東京工業大学
Tokyo Institute of Technology

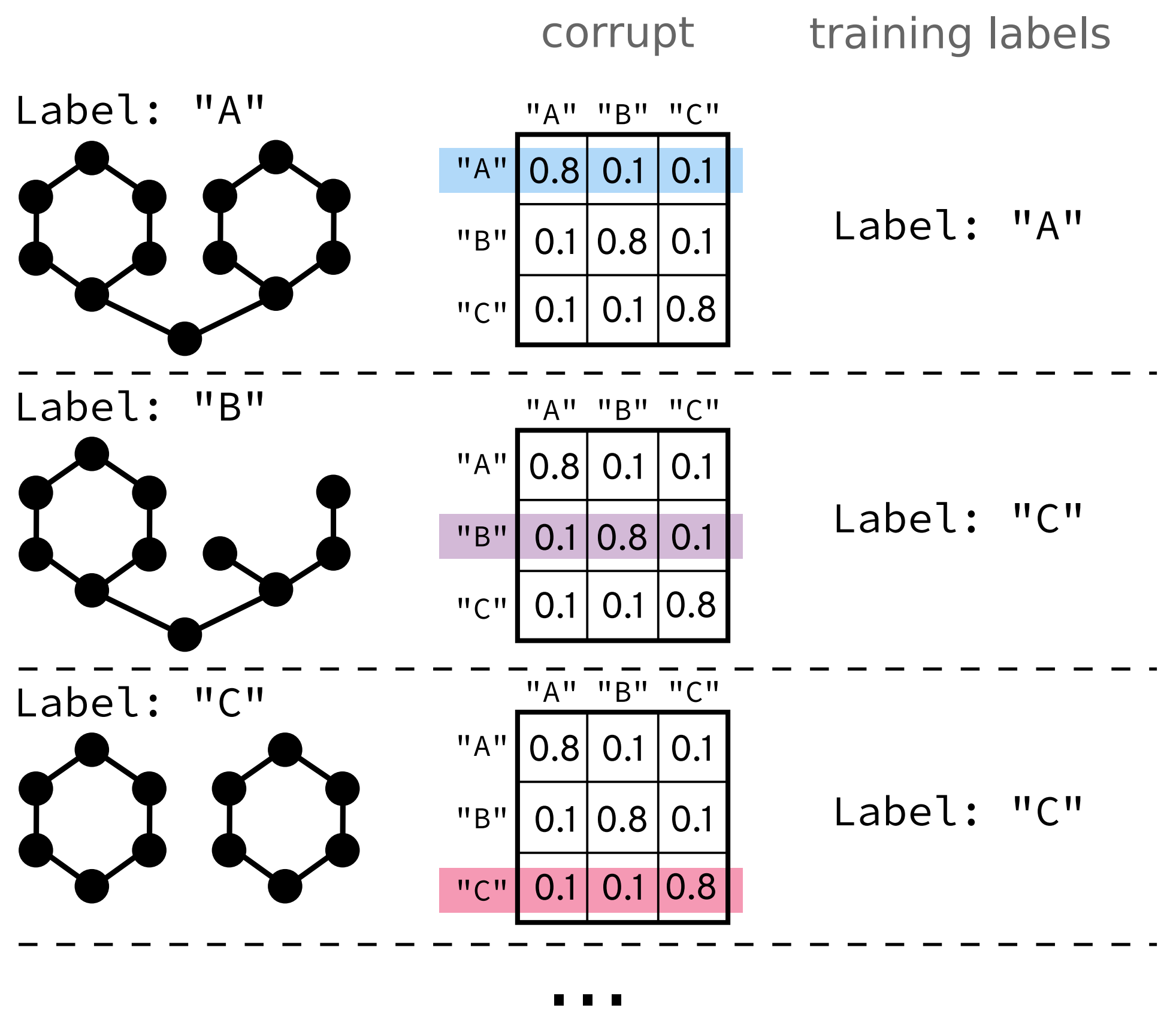
Learning GNNs with Noisy Labels

Hoang NT, Jun Jin Choong, Tsuyoshi Murata
Tokyo Institute of Technology

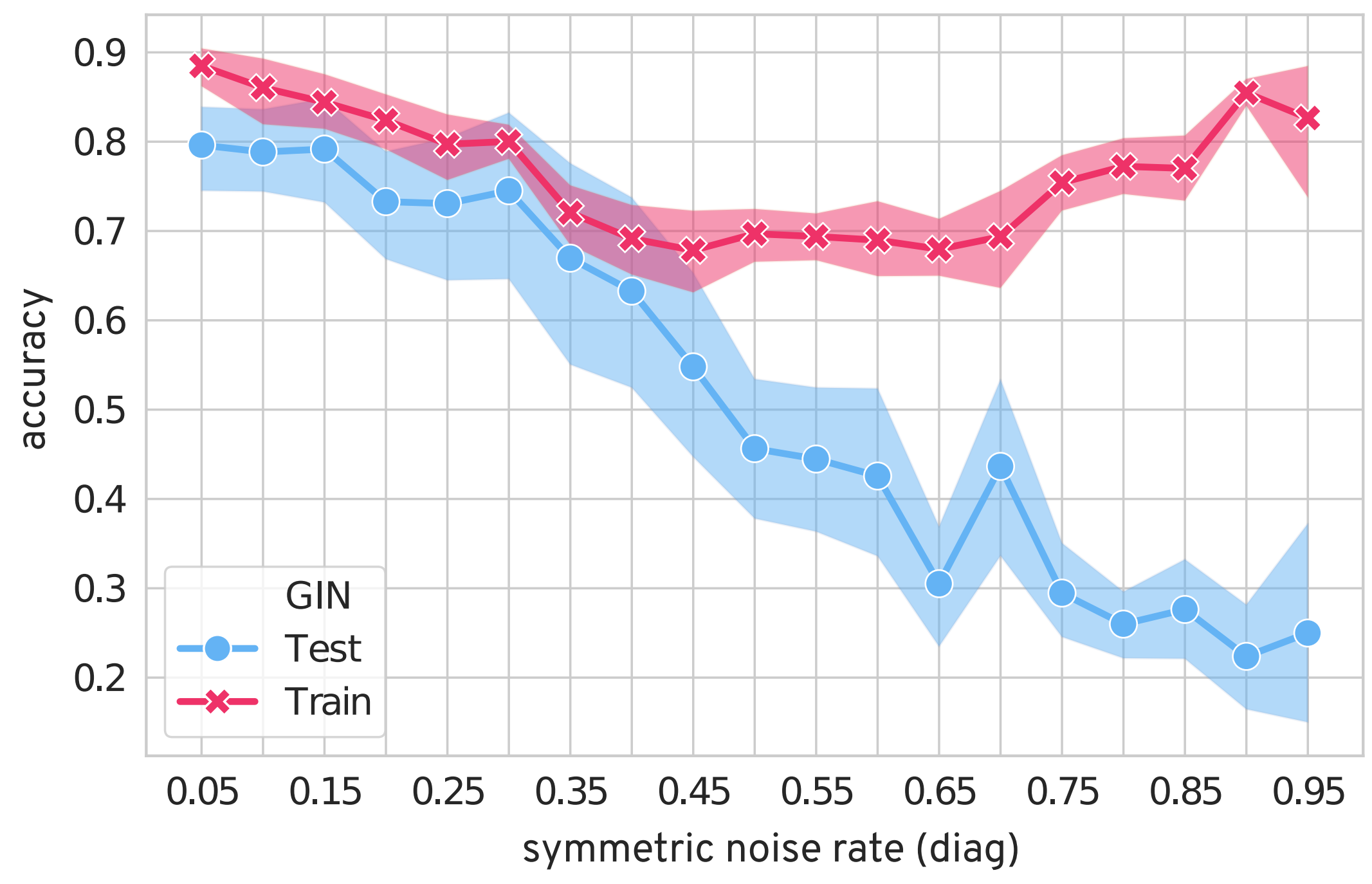
LEARNING WITH LIMITED LABELED DATA
ICLR 2019 New Orleans, USA

Introduction

We study the robustness to symmetric label noise of GNNs training procedures. By combining the nonlinear neural message-passing models (e.g. Graph Isomorphism Networks, GraphSAGE, etc.) with loss correction methods, we present a noise-tolerant approach for the graph classification task. Our experiments show that test accuracy can be improved under the artificial symmetric noisy setting.



MUTAG GENERALIZATION UNDER FOR NOISY LABELS



Graph Classification Model

We use a nonlinear message passing model similar to *GIN* [2] and *GraphSAGE* [3]. In the supervised learning setting, such model has two main steps:

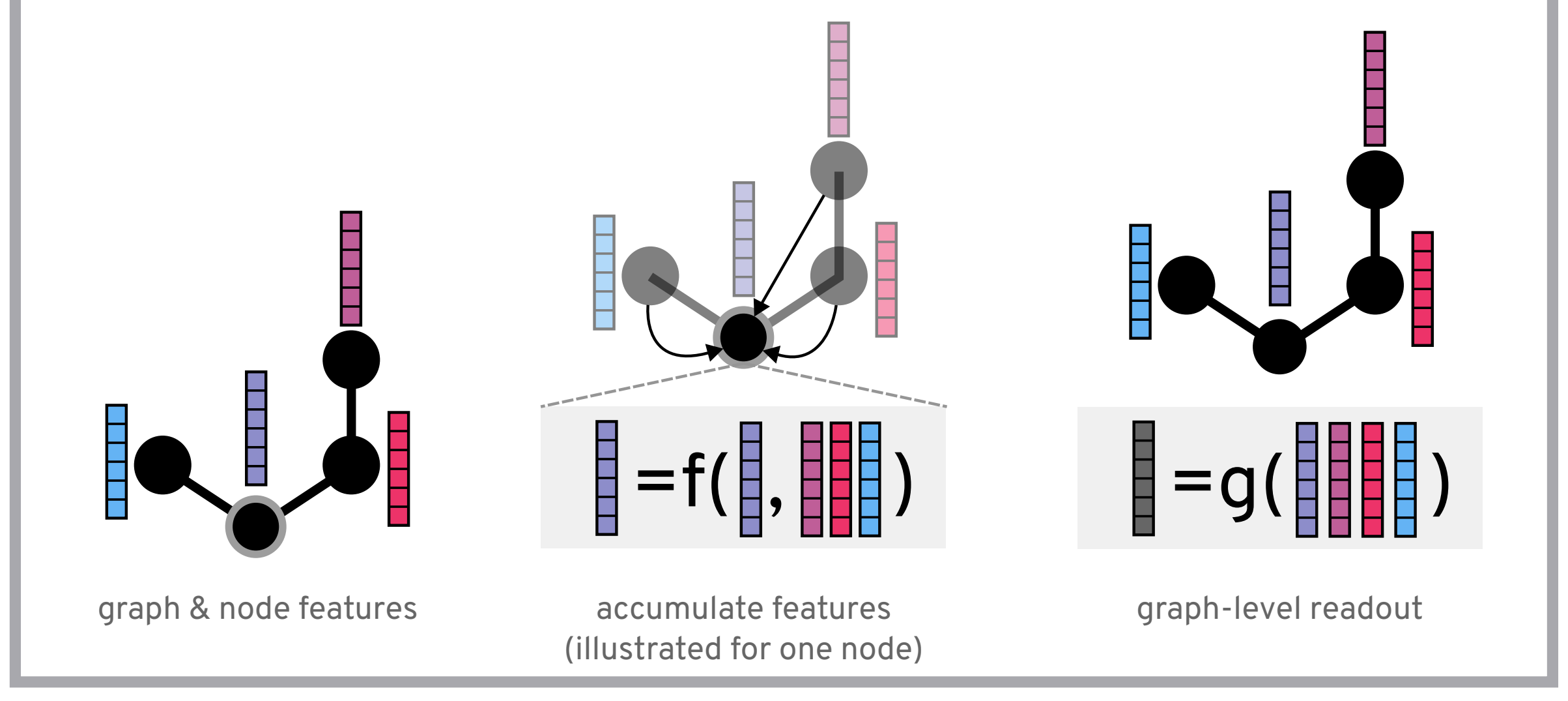
1. Accumulate neighborhood information to each vertex $\boldsymbol{v}$ and neural network layer (k):

$$\mathbf{a}_v^{(k)} = \texttt{AGGREGATE}^{(k)}(\{\mathbf{h}_u^{(k-1)} : u \in \mathcal{N}(v)\}),$$
$$\mathbf{h}_v^{(k)} = \texttt{COMBINE}^{(k)}(\mathbf{h}_v^{(k-1)}, \mathbf{a}_v^{(k)})$$

2. Employ a function to learn the overall representation of the graph, then the objective ℓ is optimized with standard backpropagation.

$$\mathbf{h}_{\mathcal{G}} = \texttt{READOUT}(\{\mathbf{h}_v^{(K)} : v \in \mathcal{G}\}),$$
$$\ell(p(y|\mathbf{h}_{\mathcal{G}}), y_{\mathcal{G}}) = \texttt{XENTROPY}(p(y|\mathbf{h}_{\mathcal{G}}), y_{\mathcal{G}})$$

$\mathbf{h}_v^{(k)}$: Feature vector of node v at iteration (k); $\mathbf{h}_{\mathcal{G}}$: Feature vector of whole graph; $y_{\mathcal{G}}$: True label of training graphs; $p(y|\mathbf{h}_{\mathcal{G}})$: A prediction model.



Short References

[1] Giorgio Patrini, Alessandro Rozza, Aditya Krishna Menon, Richard Nock, and Lizhen Q. "Making deep neural networks robust to label noise: A loss correction approach," *IEEE Conference on Computer Vision and Pattern Recognition*, pp. 1944–1952, 2017.

[2] Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. "How powerful are graph neural networks?," *International Conference on Learning Representations*, ICLR 2019.

[3] Will Hamilton, Zhitao Ying, and Jure Leskovec. "Inductive representation learning on large graphs," *Advances in Neural Information Processing Systems*, pp. 1024–1034, 2017.

[4] Thomas N. Kipf and Max Welling. "Semi-supervised classification with graph convolutional networks," *International Conference on Learning Representations*, ICLR 2017.

Loss Correction Schemes

We employ the loss correction technique from the line of work in [3]. We propose to use the *backward* surrogate loss with different estimators C for the noise matrix N:

$$\ell^{\leftarrow} = \boldsymbol{C}^{-1} \cdot \ell(\hat{p}(y|\mathcal{G}))$$

Our final loss function for the GNN model is:

$$\ell^{\leftarrow}(p(y|\mathbf{h}_{\mathcal{G}}), y_{\mathcal{G}}) = \boldsymbol{C}^{-1} \cdot \texttt{CROSS\_ENTROPY}(p(y|\mathbf{h}_{\mathcal{G}}), y_{\mathcal{G}})$$

Such loss correction can be understood as going backward one step in the noisy process. To estimate $\boldsymbol{C}$ from the noisy data (corrupted by some unknown noise process $\boldsymbol{N}$), we propose two estimation schemes:

1. **D-GNN-C** Assumes the neural network can exactly model the noisy data, hence the final softmax output is used to fill matrix $\boldsymbol{C}$. For instance, out of all sample classified as class "A" in our training data, we find the one that gives the weakest response for class "A", and use its softmax output as the values for row "A" in matrix $\boldsymbol{C}$.

2. **D-GNN-A** Uses a validation set, which does not contain noisy labels, to compute the entries for matrix $\boldsymbol{C}$.

We also propose to use directly the noise matrix $\boldsymbol{N}$ as an oracle for comparion (**D-GNN-E**).

Dataset (#classes)	diag(N)	Avg. diag($\boldsymbol{C}^{\mathrm{c}}$)	$\lVert\boldsymbol{C}^{\mathrm{c}} - N\rVert$	Avg. diag($\boldsymbol{C}^{\mathrm{a}}$)	$\lVert\boldsymbol{C}^{\mathrm{a}} - N\rVert$
IMDB-B (2)	0.8	0.99	0.76	0.77	0.12
IMDB-M (3)	0.8	0.99	1.14	0.85	0.30
RDT-B (2)	0.8	0.99	0.76	0.75	0.20
RDT-M5K (5)	0.8	0.99	1.90	0.81	0.10
COLLAB (3)	0.8	0.99	1.14	0.75	0.30
MUTAG (2)	0.8	0.99	0.76	0.74	0.24
PROTEINS (2)	0.8	0.99	0.76	0.78	0.08
PTC (2)	0.8	0.99	0.76	0.63	0.68
NCI1 (2)	0.8	0.99	0.76	0.74	0.24

Experimental Results

Dataset	#graphs	#classes	#vertices
IMDB-B	1000	2	19.8
IMDB-M	1500	3	13.0
RDT-B	2000	2	429.6
RDT-M5K	5000	5	508.5
COLLAB	5000	3	74.5
MUTAG	188	2	17.9
PROTEINS	1113	2	39.1
PTC	344	2	25.5
NCI1	4110	2	29.8

We test our framework on the set of well-studied 9 datasets for the graph classification task: 4 bioinformatics datasets (MUTAG, PTC, NCI1, PROTEINS), and 5 social network datasets (COLLAB, IMDB-BINARY, IMDB-MULTI, REDDIT-BINARY, REDDIT-MULTI5K). We follow the preprocessing suggested by [2] to use one-hot encoding as vertex degrees for social networks (except REDDIT datasets). Since these datasets have exact label for each graph, we introduce symmetric label noise artificially.

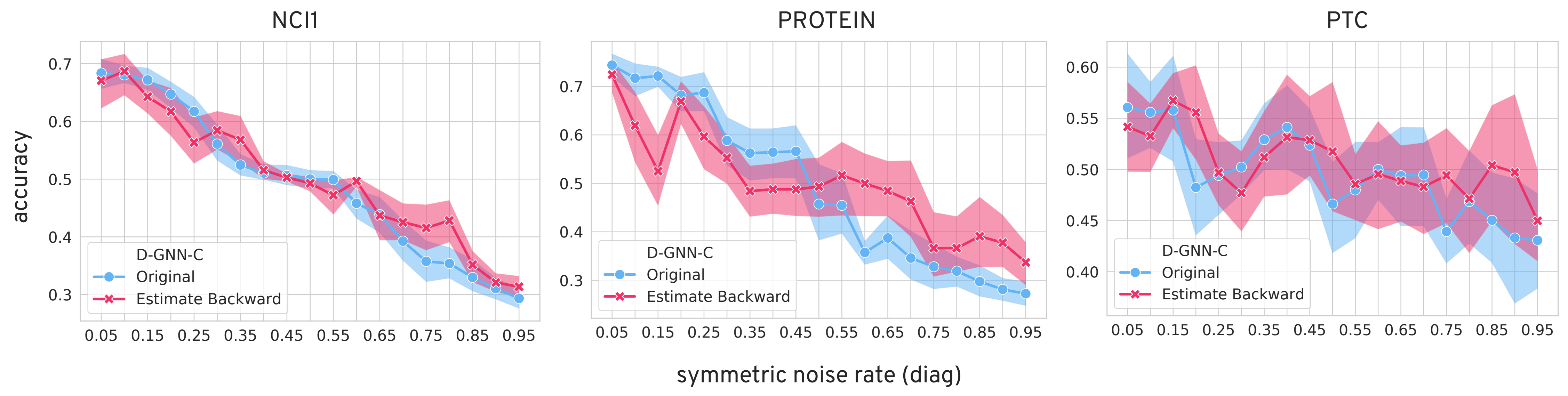
We compare our model with the original Graph Isomorphism Network (GIN) [2]. The hyperparameters are fixed across all datasets as follow: `epochs=20`, `num_layers=5`, `num_mlp_layers=2`, `batch_size=64`. Besides GIN, we consider GraphSAGE model [3] under the same noisy setting. We use the default setting for GraphSAGE.

In the table below, we fix the noise rate at 20% for the experiments and report the mean accuracy after 10 fold cross validation run.

	MUTAG	IMDB-M	RDT-B	RDT-M5K	COLLAB	IMDB-B	PROTEINS	PTC	NCI1
GIN	.7327	.4476	.6695	.3677	.6544	.6573	.6257	.4824	.6472
GraphSAGE	.7072	.4373	-	-	-	.6410	.6583	.4892	.6053
D-GNN-C	.5727	**.4747**	.5005	.2000	.5979	**.6940**	**.6693**	**.5557**	.6170
D-GNN-A	.7102	**.4505**	.5307	.2000	**.6917**	**.7088**	**.6769**	**.5001**	.6405
D-GNN-E	.7002	**.4633**	.5270	.2022	**.6960**	**.7190**	**.6917**	**.5235**	**.6638**

The worst performance variance of our model is the conservative estimation model. Due to the overestimation of softmax unit within the cross-entropy loss, the model's confidence to all training data is close to 1.0. Such overconfidence leads to wrong correction matrix estimation, which in turn leads to worse performance. In contrast to D-GNN-C, D-GNN-A and D-GNN-E have consistently outperformed the original model. Such improvement comes from the fact that the correction matrix $\boldsymbol{C}$ is correctly approximated.

Future Work Although we observed the denoising effect of our proposed model. It did not work particularly well under the conservative estimation setting. Figure below demonstrate the original performance and the loss correction performance for a range of symmetric noise. Our conservative model fails to perform in these datasets, especially under low noise.



We consider two improvements for our next model:
1) Employ unsupervised learning to estimate the loss matrix $\boldsymbol{C}$.
2) Extend the framework to node classification, which is a more common task in social network analysis.

The source code is available at: `github.com/gear/denoising-gnn`.

Acknowledgements This work was supported by JSPS Grant-in-Aid for Scientific Research (B) (Grant Number 17H01785) and JST CREST (Grant Number JPMJCR1687).