

Table 1: Comparison of training, inference times in (ms) and test accuracies on Arxiv and Proteins datasets of MPGNNs+SSMA against PNA and GPS. Golden line indicates SSMA augmented architecture. * indicates random neighbor selection while † indicates attentional neighbor selection.

Method	Train	Inference	Arxiv	Proteins
GIN*	2.768	0.988	64.217	73.921
GCN*	5.286	1.322	64.834	74.308
GAT*	5.996	1.453	64.902	75.197
PNA	6.068	1.218	59.1	74.86
GPS	7.178	1.362	63.87	73.76
GIN†	8.072	1.504	65.835	72.94
GCN†	8.347	1.666	65.368	73.132
GAT†	9.236	1.888	64.108	72.677

Table 2: Effects of positional encoding (PE) and scale on SSMA. We check how do PE and scale affect the effectiveness of SSMA augmented architectures on ZINC regression. Golden line indicates SSMA augmented architectures. We report the test MAE below.

Method/Params.	100k	500k
GPS	0.128	0.131
GPS	0.1186	0.1294
GPS+PE	0.0814	0.0785
GPS+PE	0.0778	0.0747
GIN	0.252	0.256
GIN	0.222	0.2265
GCN	0.347	0.3103
GCN	0.280	0.2768

Table 3: Accuracies (%) of SSMA augmented version of DiffPool on some of the TU datasets.

	MUTAG	IMDB-B	Proteins
Baseline	81.84	72.36	74.29
SSMA augmented	83.01	74.73	76.14

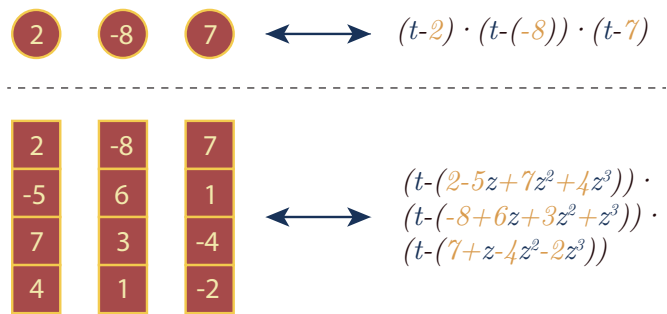


Figure 1: Illustrating the generalized DeepSets polynomial (lower) by comparing it to the original DeepSets polynomial (upper).

Table 4: Results for TU datasets & ZINC using the f-Mean aggregation as a baseline. † reproduced results. Golden line indicates SSMA augmented architectures.

Module	ENZ	PTC	MUT	PRO	IMDB	ZINC
GCN†	44.33	58.61	84.15	72.13	69.00	0.29
GCN	54.83	62.29	89.79	76.28	75.2	0.280
GAT†	50.17	59.16	83.25	73.75	68.10	0.39
GAT	56.67	66.41	89.19	80.18	74.5	0.223
GATv2†	51.67	57.43	77.05	70.96	71.8	0.26
GATv2	52.50	61.64	88.80	75.28	72.8	0.235
GIN†	15.33	57.06	70.94	68.26	57.6	0.27
GIN	51.69	61.28	90.51	75.19	74.1	0.222
GPS†	20.33	59.26	55.73	44.85	53.5	0.25
GPS	49.17	63.02	86.07	75.56	71.1	0.22

Table 5: Results for TU datasets & ZINC using the LSTM aggregation as a baseline. † indicates reproduced results. Golden line indicates SSMA augmented architectures.

Module	ENZ	PTC	MUT	PRO	IMDB	ZINC
GCN†	37.5	58.79	78.85	66.58	54.2	0.32
GCN	54.83	62.29	89.79	76.28	75.2	0.280
GAT†	32.83	61.35	74.27	64.32	48.80	0.31
GAT	56.67	66.41	89.19	80.18	74.5	0.223
GATv2†	34.33	57.06	73.16	65.07	54.90	0.30
GATv2	52.50	61.64	88.80	75.28	72.8	0.235
GIN†	37.83	58.41	78.72	71.07	50.70	0.25
GIN	51.69	61.28	90.51	75.19	74.1	0.222
GPS†	29.17	58.17	73.38	63.03	49.90	0.32
GPS	49.17	63.02	86.07	75.56	71.1	0.22