Figure 1. SGT on ZINC: Test MAE v.s. Batch Size (BS). # Training epochs are adjusted per batch-size for the same total update steps: $400 * BS/32$. The first 10% epochs are in the warmup stage.
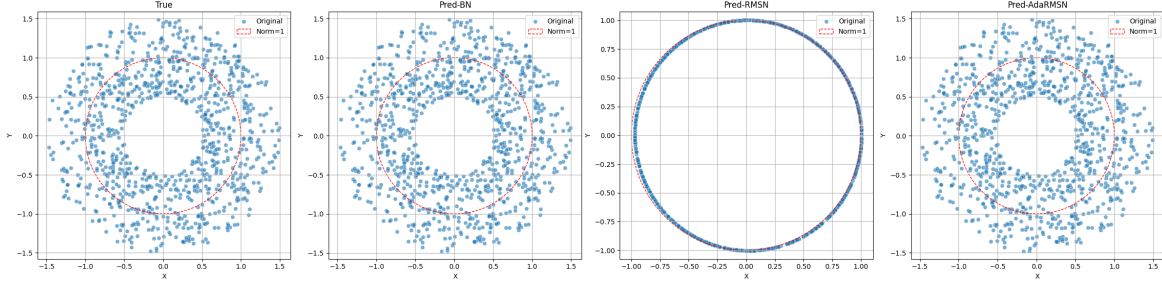

Figure 2. (Case Study of AdaRSMN) Visualization of Input and Pred data points. Ovefitting test on Auto-encoders of 2-dim (*Linear* $\to$ *BN/RMSN/AdaRMSN* $\to$ *Linear*): each model is trained 5000 epochs via AdamW without regularization. (together with Figure. 3)

Table 1. Performance on ZINC. GPS+sL_2: integrating sL_2 attention into GPS without changing other parts. (run 3 trials)

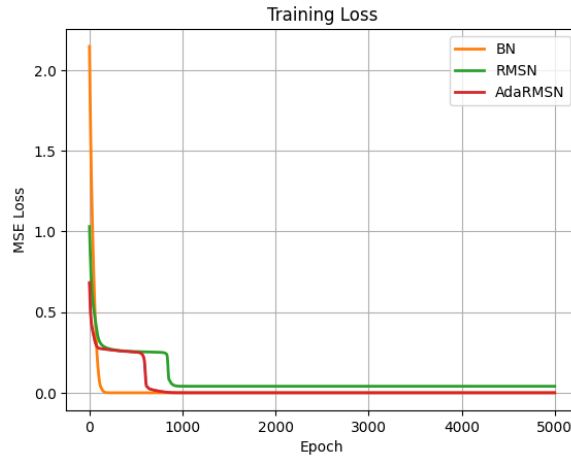| ZINC	GPS	GPS+sL_2	SGT
MAE ($\downarrow$)	0.070 ± 0.004	0.0693 ± 0.0023	0.0566 ± 0.002

Figure 3. (Case Study of AdaRSMN) Training curves of overfitting test. (together with Figure. 2)

2

Table 2. Comparison of peak GPU memory usage and per-epoch training time for GRIT and SGT. Dataset: Peptides-Structure (15K graphs); Model config.: 5 transformer layers, 96 channels, batch size 32. Hardware: a single Nvidia V100 GPU with 32GB memory, supported by 80 Intel Xeon Gold 6140 CPUs running at 2.30GHz

Model	GPU Memory (GB)	Training Time (Sec/Epoch)
GRIT	29.16	141.60
SGT	25.07	100.68
Improv.	~14.03%	~28.9%

Table 3. Performance on PCMQM4Mv2 (over 3.7M graphs). The eval. pipeline follows Rampášek et al. (2022); no 3D-info included.

PCMQM4Mv2	Val MAE ($\downarrow$)	# Param.
Graphormer	0.0864	48.3M
GPS	0.0858	19.4M
GRIT	0.0859	16.6M
SGT	0.0856	17.6M

Table 4. Performance comparison across different models on various datasets. Best results are highlighted in bold. * indicates the difference to the best is not statistically significant (by two-tail T-test)

| Model	ZINC MAE ($\downarrow$)	SP-CIFAR Acc. ($\uparrow$)	SP-MNIST Acc. ($\uparrow$)	PATTERN W.Acc. ($\uparrow$)	CLUSTER W.Acc. ($\uparrow$)	Peptides-Struct MAE ($\downarrow$)	Peptides-Func AP ($\uparrow$)
Exphormer	-	74.69±0.125	98.55±0.037	86.74±0.015	78.07±0.037	0.2481±0.0007	0.6527±0.0043
GEAET	-	76.634±0.427	98.513±0.086	86.993±0.026	-	**0.2445±0.0013**	-
GEANet	0.193±0.001	73.857±0.306	98.315±0.097	85.607±0.038	77.013±0.224	0.2512±0.0003	0.6722±0.0065
SGT	**0.0566±0.002**	**78.560±0.700**	**98.614±0.096**	**89.752±0.030**	**80.027±0.114**	0.2450±0.0017*	**0.6961±0.0062**
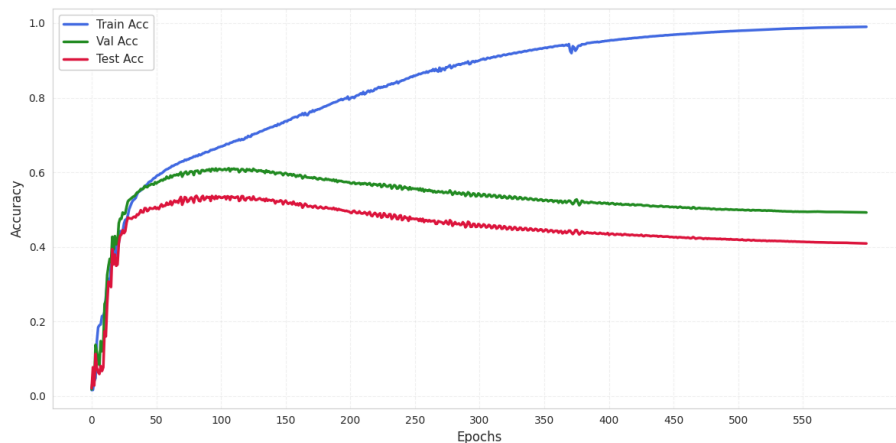
Figure 4. Sanity check of Exp-SGT on a large-scale graph in OGBN-ArXiv (169,343 nodes). Use the same configuration as Exphormer and remove all regularizations to validate the trainability via an overfitting test.