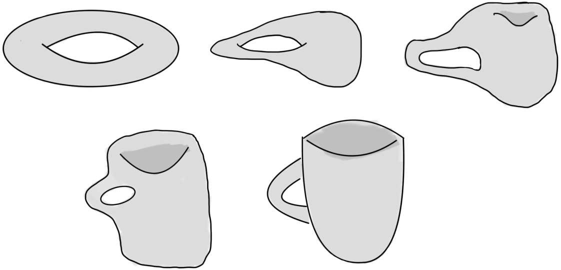
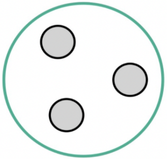


"Topology! The stratosphere of human thought! In the twenty-fourth century, it might possibly be of use to someone." — Aleksandr Solzhenitsyn, In the First Circle (1968)

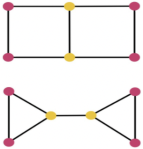
Topological Message Passing

Some problems with graph message passing

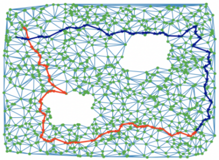
Groupwise interactions



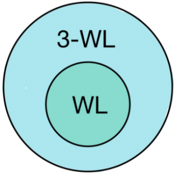
Higher-order structures



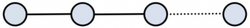
Higher-order signals



Expressive power

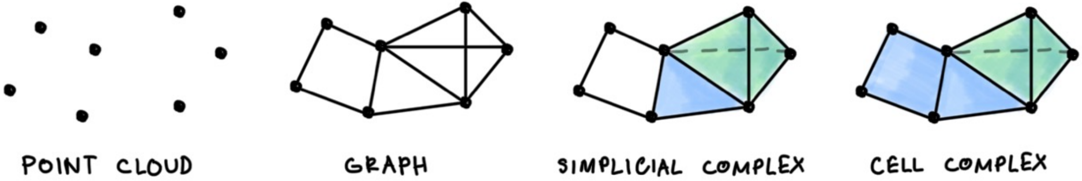


Long-range interactions



Beyond graphs

Graphs are just a type of topological space with combinatorial structure.



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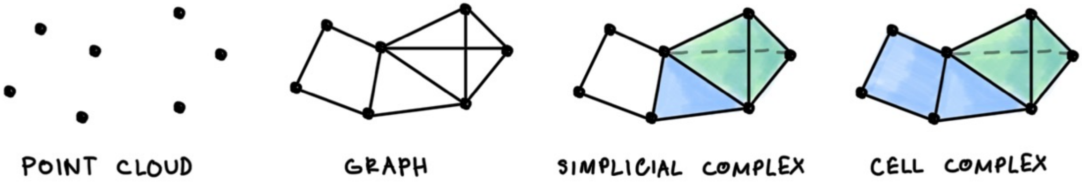
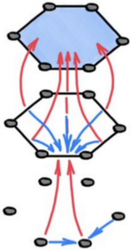


In this terminology, vertices are 0-cells, edges are 1-cells, 2D surfaces are 2-cells...

Message Passing on Cell Complexes

We can generalise message passing on graphs to cell complexes. We call this *topological message passing*.



Constructing cell complexes

But how do we obtain a cell complex?

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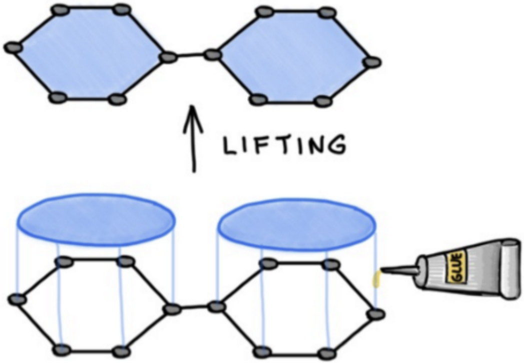
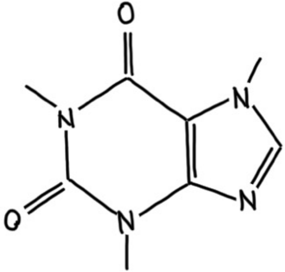
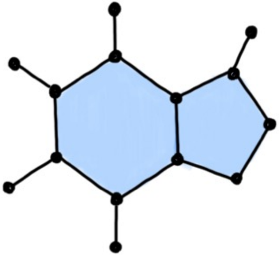


Domain alignment

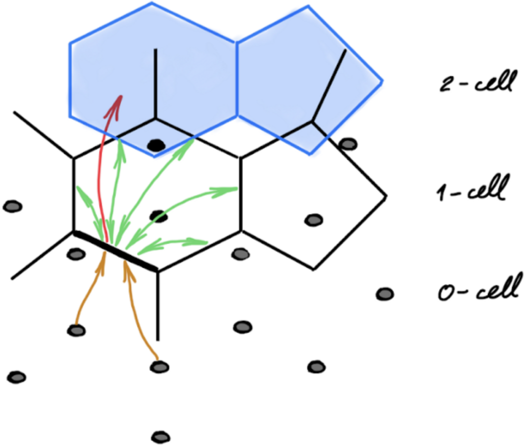
This type of space aligns well with certain applications.





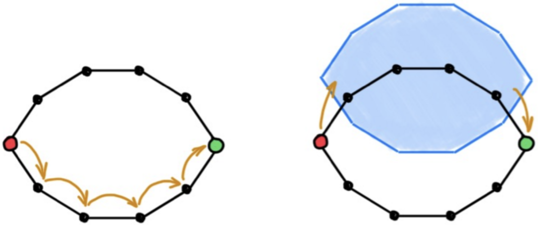
Hierarhical

The message passing becomes hierarchical.



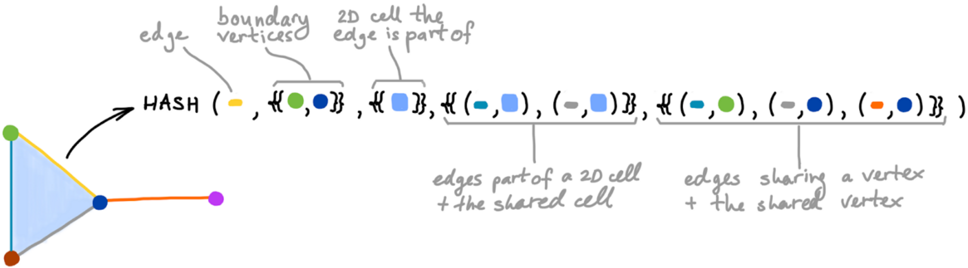
Long-range communication

Fewer layers are needed for long-range communication.



Expressivity

Topological Message Passing can distinguish more pairs of non-isomorphic graphs than message passing GNNs. This can be proven using a cellular version of the Weisfeiler-Lehman Test.



Results

Topological Message Passing can be applied to molecular property prediction.

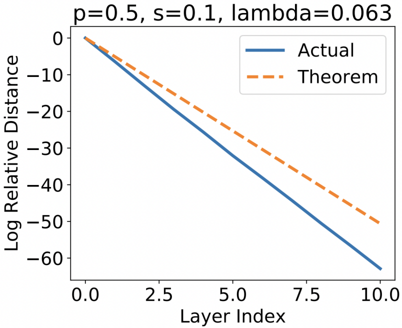
Table 3: ZINC (MAE), ZINC-FULL (MAE) and Mol-HIV (ROC-AUC).

Method	ZINC ↓ No Edge Feat.	ZINC ↓ With Edge Feat.	ZINC-FULL ↓ All methods	MOLHIV ↑ All methods
GCN [45]	0.469±0.002	N/A	N/A	76.06±0.97
GAT [67]	0.463±0.002	N/A	N/A	N/A
GatedGCN [10]	0.422±0.006	0.363±0.009	N/A	N/A
GIN [72]	0.408±0.008	0.252±0.014	0.088±0.002	77.07±1.49
PNA [19]	0.320±0.032	0.188±0.004	N/A	79.05±1.32
DGN [5]	0.219±0.010	0.168±0.003	N/A	79.70±0.97
HIMP [26]	N/A	0.151±0.006	0.036±0.002	78.80±0.82
GSN [9]	0.139±0.007	0.108±0.018	N/A	77.99±1.00
CIN-small (Ours)	0.139±0.008	0.094±0.004	0.044±0.003	80.55±1.04
CIN (Ours)	**0.115±0.003**	**0.079±0.006**	**0.022±0.002**	**80.94±0.57**

Neural Sheaf Diffusion

The Oversmoothing Problem

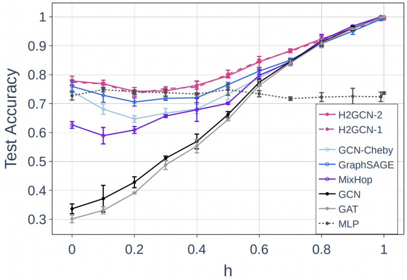
In some GNNs [Oono & Suzuki, 2020] features become progressively smoother with increased depth.



With more layers, GCN approaches a "smooth" subspace where all the node features are constant [Oono & Suzuki, 2020].

The Heterophily Problem

Numerous studies (e.g. [J. Zhu et al., 2020]) remarked that GNNs struggle in heterophilic settings (i.e. graphs where a node tends to be connected to nodes belonging to other classes).



The performance of GNNs is strongly correlated to the homophily level of a graph [J. Zhu et al., 2020].

From Heat Diffusion to Graph Convolutions

Let G be a graph with self loops, degree matrix $\mathbf{D}$, adjacency matrix $\mathbf{A}$, normalised Laplacian $\Delta_0 := I - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$, and node features $\mathbf{X} \in \mathbb{R}^{n \times d}$.

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This is strikingly similar to GCN [Kipf & Welling, 2017]:

$$\mathrm{GCN}(\mathbf{X}, \mathbf{A}) := \sigma\left(\mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}\mathbf{X}\mathbf{W}\right)$$

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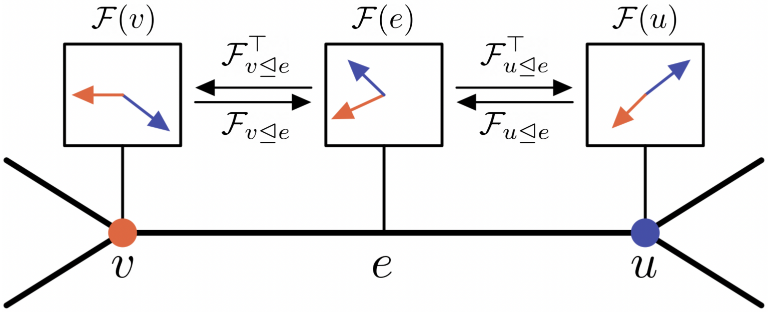
Question

How can we make the base diffusion process more powerful?

Cellular Sheaves

Cellular sheaves [Curry, 2014] are mathematical objects that attach some additional geometric structure to a graph.



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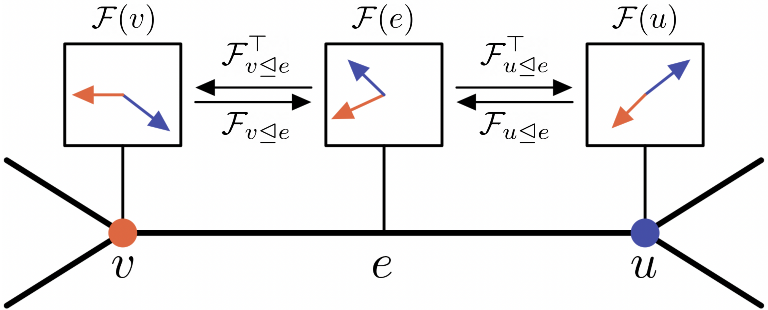
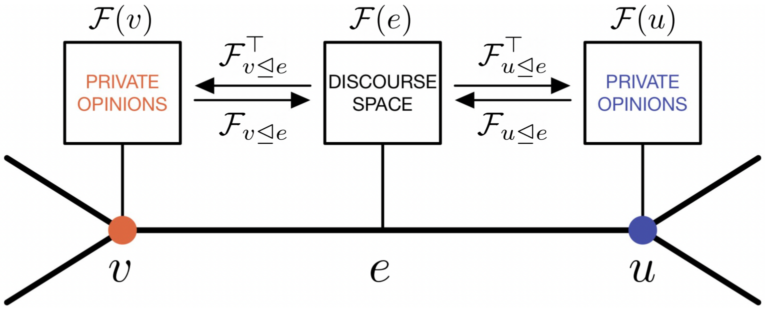


Sheaves were invented by the French mathematician Jean Leray during WWII.

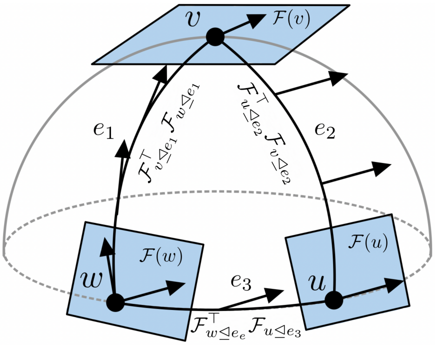
Opinion Dynamics

Opinion dynamics [Hansen & Ghrist, 2020] provides a nice mental picture of cellular sheaves.



Discrete Vector Bundles

The sheaves with orthogonal restriction maps are *discrete $O(d)$-bundles*.



Analogy between parallel transport on a sphere and transport on a discrete vector bundle. A tangent vector is moved from $\mathcal{F}(w) \to \mathcal{F}(v) \to \mathcal{F}(u)$ and back.

Expressive Power of Sheaf Diffusion

We are analysing the expressive power of the following *sheaf diffusion* PDE:

$$\mathbf{X}(0) = \mathbf{X}, \quad \dot{\mathbf{X}}(t) = -\Delta_{\mathcal{F}}\mathbf{X}(t)$$

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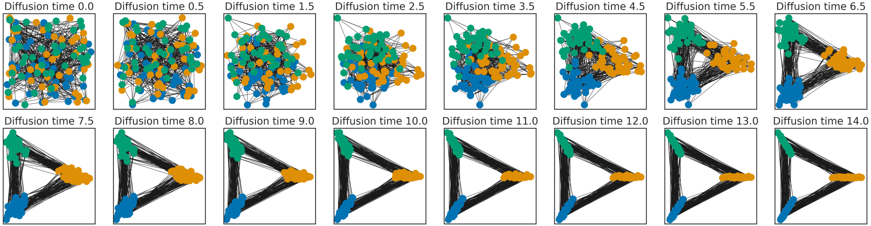

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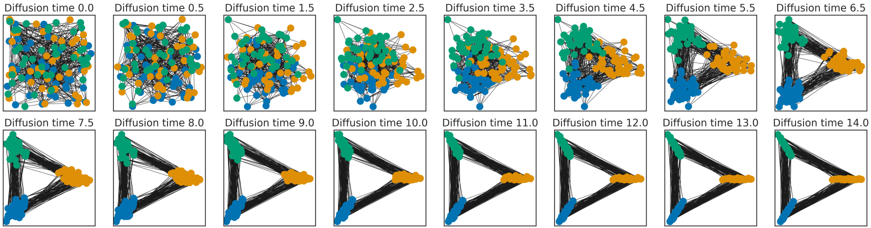


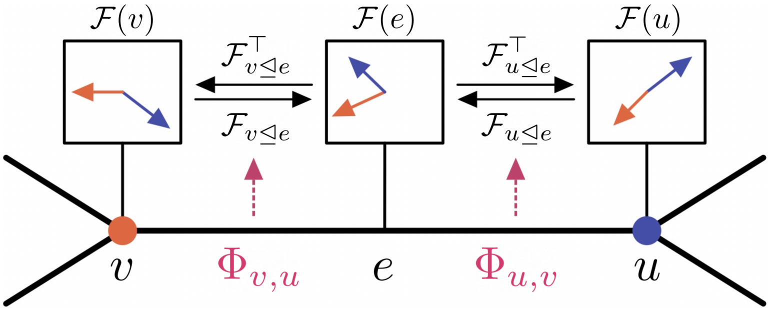
Theorem (Informal)

For any node classification task on a connected graph, there exists a sheaf that can linearly separate the classes by performing diffusion infinitely long.

Learning sheaves

Each $d \times d$ matrix $\mathcal{F}_{v \trianglelefteq e}$ is learned via a parametric function $\Phi : \mathbb{R}^{d \times 2} \to \mathbb{R}^{d \times d}$:

$$\mathcal{F}_{v \trianglelefteq e := (v,u)} = \Phi(\mathbf{x}_v, \mathbf{x}_u) \tag{3}$$



The restriction maps are learned from data.

Real-World Evaluation

We evaluate on multiple node-classifications tasks with various degrees of homophily [Rozemberczki et al, 2019, Pei et al, 2019].

	Texas	Wisconsin	Film	Squirrel	Chameleon	Cornell	Citeseer	Pubmed	Cora
Hom 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
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	43.80±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

References

Cristian Bodnar*, Fabrizio Frasca*, Yu Guang Wang*, Nina Otter, Guido Montúfar*, Pietro Liò and Michael Bronstein (2021)
Weisfeiler and Lehman Go Topological: Message Passing Simplicial Networks
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Thank you for your attention!

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