

---

# Graph Self-supervised Learning via Proximity Distribution Minimization (Supplementary Material)

---

Tianyi Zhang<sup>1</sup>

Zhenwei Dai<sup>2</sup>

Zhaozhuo Xu<sup>1</sup>

Anshumali Shrivastava<sup>1</sup>

<sup>1</sup>Department of Computer Science, Rice University, Houston, Texas, USA

<sup>2</sup>Amazon, Palo Alto, California, USA

## A TEST ACCURACY, TRAINING TIME, AND TRAINING DETAILS

The test accuracy of PDM with different proximity measures are presented in Table 1. The training time comparison of PDM with DGI Velickovic et al. [2019] is presented in Table 2. The training details and hyperparameters are shown in Table 3.

Table 1: Test accuracy of PDM with different proximity measures

	Cora	Citeseer	PubMed
PDM (heat kernel)	84.4	74.3	83.6
PDM (PPR)	84.1	74.6	83.8
PDM (SimRank)	82.2	74.6	82.3

Table 2: Training Time Comparison between DGI and PDM

	Cora			Citeseer		
	Total Training Time (ms)	Time Per Epoch (ms)	Test Accuracy	Total Training Time (ms)	Time Per Epoch (ms)	Test Accuracy
DGI	2980	14.9	82.3	4060	20.3	71.8
PDM	7340	36.7	84.4	10180	50.9	74.6

Table 3: Training details and hyper-parameters for PDM on all datasets

	Cora	Citeseer	PubMed	ogbn-arxiv	ogbn-proteins	ogbn-products
Architecture	GCN	GCN	GCN	GCN	GCN	GCN
Depth	1	1	2	3	3	3
Hidden Size	2048	2048	32	2048	2048	1024
Activation	Leaky ReLU	tanh	tanh	Leaky ReLU	Leaky ReLU	tanh
Learning Rate	5e-3	5e-4	1e-2	1e-4	1e-4	1e-4
Diffusion Type	Heat	Heat	PPR	PPR	PPR	PPR
Epochs	100	100	100	100	200	10
Optimizer	AdamW [Loshchilov and Hutter, 2019]					

## B COMPARISON WITH AUGMENTATION-FREE METHODS

We compare the performance of PDM with the augmentation-free method AFGRL [Lee et al., 2022], and the results are shown in Table 4. For AFGRL, we consider the best test accuracy for number of neighbors  $k \in \{4, 8, 16\}$ . PDM offers significant improvements over AFGRL, up to 5.1% on citeseer.

Table 4: Test Accuracy of AFGRL and PDM

	Cora	Citeseer	PubMed
AFGRL	81.1	69.5	79.2
PDM	84.4	74.6	83.8

### References

- Namkyeong Lee, Junseok Lee, and Chanyoung Park. Augmentation-free self-supervised learning on graphs. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 36, pages 7372–7380, 2022.
- Ilya Loshchilov and Frank Hutter. Decoupled weight decay regularization. In *International Conference on Learning Representations*, 2019. URL <https://openreview.net/forum?id=Bkg6RiCqY7>.
- Petar Velickovic, William Fedus, William L Hamilton, Pietro Liò, Yoshua Bengio, and R Devon Hjelm. Deep graph infomax. *ICLR (Poster)*, 2(3):4, 2019.