

Equivariant Random GNN

Table 1. New results on ZINC and ZINC-Full Datasets. Baselines results are directly from their original papers. We improves our ENGNN performance by training more epoches (1000) following previous work. Our model ENGNN outperforms all baselines include subgraph GNNs GNN-AK+,ESAN, SUN, SSWL, DRFWL, CIN, and NGNN

	zinc MAE↓	zinc-full MAE↓
GIN	0.163 \pm 0.004	0.088 \pm 0.002
GNN-AK+	0.080 \pm 0.001	—
ESAN	0.102 \pm 0.003	0.029 \pm 0.003
SUN	0.083 \pm 0.003	0.024 \pm 0.003
SSWL	0.083 \pm 0.003	0.022 \pm 0.002
DRFWL	0.077 \pm 0.002	0.025 \pm 0.003
CIN	0.079 \pm 0.006	0.022 \pm 0.002
NGNN	0.111 \pm 0.003	0.029 \pm 0.001
ENGNN	0.068 \pm 0.003	0.021 \pm 0.003

Table 2. Ablation study on ZINC-Full datasets. C=1, C=16, C=64 meaning that we use the tuned hyperparameters except setting number of noise channels to 1, 16, 64. layer=2, layer=3 means using mlp layer in deepset to 2(default) and 3 for ablation.

model	C=1	C=16	C=64	layer=2	layer=3
MAE	0.027 \pm 0.004	0.021 \pm 0.003	0.024 \pm 0.003	0.021 \pm 0.003	0.025 \pm 0.003

Table 3. Apply Equivariant Layer to GPS Graph Transformer on ZINC dataset. By replacing the message passing layer in GPS with our equivariant noise layer and use the original hyperparameters, we achieve good performance on ZINC.

model	GPS	GPS-ENGNN
MAE	0.070 \pm 0.003	0.071 \pm 0.004

Table 4. Comparison between ENGNN and GNN-RNI (Abboud et.al.) on EXP dataset. Baseline results are directly from GNN-RNI origin paper. We keep the same hidden dimension and training epochs.

Model	GCN-RNI	PPGN	1-2-3-GCN-L	3-GCN	ENGNN
Acc (%)	98.0 \pm 1.85	50.0	50.0	99.7 \pm 0.00	100.0 \pm 0.00

Table 5. Comparison between ENGNN and rGIN (Sato et.al.) on rGIN’s dataset. Baseline results are directly from the origin paper. We keep the same hidden dimension and training epochs. Results are all in roc-auc score \uparrow .

dataset	TRI(N)	TRI(X)	LCC(N)	LCC(X)	MDS(N)	MDS(X)	MUTAG	NCII	PROTEINS
GINs	0.500	0.500	0.500	0.500	0.500	0.500	0.946 \pm 0.034	0.870 \pm 0.009	0.806 \pm 0.029
rGINs	0.908	0.926	0.811	0.852	0.807	0.810	0.949 \pm 0.040	0.876 \pm 0.010	0.810 \pm 0.020
ENMPNN	1.000	1.000	1.000	1.000	0.936 \pm 0.030	0.934 \pm 0.04	0.956 \pm 0.054	0.922 \pm 0.022	0.814 \pm 0.023

Table 6. Results on node classification datasets: Mean accuracy (%) \pm standard variation.

DATASETS	GIN	GAT	GCN	APPNP	CHEBYNET	GPRGNN	BERNNET	ENGNN	MPNN	NMPNN
CORA	86.58 \pm 0.97	88.03 \pm 0.79	87.14 \pm 1.01	88.14 \pm 0.73	86.67 \pm 0.82	88.57 \pm 0.69	88.52 \pm 0.95	88.85\pm0.96	87.36 \pm 0.52	20.11 \pm 2.01
CITESEER	77.11 \pm 0.76	80.52 \pm 0.71	79.86 \pm 0.67	80.47\pm0.74	79.11 \pm 0.75	80.12 \pm 0.83	80.09 \pm 0.79	79.97 \pm 0.79	79.62 \pm 0.75	20.80 \pm 2.63
PUBMED	86.93 \pm 0.26	87.04 \pm 0.24	86.74 \pm 0.27	88.12 \pm 0.31	87.95 \pm 0.28	88.46 \pm 0.33	88.48 \pm 0.41	89.79\pm0.64	89.53 \pm 0.29	69.28 \pm 3.14
COMPUTERS	58.87 \pm 7.55	83.23 \pm 0.39	83.32 \pm 0.33	85.32 \pm 0.37	87.54 \pm 0.43	86.85 \pm 0.25	87.64 \pm 0.44	90.48\pm0.31	89.53 \pm 0.83	66.42 \pm 1.39
PHOTO	87.13 \pm 4.52	90.94 \pm 0.68	88.26 \pm 0.73	88.51 \pm 0.31	93.77 \pm 0.32	93.85 \pm 0.28	93.63 \pm 0.35	95.24\pm0.58	94.74 \pm 0.25	65.12 \pm 1.95
CHAMELEON	66.87 \pm 2.72	63.13 \pm 1.93	59.61 \pm 2.21	51.84 \pm 1.82	59.28 \pm 1.25	67.28 \pm 1.09	68.29 \pm 1.58	71.40\pm1.29	67.18 \pm 1.07	41.25 \pm 1.38
ACTOR	36.66 \pm 7.53	33.93 \pm 2.47	33.23 \pm 1.16	39.66 \pm 0.55	37.61 \pm 0.89	39.92 \pm 0.67	41.79\pm1.01	40.64 \pm 0.67	40.41 \pm 1.53	23.73 \pm 2.36
SQUIRREL	40.53 \pm 1.16	44.49 \pm 0.88	46.78 \pm 0.87	34.71 \pm 0.57	40.55 \pm 0.42	50.15 \pm 1.92	51.35 \pm 0.73	52.77\pm1.43	51.99 \pm 1.78	38.25 \pm 1.04