A Experimental Details

A.1 Hyperparameters

For experiments of baselines and LC versions, we set hyperparameters similarly to [18],

- Activation: ReLU
- Batch size for precomputation-based GNNs: 4096
- Patience: 300
- Maximum number of epochs: 2000
- Hidden dimension: 256

We show hyperparameter search space for each GNN as follows.

GCN. The hyperparameter search space of GCN is listed as follows:

- Weight decay: [1e-8, 1e-7, 1e-6, 1e-5]
- Learning rate: [0.005, 0.01, 0.02]
- Dropout: [0, 0.5]
- Number of layers: [2]

JKNet. The hyperparameter search space of JKNet is listed as follows:

- Weight decay: [1e-8, 1e-7, 1e-6, 1e-5]
- Learning rate: [0.001, 0.005, 0.01]
- Dropout: [0, 0.5]
- Number of layer: [3]
- Pooling: [concat, max]

GPRGNN. The hyperparameter search space of JKNet is listed as follows:

- Weight decay: [0, 1e-10, 1e-9, 1e-8]
- Learning rate: [0.005, 0.01, 0.02]
- Dropout for MLP: [0.5]
- Dropout before propagation: [0, 0.5, 0.7]
- Parameter initializing attention: [0, 0.1, 0.5, 0.9, 1]
- Number of propagation layer: [5]
- Number of layer of MLP: [4]

SGC. The hyperparameter search space of SGC is listed as follows:

- Weight decay: [1e-9, 1e-8, 1e-7, 1e-6, 1e-5]
- Learning rate: [1e-4, 0.001, 0.01]
- Number of layers: [2]

FSGNN. The hyperparameter search space of FSGNN is listed as follows:

- Weight decay1: [1e-5, 1e-4, 1e-3]
- Learning rate1: [1*e*-4, 0.001, 0.01]
- Weight decay2: [1e-6, 1e-5, 1e-4, 1e-3]

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- Learning rate2: [1e-4, 0.001, 0.01]
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- Weight decay3: [1e-6, 1e-5, 1e-4, 1e-3]

- Learning rate3: [1*e*-4, 0.001, 0.01]

- Weight decay for attention: [1e-6, 1e-5, 1e-4, 0.001]

- Learning rate for attention: [0.001, 0.01, 0.1]

- Dropout1: [0.5, 0.6, 0.7]

- Dropout2: [0.5, 0.6, 0.7]

- Number of layers: [3]

GCN_LC. The hyperparameter search space of GCN_LC is listed as follows:

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- Weight decay: [1e-7, 1e-6, 1e-5, 1e-4]
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- Learning rate: [5e-5, 1e-4, 0.001, 0.01]

- Dropout: [0, 0.5]

- Number of layers: [2]

JKNet_LC. The hyperparameter search space of JKNet_LC is listed as follows:

- Weight decay: [1e-6, 1e-5, 1e-4, 0.001]

- Learning rate: [1e-4, 0.001]

- Dropout: [0, 0.5]

- Number of layers: [3]

- Pooling: [concat, max]

GPRGNN_LC. The hyperparameter search space of GPRGNN_LC is listed as follows:

- Weight decay: [0, 1*e*-8, 1*e*-7]

- Learning rate: [1*e*-4, 0.001, 0.01]

– Dropout for MLP: [0.5]

- Dropout before propagation: [0, 0.5, 0.7]

- Parameter initializing attention: [0, 0.1, 0.5, 0.9, 1]

- Number of propagation layer: [5]

- Number of layer of MLP: [4]

We choose the best parameter set from these candidates by utilizing Optuna [2] for 50 trials. Configuration of baselines and LC versions to reproduce experiments in our paper is shown in Table 5.

Table 5: Configuration for Table 2 and 4. OOM indicates that the execution is out of memory. "-" indicates that the parameter is not used for the GNN.

| | Dataset | Weight decay | Learning rate | Dropout | Number of layers | Pooling | Attention initialing parameter |
|-----------|--------------|-----------------|----------------|---------------------|------------------|---------|--------------------------------|
| | | | | | | | mittainig parameter |
| | Flickr | 1e-6 | 0.02 | 0 | 2 | - | - |
| GCN | Reddit | 1e-7 | 0.02 | 0 | 2 | - | - |
| | arxiv | 1e-5 | 0.02 | 0 | 2 | - | - |
| | papers100M | OOM | OOM | OOM | OOM | OOM | OOM |
| | Flickr | 1e-5 | 0.01 | 0 | 3 | concat | - |
| JKNet | Reddit | 1e-7 | 0.005 | 0.5 | 3 | concat | - |
| | arxiv | 1e-7 | 0.001 | 0.5 | 3 | concat | - |
| | papers100M | OOM | OOM | OOM | OOM | OOM | OOM |
| GPRGNN | Flickr | 0 | 0.005 | MLP: 0.5 | MLP: 4 | _ | 0.1 |
| | | | | Propagation : 0.5 | | | |
| | Reddit | 1e-9 | 1e-4 | MLP: 0.5 | MLP: 4 | _ | 0.1 |
| | | | | Propagation: 0.5 | | | 0.1 |
| | arxiv | 1e-9 | 0.005 | MLP: 0.5 | MLP: 4 | _ | 0.9 |
| | | | | Propagation: 0 | Propagation: 5 | | |
| | papers100M | OOM | OOM | OOM | OOM | OOM | OOM |
| | Flickr | 1e-6 | 0.01 | - | 2 | - | - |
| SGC | Reddit | 1e-9 | 0.01 | - | 2 | - | - |
| | arxiv | 1e-9 | 0.01 | - | 2 | - | - |
| | papers100M | 1e-8 | 0.01 | - | 2 | - | - |
| FSGNN | Flickr | wd1 : 1e-4 | lr1:1e-4 | | | - | |
| | | wd2 : 1e-4 | lr2:0.001 | dp1:0.7 | 3 | | |
| | | wd3:1e-4 | lr3:0.001 | dp2:0.7 | 3 | | |
| | Reddit | wd_att : 0.01 | lr_att : 0.001 | | | | |
| | | wd1 : 1e-5 | lr1:1e-4 | | | | |
| | | wd2: 0.001 | lr2:0.001 | dp1:0.6 | 3 - | _ | |
| | | wd3 : 1e-4 | lr3:0.001 | dp2:0.5 | | | = |
| | | wd_att : 0.001 | lr_att : 0.01 | | | | |
| | arxiv | wd1 : 1e-5 | lr1:1e-4 | | | | |
| | | wd2 : 1e-5 | lr2:0.001 | dp1:0.7 | 3 - | | |
| | | wd3:1e-4 | lr3:0.001 | dp2:0.6 | | - | - |
| | | wd_att: 0.001 | lr_att : 0.01 | | | | |
| | | wd1 : 1e-4 | lr1:1e-4 | | | | |
| | papers100M | wd2 : 1e-5 | lr2:1e-4 | dp1:0.5 | 3 | _ | |
| | papersiooivi | wd3:1e-6 | lr3:0.001 | dp2:0.5 | 3 | - | - |
| | | wd_att : 1e-4 | lr_att : 0.1 | | | | |
| | Flickr | 1e-5 | 1e-4 | 0 | 2 | - | - |
| GCN_LC | Reddit | 1e-7 | 0.001 | 0.5 | 2 | - | - |
| | arxiv | 1e-4 | 0.001 | 0 | 2 | - | - |
| | papers100M | 1e-6 | 0.001 | 0 | 2 | - | - |
| JKNet_LC | Flickr | 1e-4 | 1e-4 | 0 | 3 | concat | - |
| | Reddit | 1e-6 | 1e-4 | 0.5 | 3 | concat | - |
| | arxiv | 1e-6 | 1e-4 | 0.5 | 3 | concat | - |
| | papers100M | 1e-6 | 0.001 | 0 | 3 | concat | - |
| GPRGNN.LC | Flickr | 0 | 1e-4 | MLP: 0.5 | MLP: 4 | | 0.1 |
| | PHENI | U | 16-4 | Propagation: 0 | Propagation: 5 | - | 0.1 |
| | Reddit | 0 | 1e-4 | MLP: 0.5 | MLP: 4 | - | 0.5 |
| | | | | Propagation: 0 | Propagation: 5 | | |
| | arxiv | 1e-8 | 0.001 | MLP: 0.5 | MLP: 4 | | 0.9 |
| | | | | Propagation: 0.5 | Propagation: 5 | - | |
| | papers100M | 1e-7 | 0.001 | MLP: 0.5 | MLP: 4 | | 1 |
| | papersroom | 10-1 | 0.001 | Propagation: 0 | Propagation: 5 | - | 1 |
| | | | | | | | |