Reverse Graph Learning for Graph Neural Network

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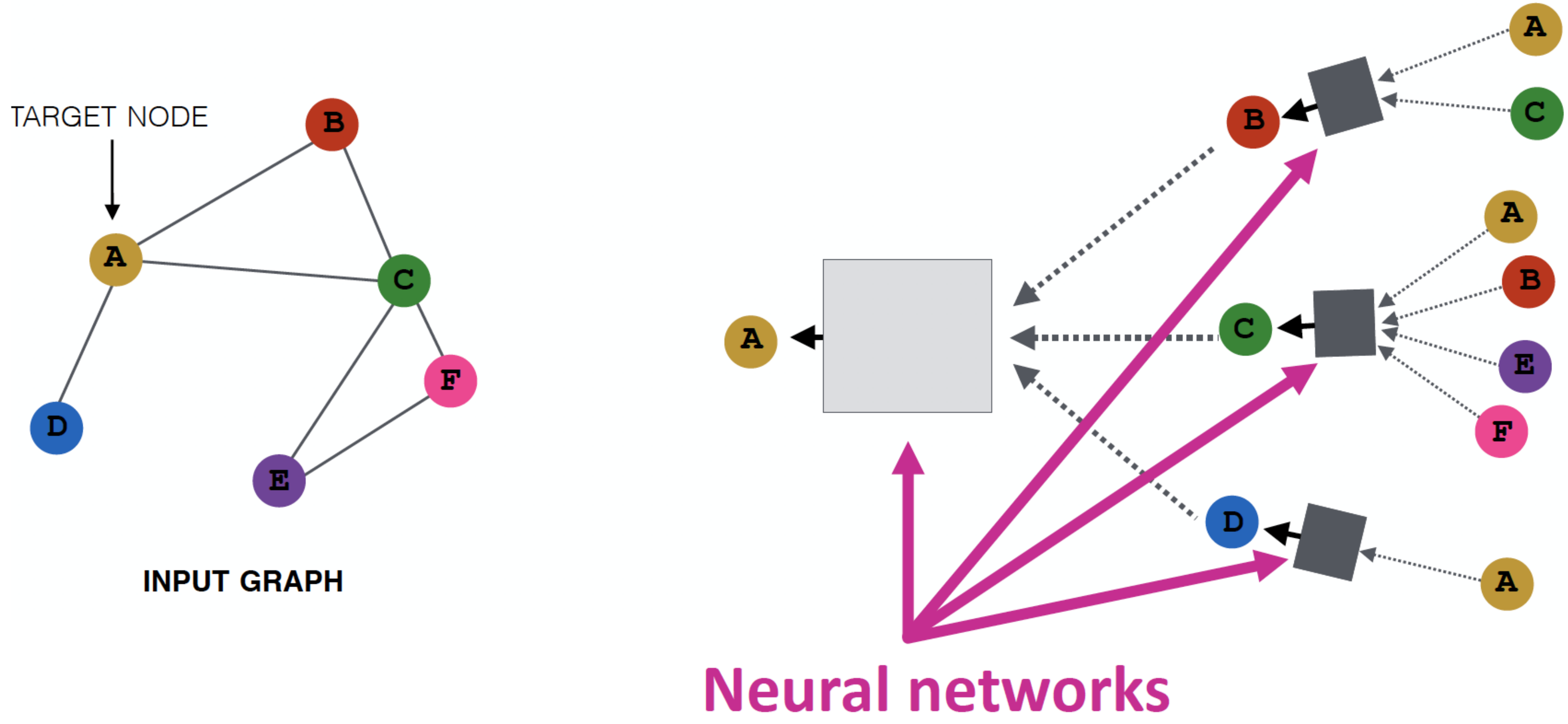
Index - 1

1. 논문 목적 (why)
2. Preliminaries
3. Method
4. Experiment
5. Result (+생각)

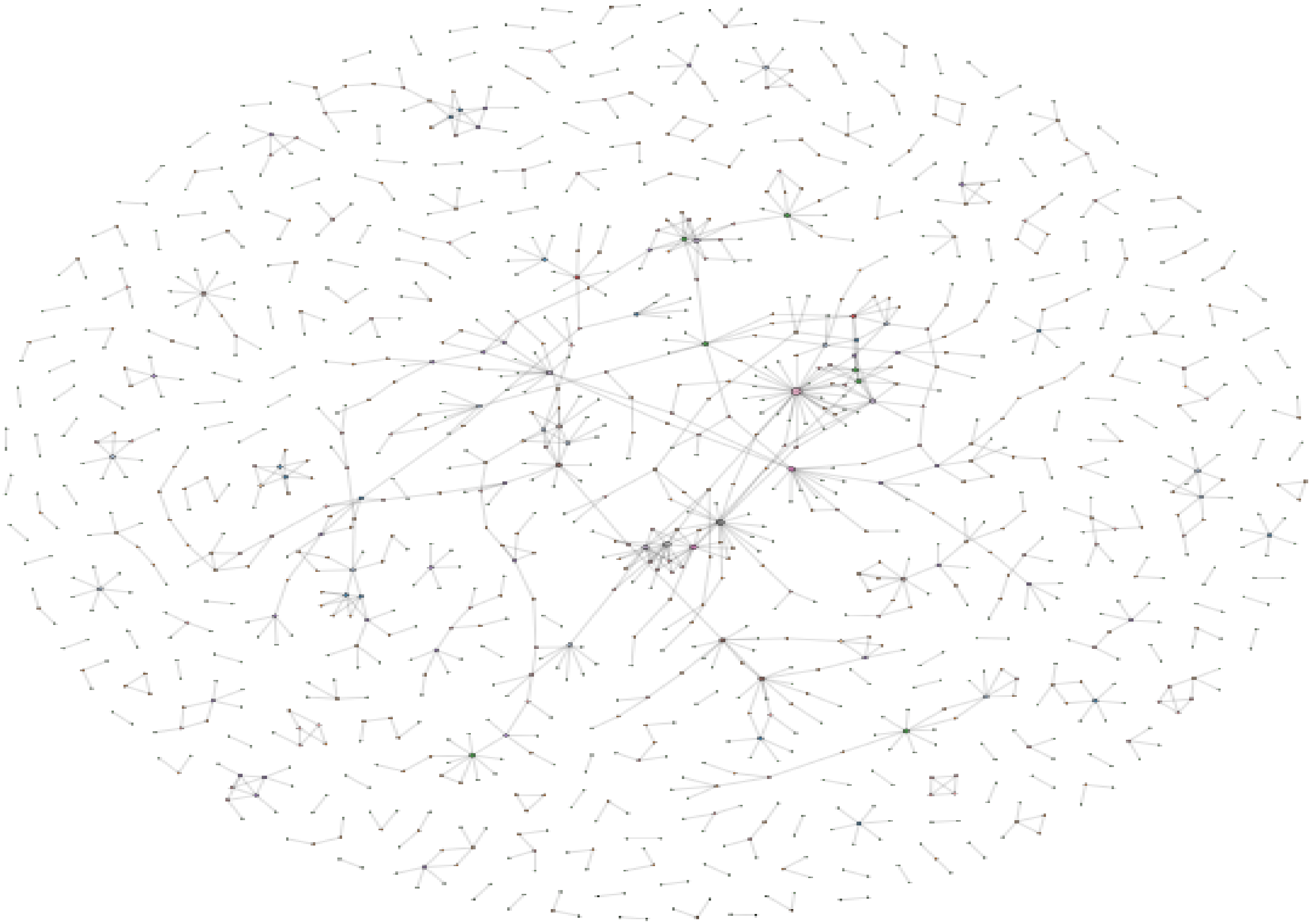
논문 목적 (why) - 2

Basic GNN Models



논문 목적 (why) - 3

Is the graph properly structured?



논문 목적 (why) - 4

Preliminaries

1. GCN
2. Graph Learning

Preliminaries -5

1. GCN

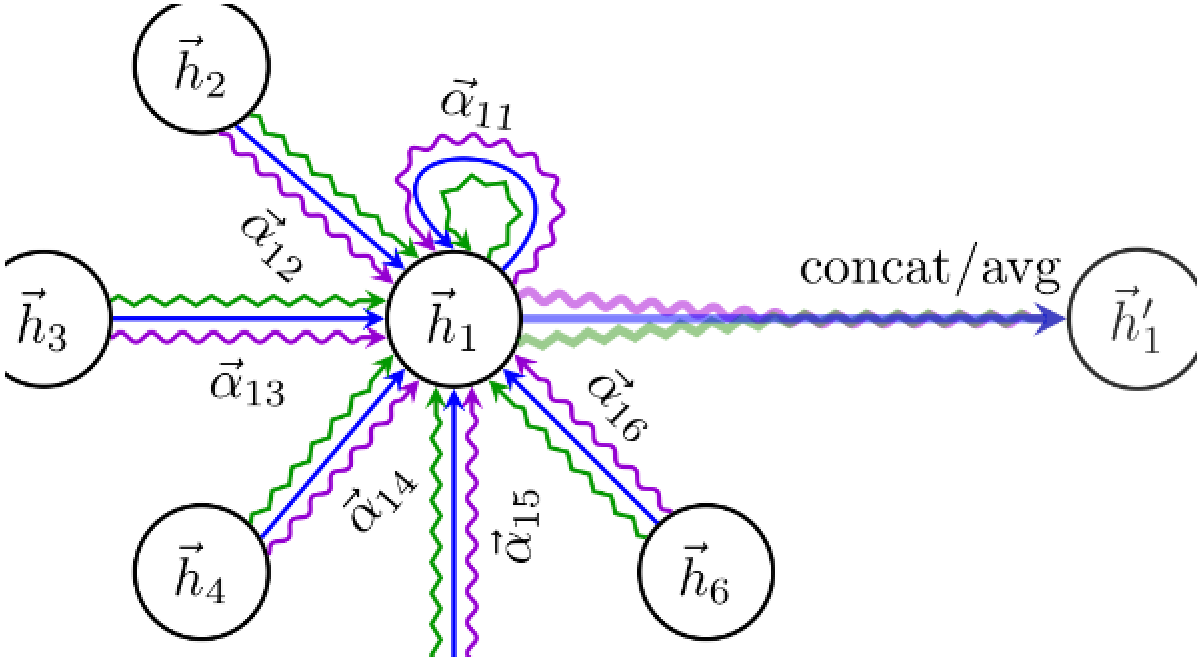
$$\mathbf{H}^{l+1} = \sigma\left(\mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{\frac{1}{2}}\mathbf{H}^{l}\mathbf{W}^{l}\right)$$

Preliminaries -6

Preliminaries

2. Graph Learning

Like GAT



Limitation -> Just reduce edge

Preliminaries -7

Preliminaries

2. Graph Learning (GLCN loss)

$$S_{ij} = g(x_i, x_j) = \frac{\exp(\mathrm{ReLU}(a^T|x_i - x_j|))}{\sum_{j=1}^{n} \exp(\mathrm{ReLU}(a^T|x_i - x_j|))}$$

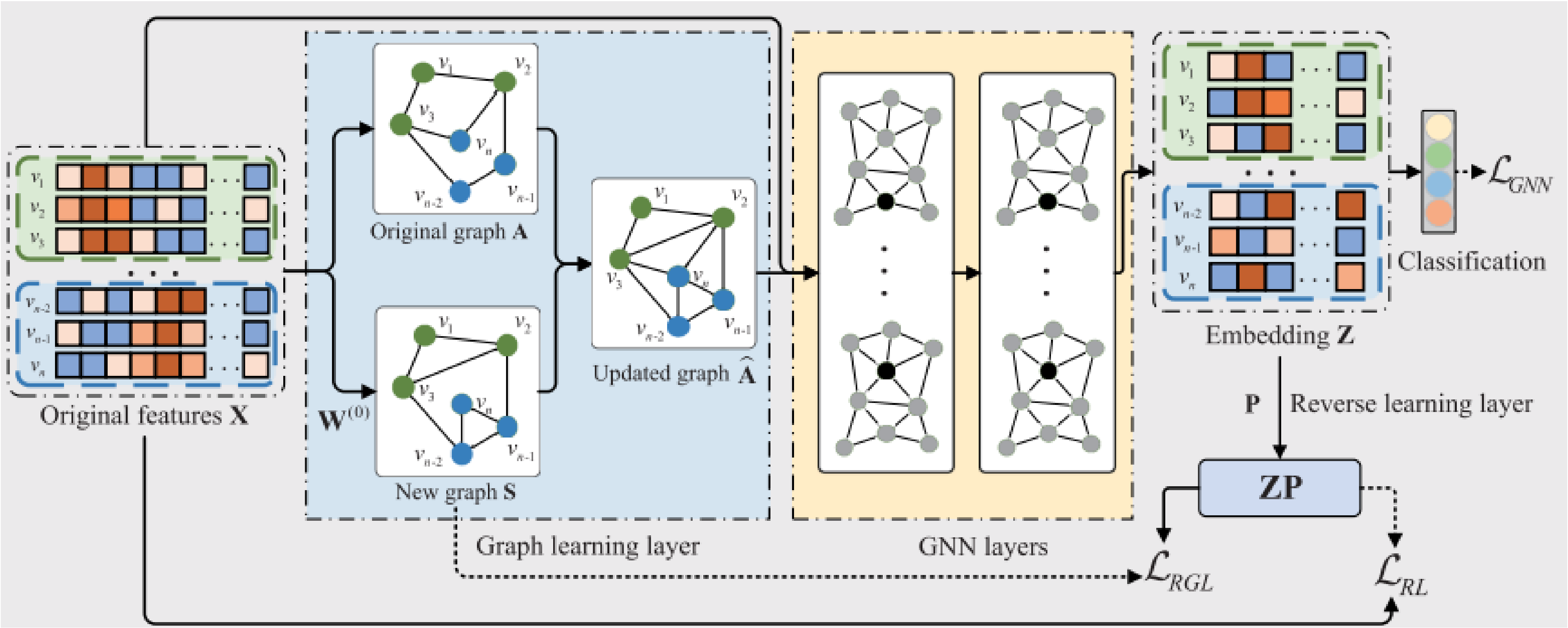
$$\mathcal{L}_{\mathrm{GL}} = \sum_{i,j=1}^{n} \|x_i - x_j\|_2^2 S_{ij} + \gamma\|S\|_F^2$$

S : new graph(learnable)

L_GL : new loss function

L_GLCN : L_GCN + lamda*L_GL (lamda is parameter)

method - 8



Original features X
W(0)
Original graph A
New graph S
Updated graph Â
Graph learning layer
GNN layers
Embedding Z
Classification
P
Reverse learning layer
ZP
$\mathcal{L}_{GNN}$
$\mathcal{L}_{RGL}$
$\mathcal{L}_{RL}$

method - 9

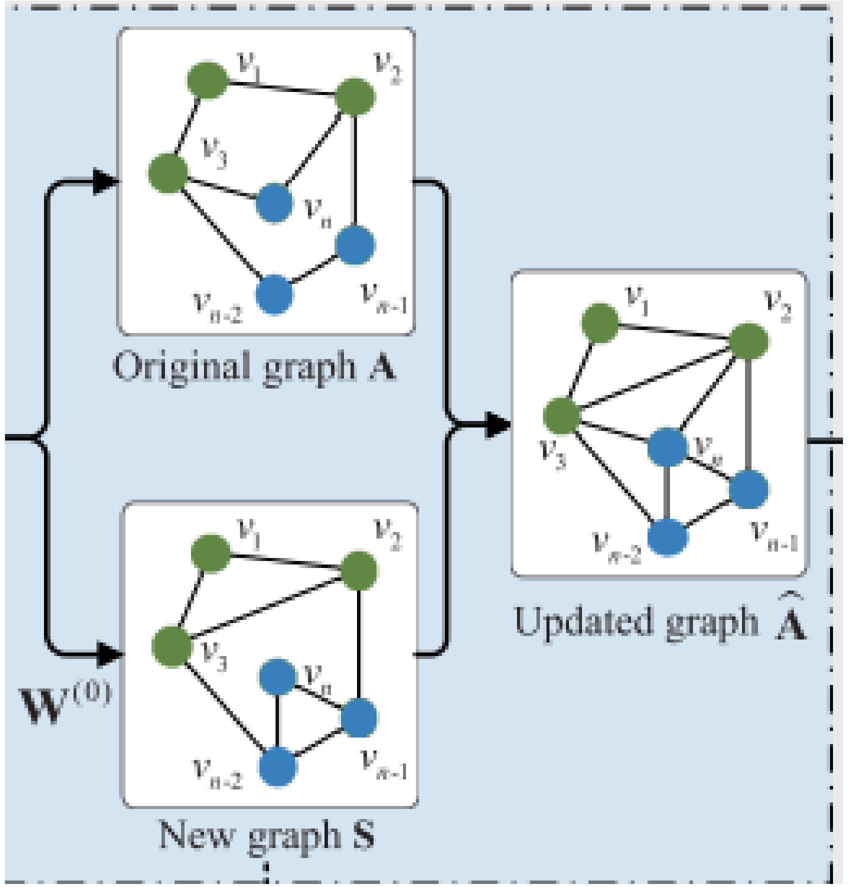
method

총 3종류의 layer가 존재함

1. Graph learning layers

$$\mathcal{L}_{\mathrm{RGL}}: \quad \min_{\mathbf{S}} \sum_{ij}^{n} \|\mathbf{z}_i\mathbf{P} - \mathbf{z}_j\mathbf{P}\|_2^2 s_{ij} + \|\mathbf{S}\|_F^2$$

$$\hat{\mathbf{A}} = (1-\eta)\mathbf{A} + \eta\mathbf{S}$$

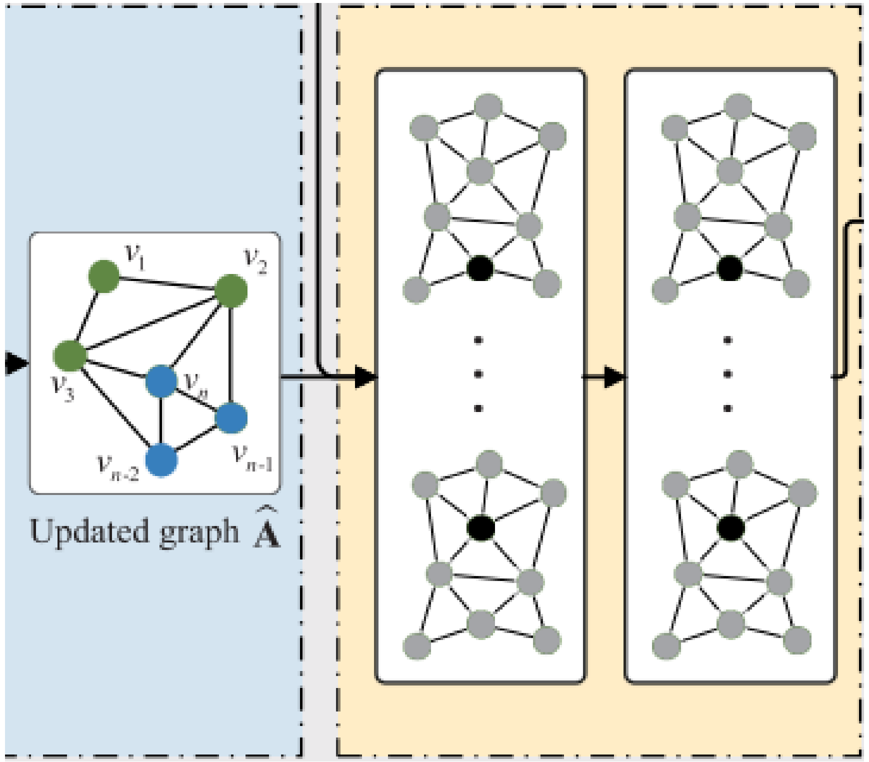


method - 10

method

총 3종류의 layer가 존재함

2. GNN layers



method - 11

method

총 3종류의 layer가 존재함

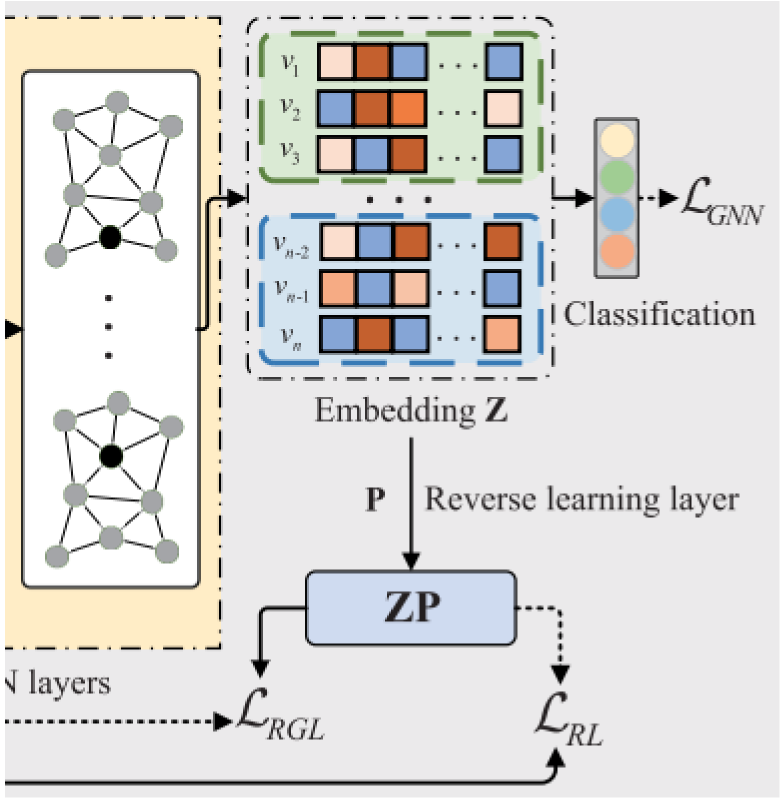
3. Reverse learning layer

$$\mathcal{L}_{\mathrm{RGL}}: \quad \min_{\mathbf{S}} \sum_{ij}^{n} \|\mathbf{z}_i\mathbf{P} - \mathbf{z}_j\mathbf{P}\|_2^2 s_{ij} + \|\mathbf{S}\|_F^2$$

$$\text{s.t.,} \quad \sum_{j=1}^{n} s_{ij} = 1, \quad s_{ij} > 0, \;\; i, j = 1, \ldots, n$$

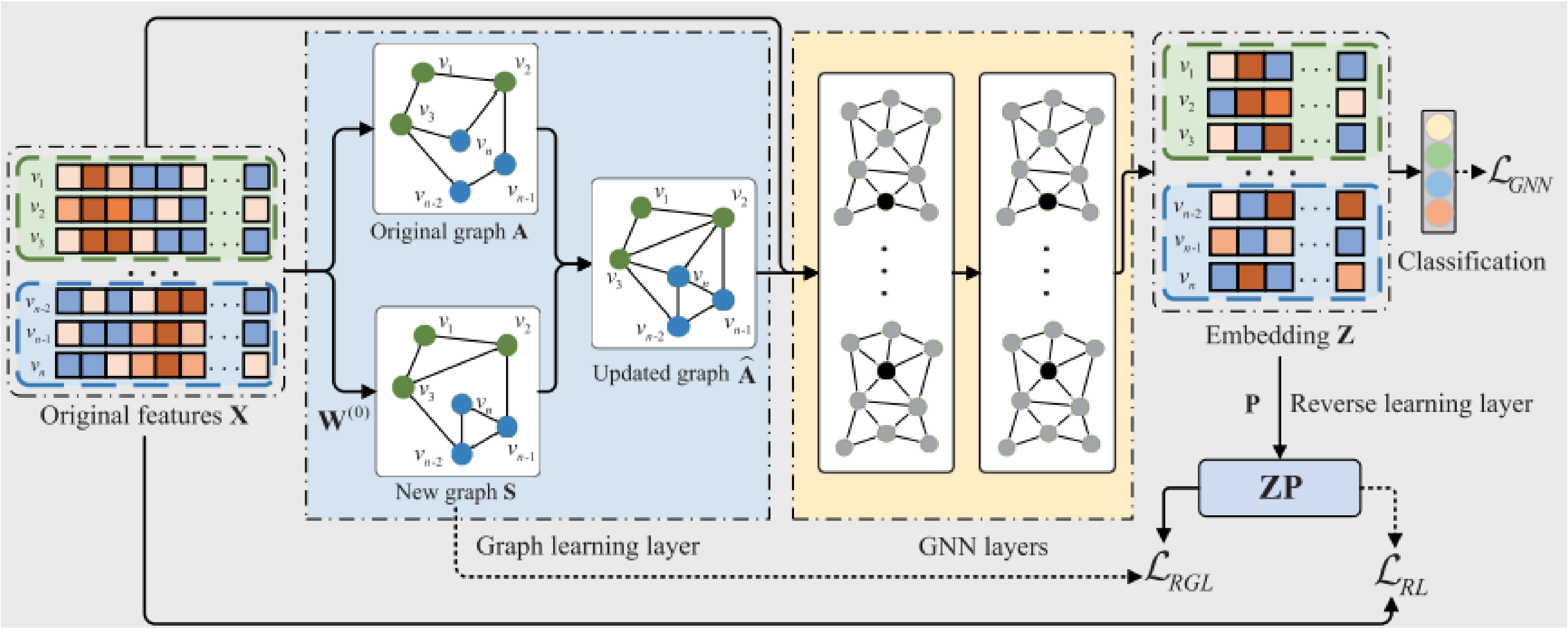
$$\mathcal{L}_{\mathrm{RL}}: \quad \min_{\mathbf{P}, \mathbf{P}^T\mathbf{P}=\mathbf{I}} \|\mathbf{X} - \mathbf{Z}\mathbf{P}\|_F^2$$

$$\mathcal{L} = \mathcal{L}_{\mathrm{GNN}} + \beta\,\mathcal{L}_{\mathrm{RGL}} + \gamma\,\mathcal{L}_{\mathrm{RL}}$$



method - 12

method



method - 13

method

Out of sample

$$\mathbf{S}_q = \cos(\mathbf{x}_q \mathbf{W}^{(0)}, \mathbf{X}_{\text{train}} \mathbf{W}^{(0)}).$$

We then select the neighborhood by

$$\mathcal{N}_q \leftarrow \text{topk}(\mathbf{S}_q).$$

S_q : new data q가 어디에 유사한지

X_q : new data q

W^(0) : graph learning layer

Experiment - 14

Experiment

Node classification

CLASSIFICATION ACCURACY OF ALL METHODS ON NINE DATASETS FOR SEMI-SUPERVISED NODE CLASSIFICATION

Methods	Cora	Citeseer	Handwritten	Caltech	AWA	BBC	WebKB	3sources	Flower
GCN	$81.06_{\pm 0.5}$	$71.22_{\pm 0.6}$	$93.38_{\pm 0.8}$	$80.48_{\pm 1.2}$	$56.29_{\pm 0.9}$	$72.56_{\pm 0.8}$	$72.28_{\pm 1.1}$	$79.61_{\pm 0.6}$	$45.51_{\pm 1.2}$
GLCN	$81.80_{\pm 0.7}$	$70.56_{\pm 0.9}$	$94.22_{\pm 0.9}$	$79.36_{\pm 1.4}$	$55.81_{\pm 0.7}$	$73.36_{\pm 1.0}$	$75.76_{\pm 0.9}$	$79.22_{\pm 0.6}$	$46.65_{\pm 1.0}$
DIAL	$82.41_{\pm 0.4}$	$71.68_{\pm 0.7}$	$93.75_{\pm 1.2}$	$76.79_{\pm 1.2}$	$56.57_{\pm 0.7}$	$71.39_{\pm 1.2}$	$70.33_{\pm 1.0}$	$78.18_{\pm 0.4}$	$45.49_{\pm 1.0}$
JLGCN	$83.66_{\pm 0.5}$	$72.94_{\pm 0.6}$	$94.60_{\pm 0.8}$	$82.74_{\pm 0.8}$	$58.96_{\pm 0.5}$	$76.12_{\pm 0.6}$	$75.65_{\pm 0.8}$	$75.46_{\pm 0.8}$	$50.61_{\pm 0.8}$
Proposed	$\mathbf{83.89}_{\pm 0.7}$	$\mathbf{73.35}_{\pm 0.8}$	$\mathbf{95.89}_{\pm 0.9}$	$\mathbf{83.92}_{\pm 0.6}$	$\mathbf{61.60}_{\pm 0.5}$	$\mathbf{80.81}_{\pm 0.5}$	$\mathbf{77.39}_{\pm 0.7}$	$\mathbf{81.43}_{\pm 0.3}$	$\mathbf{50.79}_{\pm 0.7}$

Experiment - 15

Experiment

Out of sample

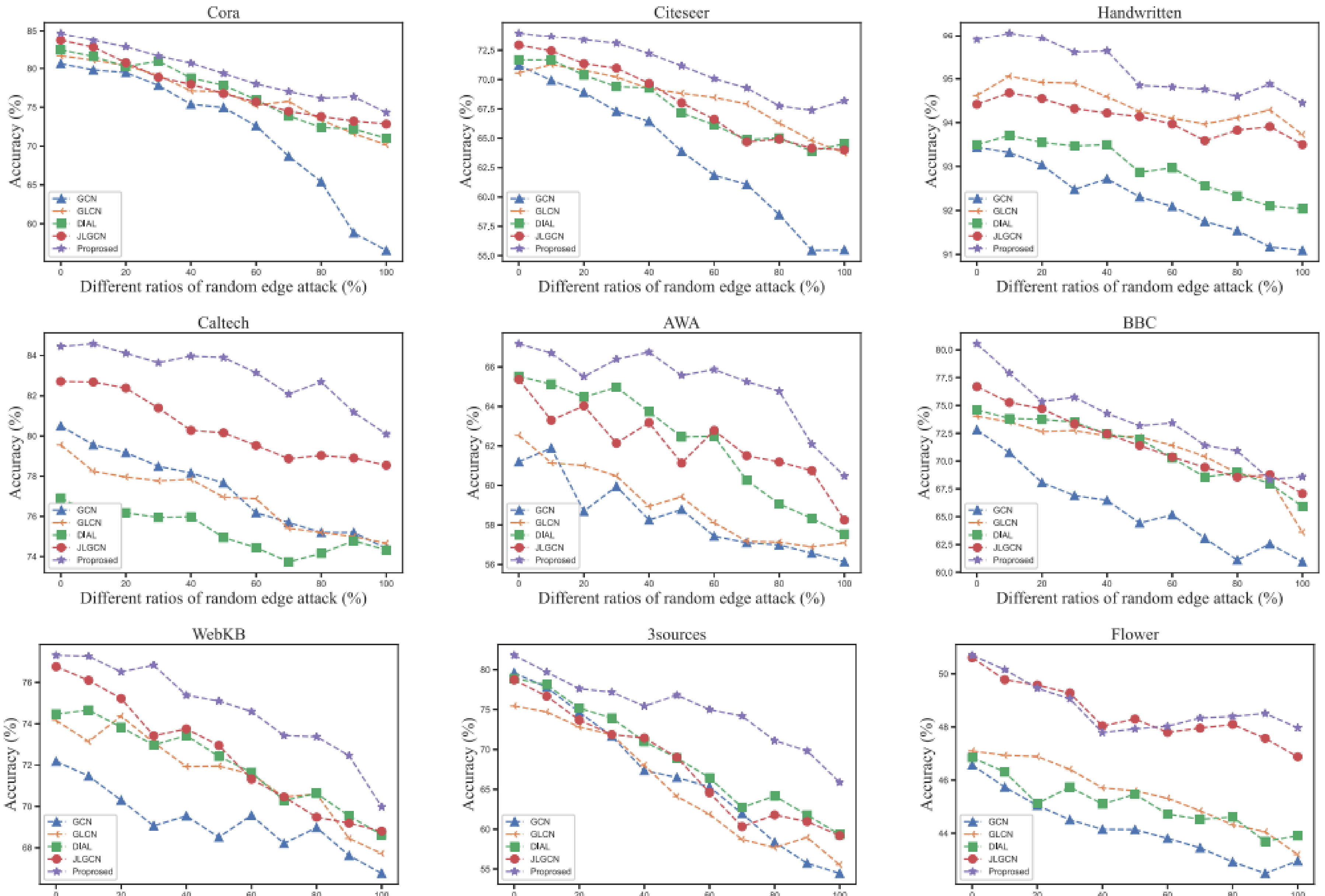
Classification Accuracy of All Methods on Nine Datasets for Out-of-Sample Extension

	Cora	Citeseer	Handwritten	Caltech	AWA	BBC	WebKB	3sources	Flower
Deepwalk	85.23±0.2	61.81±0.1	96.94±0.1	83.45±0.3	61.88±0.2	78.91±0.2	79.29±0.2	83.47±0.4	53.12±0.6
GraphSAGE	84.68±0.4	72.97±0.3	96.72±0.1	**83.69**±0.2	65.21±0.3	79.50±0.3	76.27±0.7	85.52±0.5	58.52±0.7
SGC	73.43±0.3	68.32±0.5	88.95±0.2	81.14±0.4	62.63±0.4	74.74±0.4	61.83±1.2	70.22±0.4	50.59±0.5
GCN*	78.30±0.5	76.70±0.3	92.50±0.2	82.09±0.4	64.83±0.5	84.89±0.3	82.79±0.4	79.48±0.3	56.54±0.7
GCN**	88.71±0.2	81.29±0.4	97.05±0.1	81.61±0.3	64.92±0.5	85.61±0.3	80.93±0.6	89.47±0.1	56.03±0.6
QFE	79.85±0.2	70.12±0.3	97.00±0.1	80.27±0.5	62.11±0.5	84.31±0.1	80.72±0.7	87.37±0.2	49.93±0.9
Proposed	**89.26**±0.2	**81.47**±0.4	**97.90**±0.1	83.50±0.2	**70.30**±0.5	**92.95**±0.1	**89.77**±0.3	**92.63**±0.2	**62.36**±0.6

Experiment - 16

Experiment

Random edge attack



Result - 17

Result

1. Graph 변형으로 한계 극복
2. Model 비교 적음(아쉬움)
3. Random attack 실험