

Figure 1: Illustration of the graph-signal cut distance. Left: a stochastic block model (SBM) with a signal. The color of the block represents the value of the signal at this block. The thickness of the edges between the blocks (including self-loops) represents the probability/density of edges between the blocks. Middle: a small graph-signal which looks like was sampled from the SMB. The color of the nodes represent the signal values. Right: a large graph-signal which looks like was sampled from the SMB. In graphon-signal cut distance, these two graph-signals are close to each other.

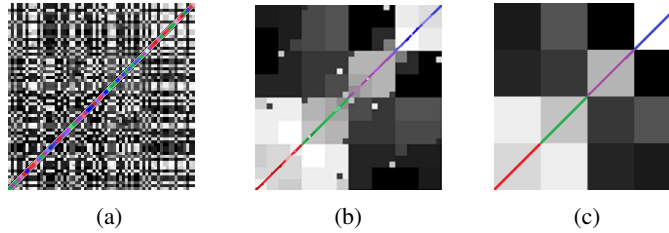


Figure 2: Illustration of the graphon-signal regularity lemma. The values of the graphon are in gray scale over $[0, 1]^2$, and the signal is plotted in color on the diagonal of $[0, 1]^2$. (a) A graphon-signal. (b) Representation of the same graphon-signal under the “good” permutation/measure preserving bijection guaranteed by the regularity lemma. (c) The approximating step graphon-signal guaranteed by the regularity lemma.

Table 1: Comparison of the assumptions made by different GNN generalization analysis papers.

Generalization analysis paper	Assumption on the graphs	No weight sharing	General MPL	Dependency on N
Generalization Limits of GNNs [13]	bounded degree	✗	✗	$N^{-1/2}$
PAC-bayesian MPNN [22]	bounded degree	✗	✗	$N^{-1/2}$
PAC-bayesian GCN [22]	bounded degree	✓	✗	$N^{-1/2}$
VC meets IWL [29]	bounded color complexity	✓	✗	$N^{-1/2}$
Generalization Analysis of MPNNs [25]	sampled from a small set of graphons	✓	✓	$N^{-1/2}$
Our graphon-signal theory	non	✓	✓	$\xi^{-1}(N)$

Table 2: Standard MPNN architectures with normalized sum aggregation (nsa) and mean aggregation (ma), 3-layers with 512-hidden-dimension, and global mean pooling, denoted by “MPNN-nsa” and “MPNN-ma.” We use the MPNNs GIN [34] and GraphConv [28], and report the mean accuracy \pm std over ten data splits. Nsa has good generalization and better performance than ma.

Accuracy \uparrow	MUTAG	IMDB-BINARY	IMDB-MULTI	NCII	PROTEINS	REDDIT-BINARY
GIN-nsa (train)	83.94 \pm 3.25	70.54 \pm 0.79	47.01 \pm 0.8	83.12 \pm 0.59	74.06 \pm 0.44	90.43 \pm 0.53
GIN-nsa (test)	79.36 \pm 2.93	69.83 \pm 0.93	46.01 \pm 1.01	78.55 \pm 0.3	73.11 \pm 0.81	89.38 \pm 0.57
GIN-ma (trained)	74.63 \pm 2.93	49.48 \pm 1.56	33.70 \pm 1.35	73.74 \pm 0.45	71.53 \pm 0.93	50.04 \pm 0.70
GIN-ma (untrained)	72.46 \pm 2.56	49.18 \pm 1.83	33.03 \pm 1.12	77.16 \pm 0.39	70.33 \pm 0.95	49.90 \pm 0.83
GraphConv-nsa (train)	82.48 \pm 0.99	59.34 \pm 2.34	40.53 \pm 1.85	63.14 \pm 0.55	71.07 \pm 0.5	82.4 \pm 0.19
GraphConv-nsa (test)	82.04 \pm 1.05	59.03 \pm 2.77	40.25 \pm 1.59	63.16 \pm 0.32	70.92 \pm 0.7	82.38 \pm 0.26
GraphConv-ma (trained)	65.87 \pm 3.24	49.32 \pm 1.35	33.15 \pm 1.19	54.39 \pm 1.25	66.76 \pm 0.96	49.68 \pm 0.82
GraphConv-ma (untrained)	63.30 \pm 3.55	48.80 \pm 1.91	32.51 \pm 0.90	55.84 \pm 0.53	70.73 \pm 0.69	49.39 \pm 0.48