

# **Semi-supervised classification with graph convolutional networks**

Kipf, Thomas N., and Max Welling., ICLR 2017.

2020-05-14

KIM INA (dodary0214@gmail.com)

# Contents

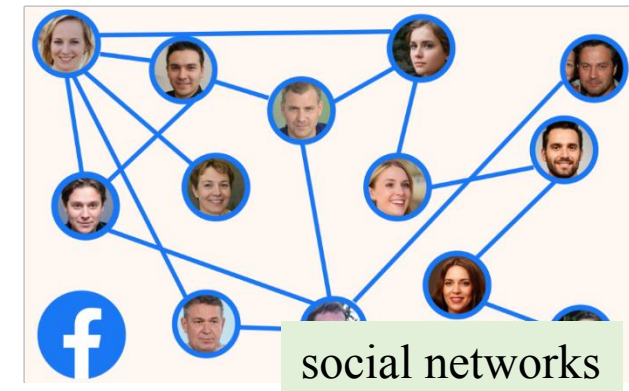
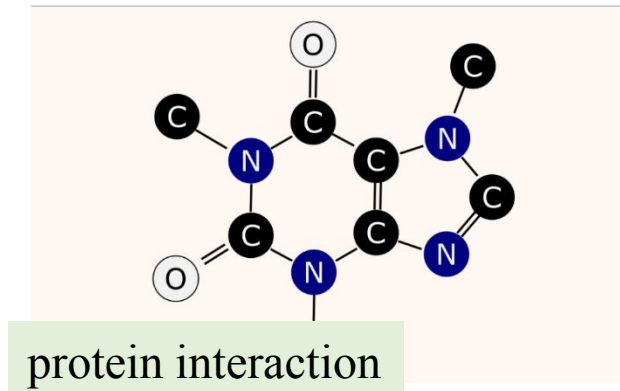
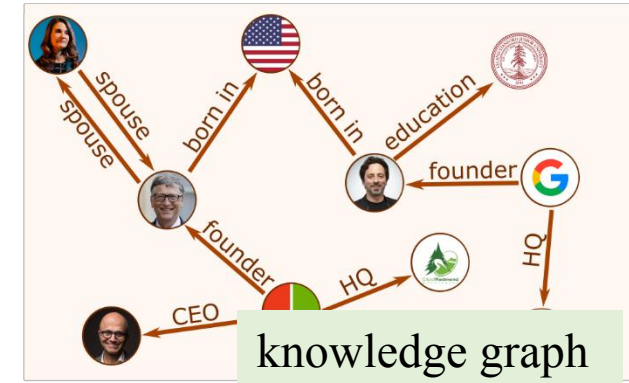
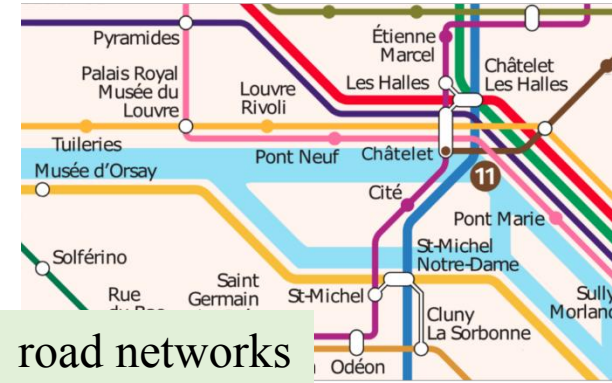
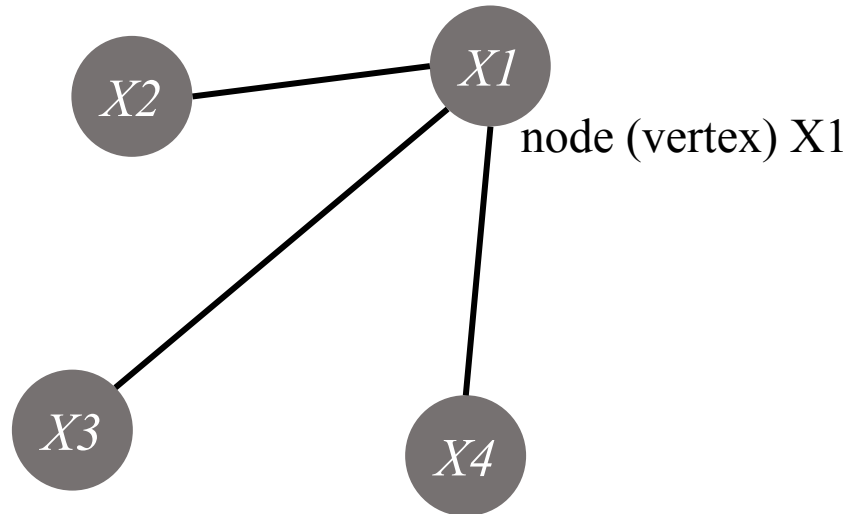
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- Background
- Introduction
- Fast approximate convolutions on graphs
  - Spectral graph convolutions
  - Layer-wise linear model
- Semi-supervised node classification
- Experiments
- Conclusions and limitations

# Graph

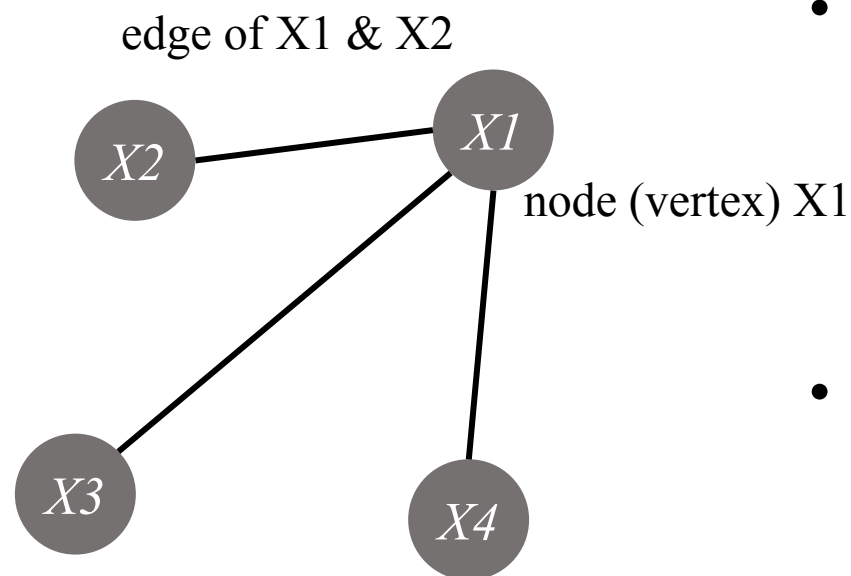
- Graph  $G = (V, E)$
- A set of vertices  $V = \{X_1, \dots, X_n\}$
- A set of edges  $E = \{E_{ij}, X_i, X_j \in V\}$

edge of  $X_1$  &  $X_2$

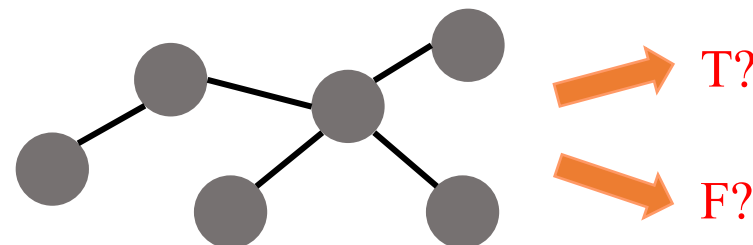


# Graph Tasks

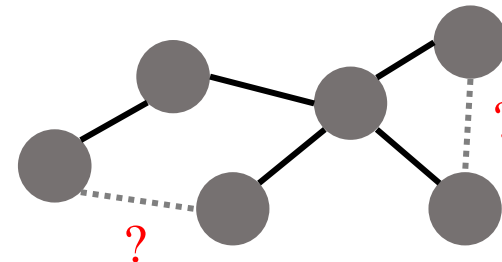
- Graph  $G = (V, E)$
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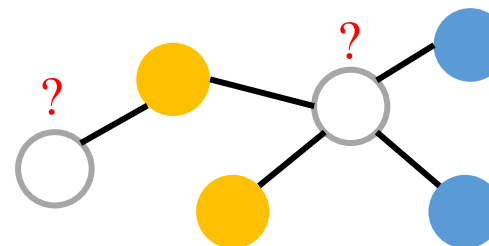
- Graph-level: graph classification



- Edge-level: edge classification, link prediction



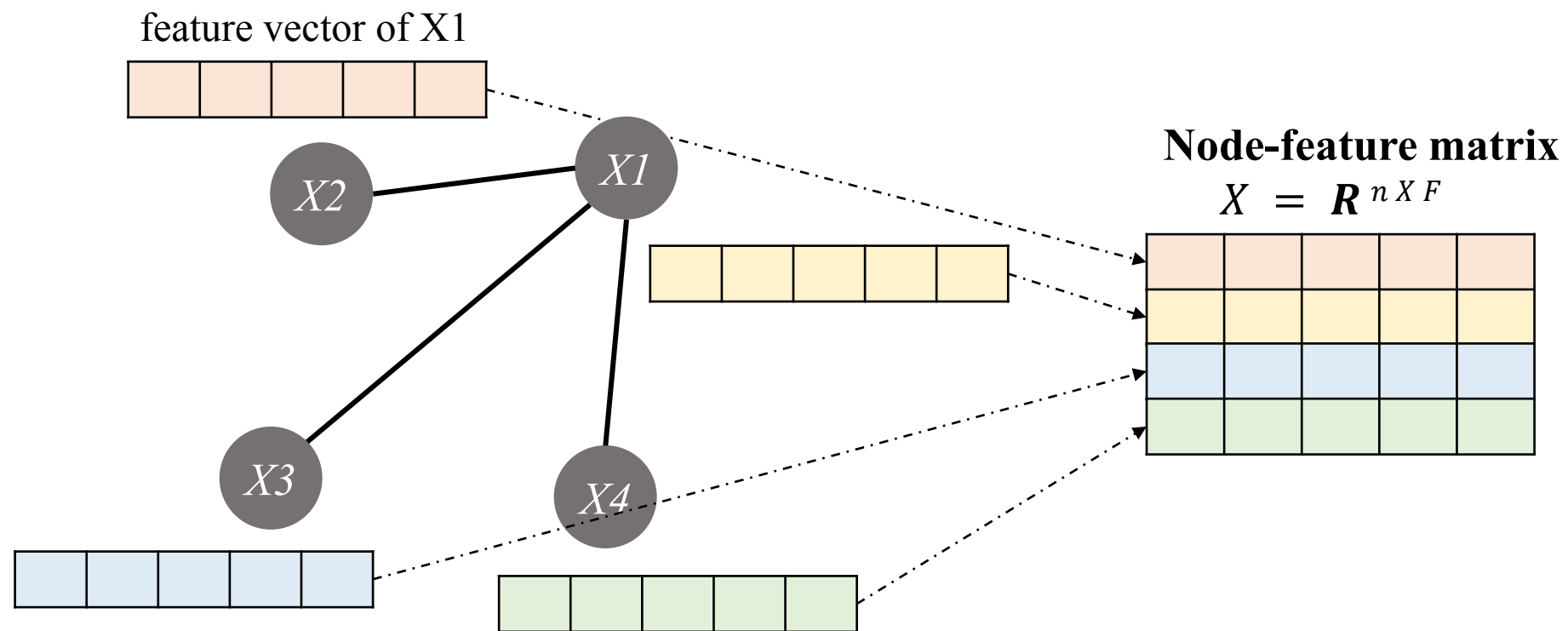
- Node-level: node classification



<https://towardsdatascience.com/graph-convolutional-networks-deep-99d7fee5706f>

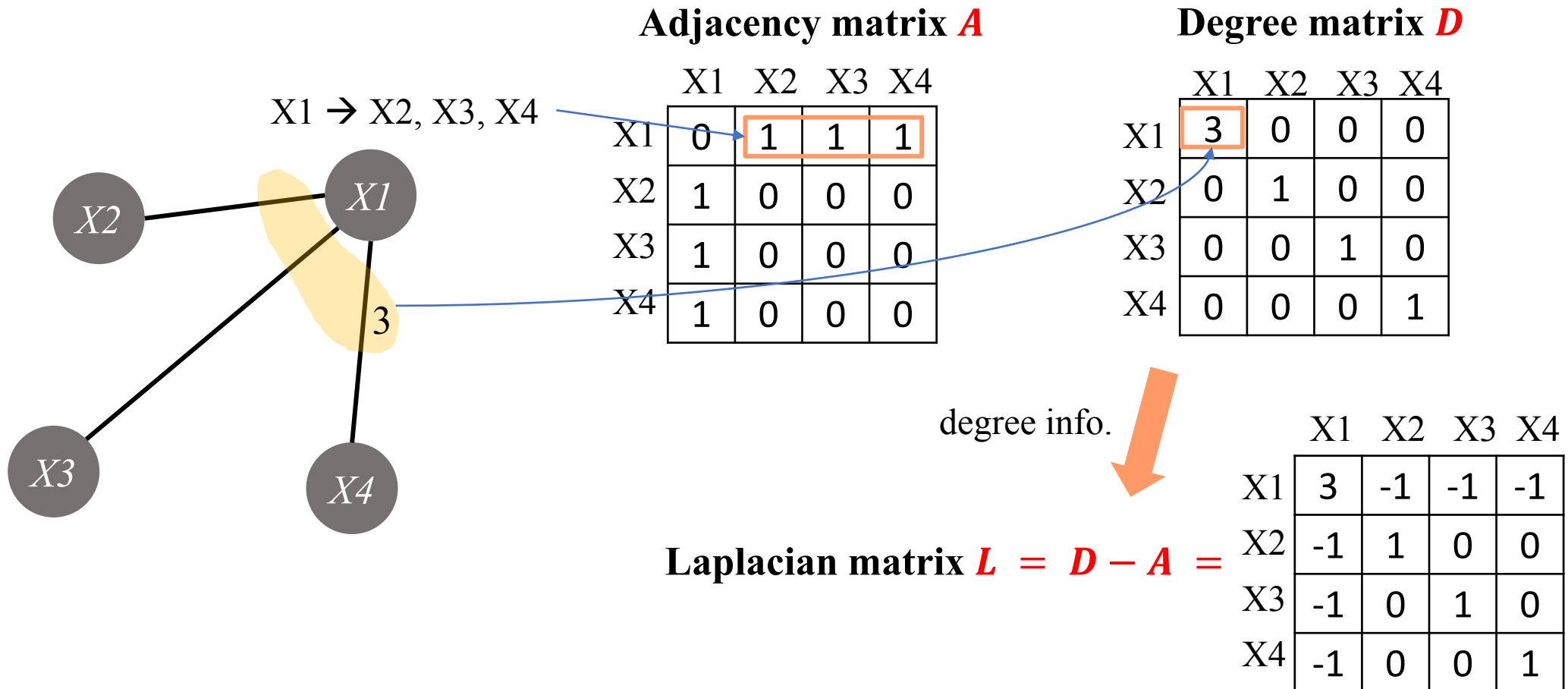
# Graph Representation – Node-Feature Matrix

Representation structures : **Node-feature matrix**, Adjacency matrix, Degree matrix, Laplacian matrix



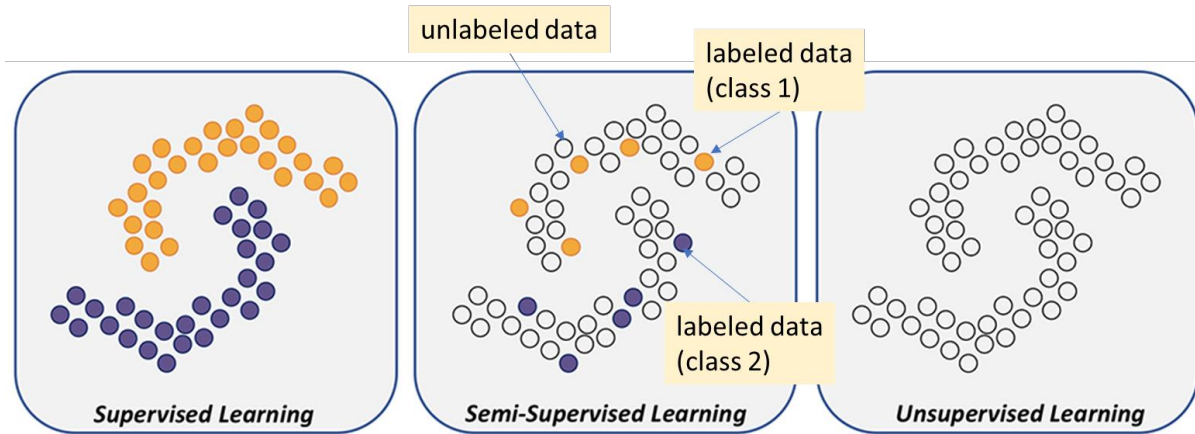
# Graph Representation – Graph Structure Representation

Representation structures : Node-feature matrix, **Adjacency matrix**, **Degree matrix**, **Laplacian matrix**



# Semi-Supervised Classification with Graph Convolutional Networks

## Semi-Supervised Classification



<https://blog.est.ai/2020/11/ssl/>

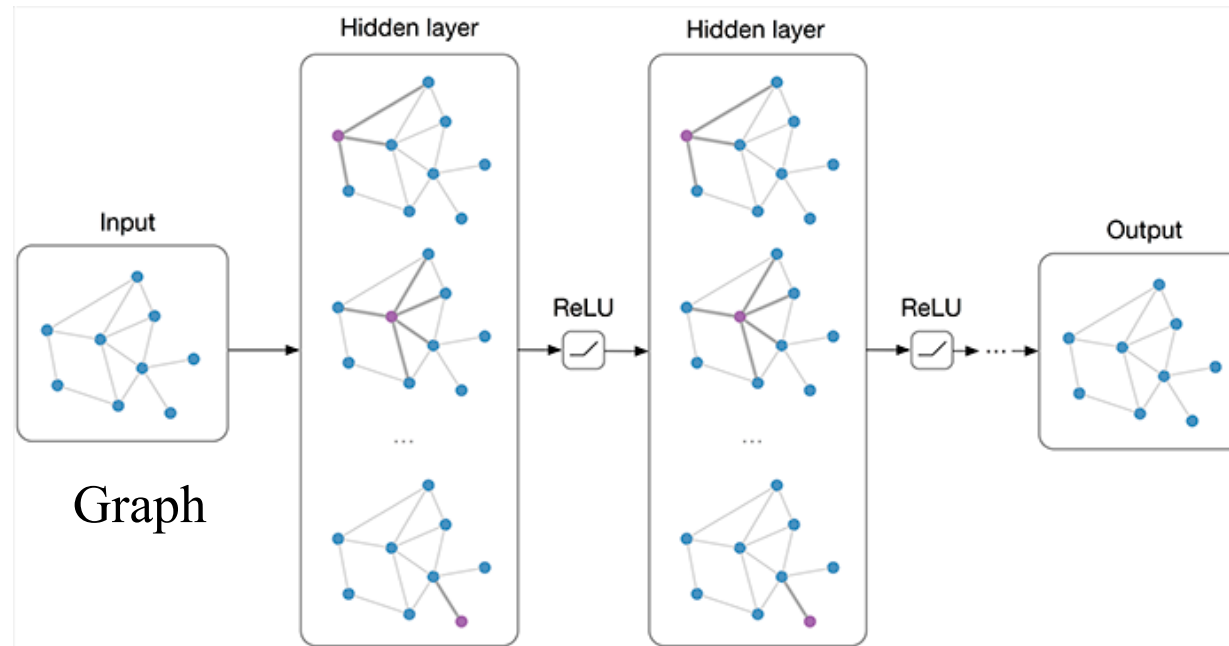
## Graph Convolutional Network

$$\text{GNN} + \text{CNN} = \text{GCN}$$

# Graph Neural Network (GNN)

### ➤ GNN

- 그래프 구조에서 사용하는 Neural Network로, Graph를 입력으로 받음
- Graph와 관련된 모든 Neural Network를 GNN으로 칭함



<https://tkipf.github.io/graph-convolutional-networks/>

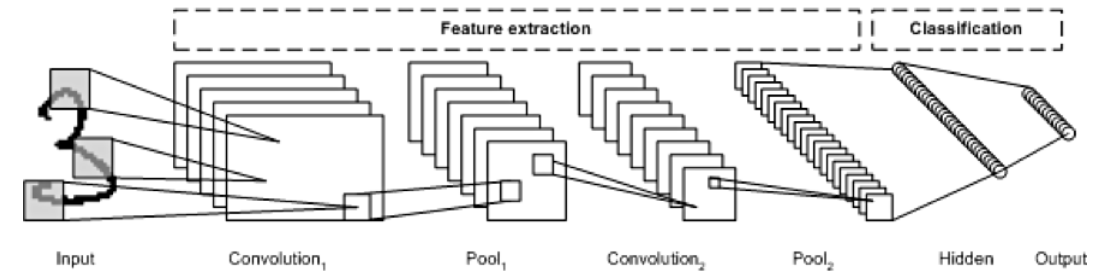


# 1 INTRODUCTION

## Convolution

### ➤ CNN

- 이미지에 대하여 Filter를 사용해 정보를 Aggregate
- Convolution values (i.e., weight, filter)를 학습

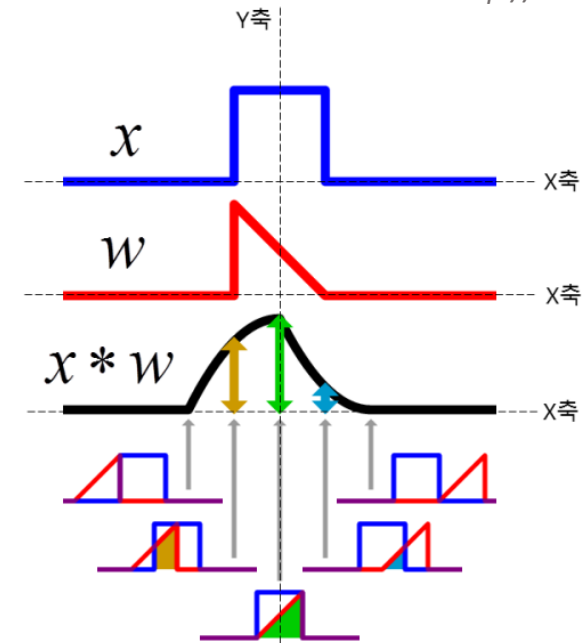


<http://taewan.kim/post/cnn/>

### ➤ Convolution (합성곱)

- f, g 가운데 하나의 함수를 반전, 전이 시킨 후 다른 하나의 함수와 곱한 결과를 적분
- 현재 합성곱의 값은 이전 시간의 결과를 포함

$$(f * g)(t) = \int_{-\infty}^{\infty} f(\tau)g(t - \tau) d\tau \quad * \text{ convolution symbol}$$

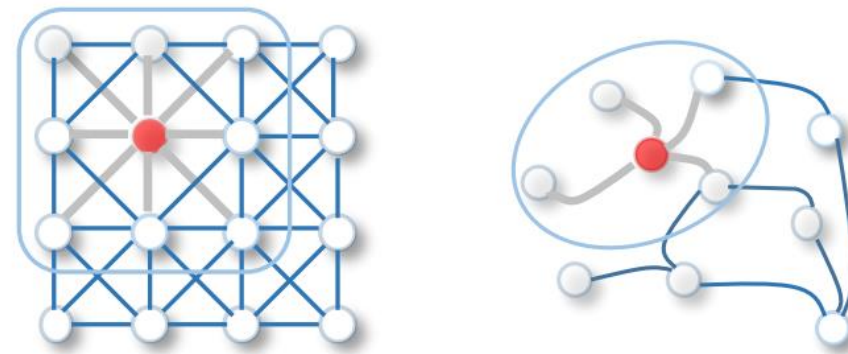


<https://en.wikipedia.org/wiki/Convolution>

# Convolution on Graph

## ➤ Graph convolution

- Convolution filter를 사용해서, 그래프 노드와 인접 노드간의 관계 계산 목적
- 전체 데이터에서 Local feature 추출 목적
- Filter들이 Spatial location에 따라 변하지 않음



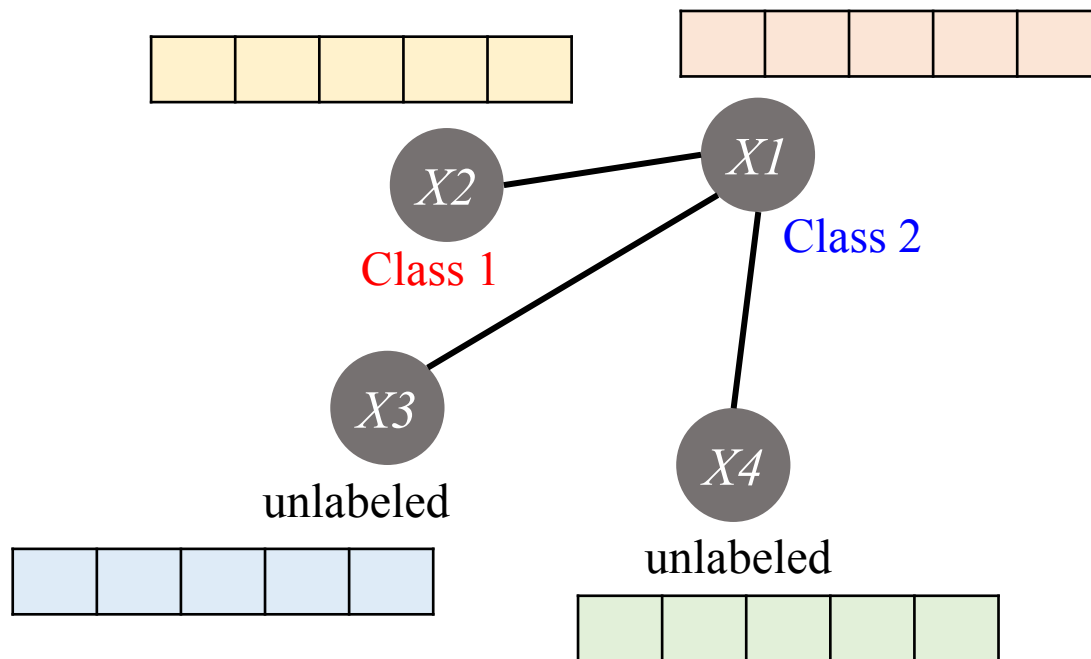
## ➤ Convolution theorem

- 한 domain 의 convolution은 다른 domain의 point-wise multiplication과 같음 → Graph domain의 convolution은 Fourier domain의 point-wise multiplication과 같음
- Convolution의 laplace 변환은 point-wise multiplication으로 변함

$$\mathcal{F}(f \star g) = \mathcal{F}\{f\} \odot \mathcal{F}\{g\} \quad x *_G g = \mathcal{F}^{-1}(\mathcal{F}(x) \odot \mathcal{F}(g))$$

# Graph-based Semi-Supervised Learning

$$\mathcal{L} = \mathcal{L}_0 + \lambda \mathcal{L}_{\text{reg}}, \quad \text{with} \quad \mathcal{L}_{\text{reg}} = \sum_{i,j} A_{ij} \|f(X_i) - f(X_j)\|^2 = f(X)^\top \Delta f(X)$$



Node-feature matrix

$$X \in \mathbf{R}^{n \times F}$$

orange	orange	orange	orange	orange
yellow	yellow	yellow	yellow	yellow
light blue	light blue	light blue	light blue	light blue
light green	light green	light green	light green	light green

Adjacency matrix

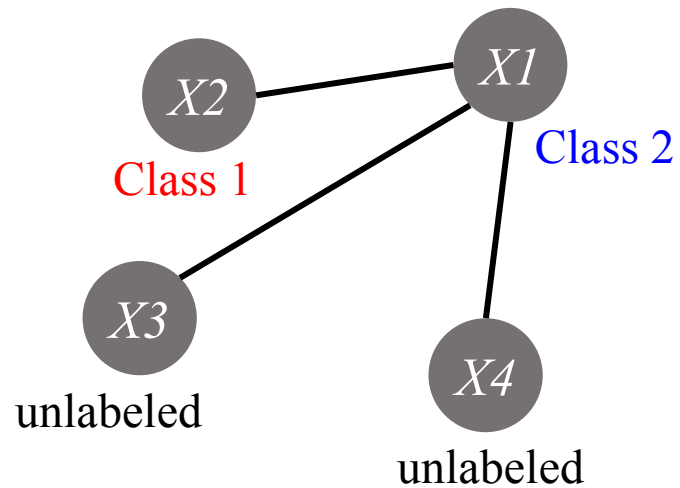
$$A \in \mathbf{R}^{n \times n}$$

0	1	1	1
1	0	0	0
1	0	0	0
1	0	0	0

# Graph-based Semi-Supervised Learning

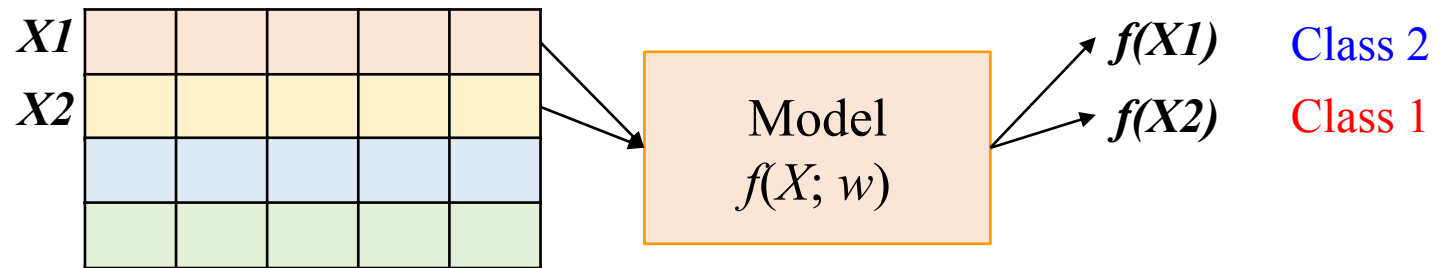
the supervised loss  
w.r.t. **the labeled part** of the graph

$$\mathcal{L} = \mathcal{L}_0 + \lambda \mathcal{L}_{\text{reg}}$$



**Node-feature matrix**

$$X \in \mathbb{R}^{n \times F}$$



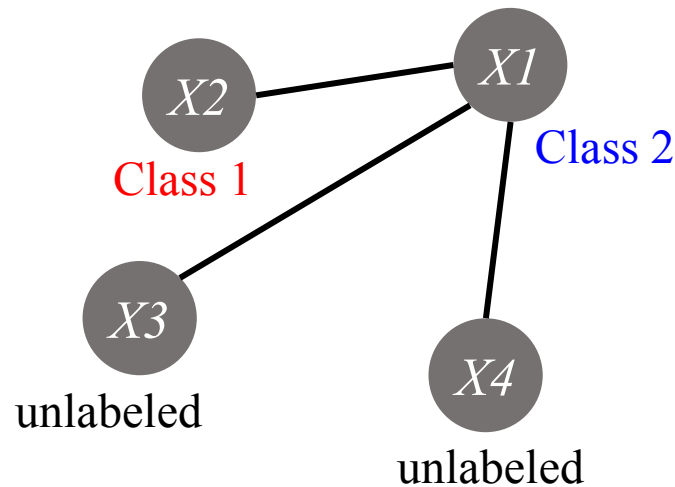
# Graph-based Semi-Supervised Learning

graph laplacian regularization term

$$\mathcal{L} = \mathcal{L}_0 + \lambda \mathcal{L}_{\text{reg}}$$

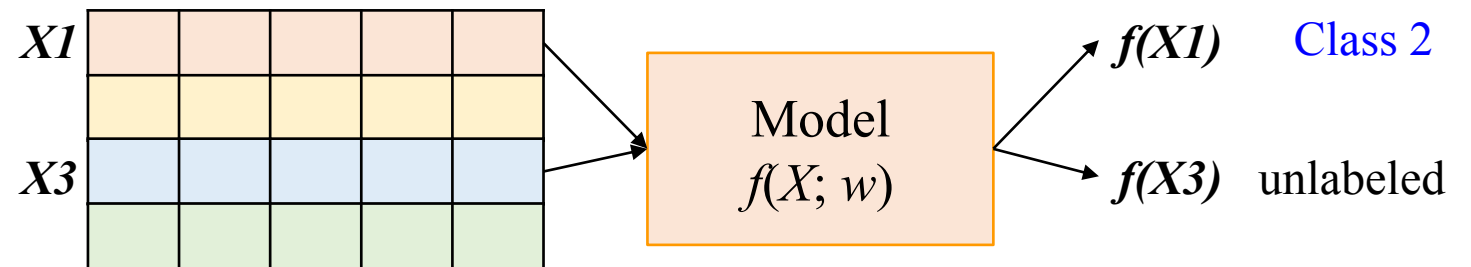
$$\mathcal{L}_{\text{reg}} = \sum_{i,j} A_{ij} \|f(X_i) - f(X_j)\|^2 = f(X)^\top \Delta f(X)$$

$f(X1)$        $f(X3)$



Node-feature matrix

$$X \in \mathbf{R}^{n \times F}$$



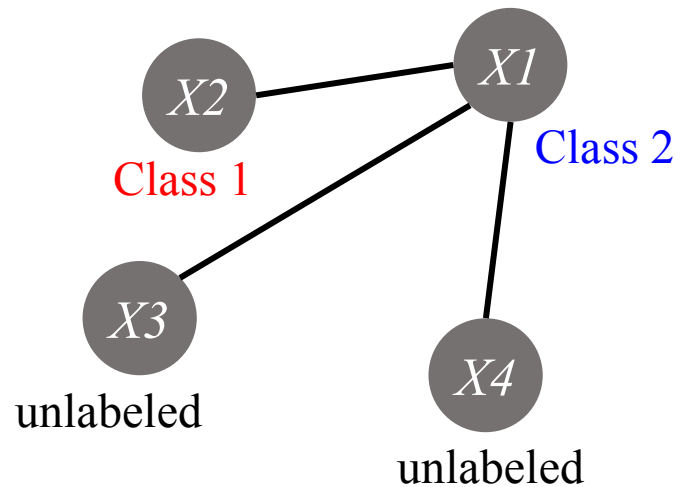
# Graph-based Semi-Supervised Learning

graph laplacian regularization term

$$\mathcal{L} = \mathcal{L}_0 + \lambda \mathcal{L}_{\text{reg}}$$

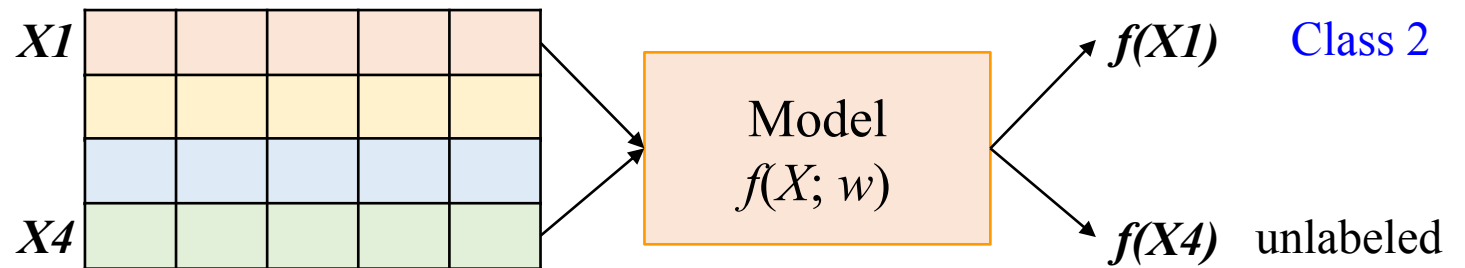
$$\mathcal{L}_{\text{reg}} = \sum_{i,j} A_{ij} \|f(X_i) - f(X_j)\|^2 = f(X)^\top \Delta f(X)$$

$f(X1) \quad f(X4)$



Node-feature matrix

$$X \in \mathbf{R}^{n \times F}$$



# Contributions

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- Graph-based Semi-Supervised Learning
  - ✓ Assumption: connected nodes in the graph  $\rightarrow$  share same labels
  - ✓ Limitation: could not contain additional information of the graph
- This work
  - ✓ Encode the graph structure using a neural network model  $f(\mathbf{X}, \mathbf{A})$   $\mathbf{X}$ : node-feature matrix,  $\mathbf{A}$ : Adjacency matrix
  - ✓ Can be used for fast and scalable semi-supervised classification of nodes in a graph

# Graph Convolutional Networks (GCN)

Graph convolution (Layer-wise propagation rule)

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

- $H^{(l)}$ : hidden state of the  $l$ -th layer
- $\tilde{A}$ :  $A$  (adjacency matrix) +  $I$  (Identity matrix)
- $\tilde{D}$ :  $\tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$
- $W^{(l)}$ : layer-specific trainable weight matrix
- $\sigma$ : activation function  $ReLU(\cdot)$

Multi-layers

$$Z = f(X, A) = \text{softmax} \left( \hat{A} \text{ReLU} \left( \hat{A} X W^{(0)} \right) W^{(1)} \right)$$

Layer 1

Layer 2



# Spectral Graph Convolutions

## ➤ Graph에 대한 Spectral convolution

- Graph domain  $\rightarrow$  Fourier domain
- **signal**  $x \in R^N \times$  **filter**  $g_\theta = \text{diag}(\theta)/\theta \in R^N$

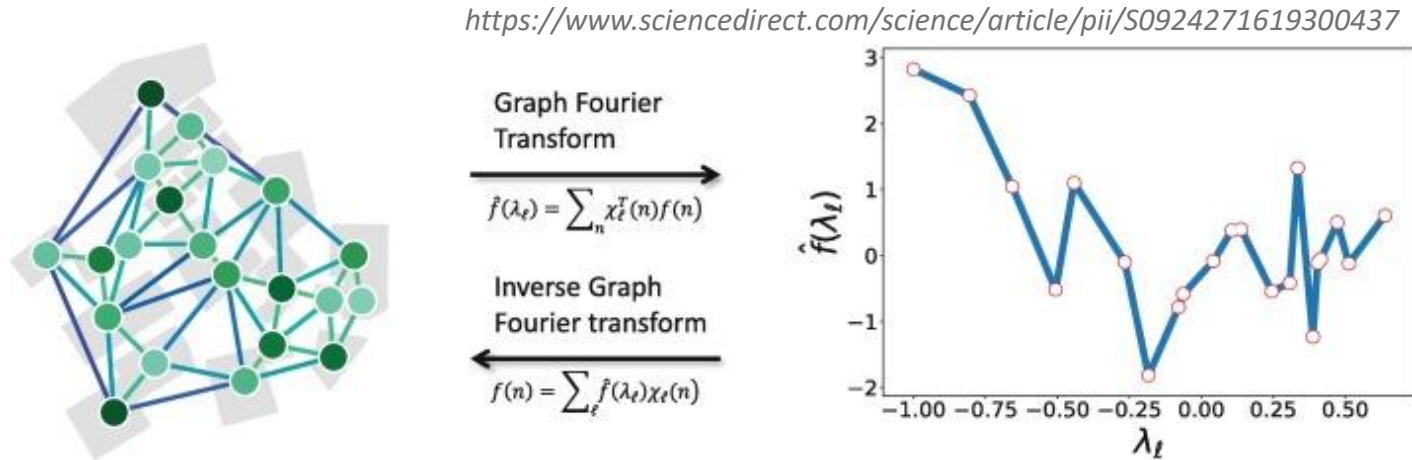
<p>Convolution theorem</p> $\mathcal{F}(f \star g) = \mathcal{F}\{f\} \odot \mathcal{F}\{g\}$		<p>signal <math>x \times</math> filter <math>g_\theta</math> in Fourier domain</p> $g_\theta * x = U g_\theta^* U^T x$
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## ➤ Graph Fourier Transform

- Graph를 signal / filter의 point-wise multiplication으로 적용하기 위해서, Fourier transform 적용 필요

## 2.1 SPECTRAL GRAPH CONVOLUTIONS

# Graph Fourier Transform



✓ Graph signal(Graph node features)을 Frequency(Features 간 차이)로 분해

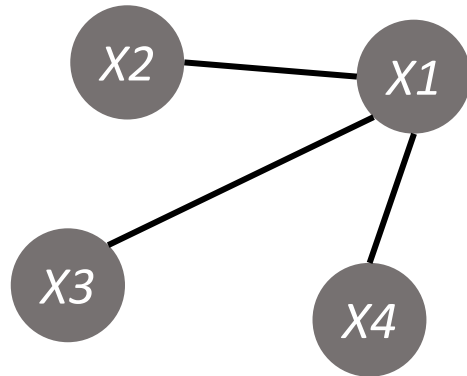
- Fourier Transform
  - 어떤 형태의 주파수가 Signal에 어느 정도로 포함되어 있는지 측정 가능
- Graph Fourier Transform
  - 어떤 형태의 그래프 관계가 Signal에 어느 정도로 포함되어 있는지 측정 가능
- GFT → Filtering → IGFT = Laplacian matrix를 Feature vector와 곱하는 것과 같음
  - Laplacian의 Eigen-vector가 Fourier Basis 역할을 함
  - GFT를 적용하여 Frequency가 낮은 관계들 (i.e., 유사 노드)을 우선적으로 반영

# Graph Laplacian (Laplacian Matrix)

## ➤ Graph laplacian:

- 한 노드의 특징  $\rightarrow$  해당 노드와 연결된 이웃노드와의 관계 관점에 표현
- 이웃 노드와의 차이 (변화)를 고려한 것  $\rightarrow$  그래프의 유용한 특성 반영

$$(\Delta\phi)(v) = \sum_{w:d(w,v)=1} [\phi(v) - \phi(w)]$$



Central node와 Neighbor node 간 차이

$$\Delta\phi(X1) = 3\phi(X1) - \phi(X2) - \phi(X3) - \phi(X4)$$

$$\Delta\phi(X2) = \phi(X2) - \phi(X1)$$

$$\Delta\phi(X3) = \phi(X3) - \phi(X1)$$

$$\Delta\phi(X4) = \phi(X4) - \phi(X1)$$

$$L = (\Delta\phi)(X) =$$

3	-1	-1	-1
-1	1	0	0
-1	0	1	0
-1	0	0	1

$$\begin{bmatrix} \phi(X1) \\ \phi(X2) \\ \phi(X3) \\ \phi(X4) \end{bmatrix} = D - A$$

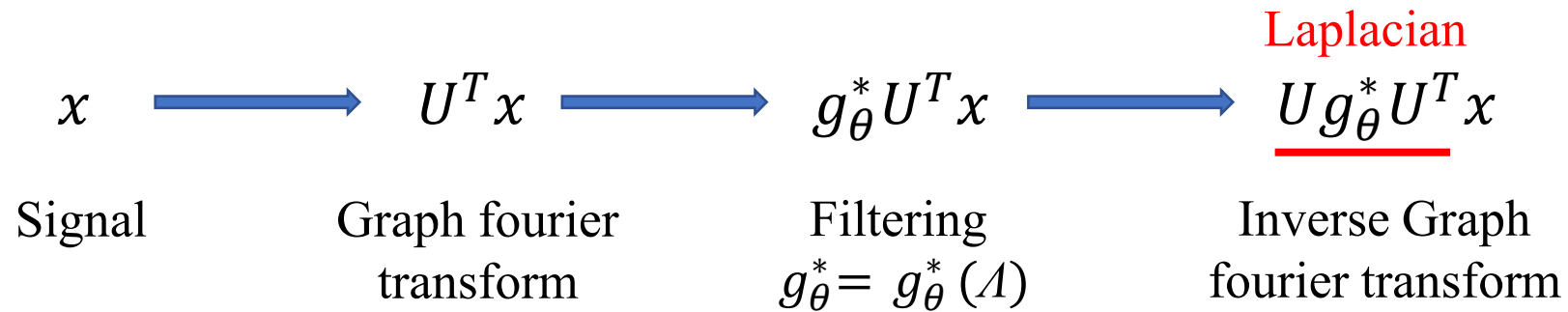
# Graph Laplacian (Laplacian Matrix)

signal  $x$   $\times$  filter  $g_\theta$  in Fourier domain

$$g_\theta * x = U g_\theta^* U^T x$$

Eigen decomposition

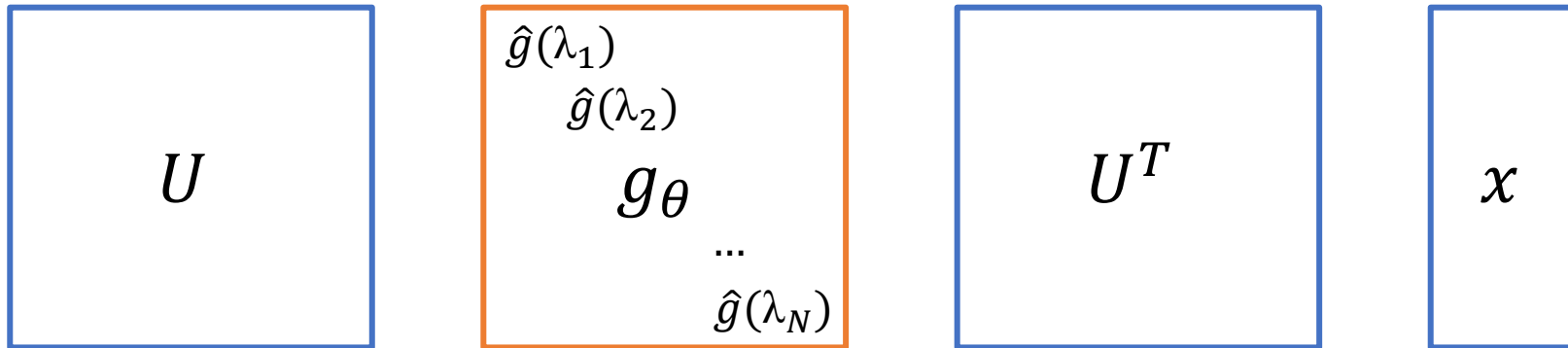
$$L = U \Lambda U^T$$



## Graph Laplacian (Laplacian Matrix)

signal  $x \times$  filter  $g_\theta$  in Fourier domain

$$g_\theta * x = U g_\theta^* U^T x$$



→ filter  $g_\theta$  is non-parametric  
High computation for eigen-decomposition

# Chebyshev Polynomials

$$\text{filter } g'_\theta(\Lambda) = \sum_{k=0}^K \theta'_k \Lambda^k = \theta'_0 \Lambda^0 + \theta'_1 \Lambda^1 + \dots + \theta'_K \Lambda^K$$

$$\Rightarrow g_\theta * x = U g'_\theta U^T x = U \left( \sum_{k=0}^{K-1} \theta_k \Lambda^k \right) U^T x = \sum_{k=0}^{K-1} \theta_k U \Lambda^k U^T x = \underline{\sum_{k=0}^{K-1} \theta_k L^k x}$$

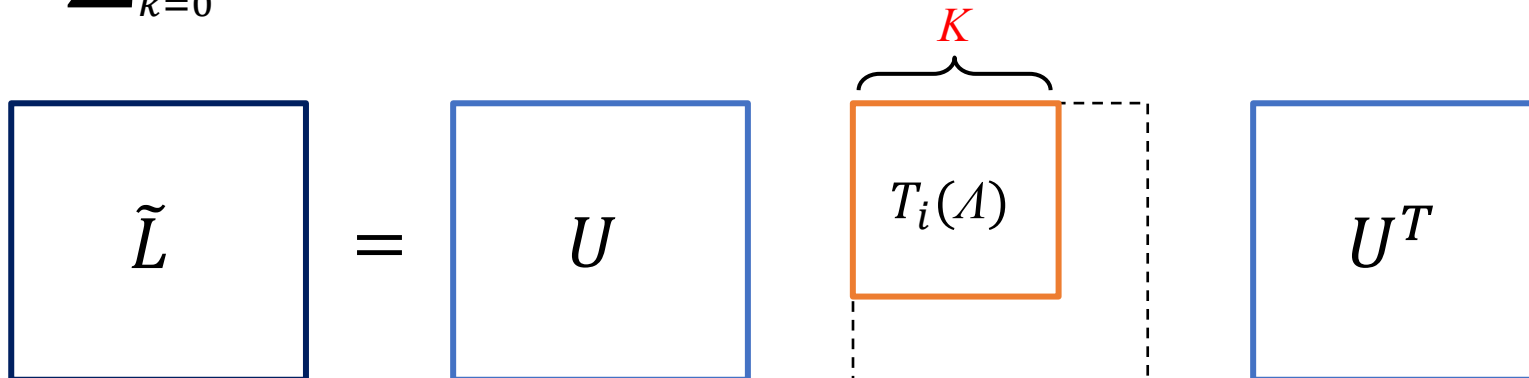
*K-Localized (K: neighbors)*

Chebyshev Polynomials  $T_k(x)$  활용하여 근사화

$$T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$$



$$\Rightarrow g'_\theta * x \approx \sum_{k=0}^K \theta'_k T_k(\tilde{L})x = \theta'_0 T_0(\tilde{L})x + \theta'_1 T_1(\tilde{L})x + \theta'_2 T_2(\tilde{L})x + \dots + \theta'_K T_K(\tilde{L})x$$



## Layer-wise Linear Model

### Chebyshev Polynomials

$$\Rightarrow g'_\theta * x \approx \sum_{k=0}^K \theta'_k T_k(\tilde{L})x = \theta'_0 T_0(\tilde{L})x + \theta'_1 T_1(\tilde{L})x + \theta'_2 T_2(\tilde{L})x + \cdots + \theta'_K T_K(\tilde{L})x$$

### Chebyshev Polynomials (K=1)

$$\begin{aligned} \Rightarrow g'_\theta * x &\approx \theta'_0 T_0(\tilde{L})x + \theta'_1 T_1(\tilde{L})x \\ &\approx \theta'_0 \cdot 1 \cdot x + \theta'_1 (L - I_N)x \\ &\approx \theta'_0 \cdot 1 \cdot x + \theta'_1 D^{-1/2} A D^{-1/2} x \\ &\approx \theta \left( I_N + D^{-\frac{1}{2}} A D^{-\frac{1}{2}} \right) x \end{aligned}$$

$$\Rightarrow Z = \tilde{D}^{-\frac{1}{2}} A \tilde{D}^{-\frac{1}{2}} X \Theta$$

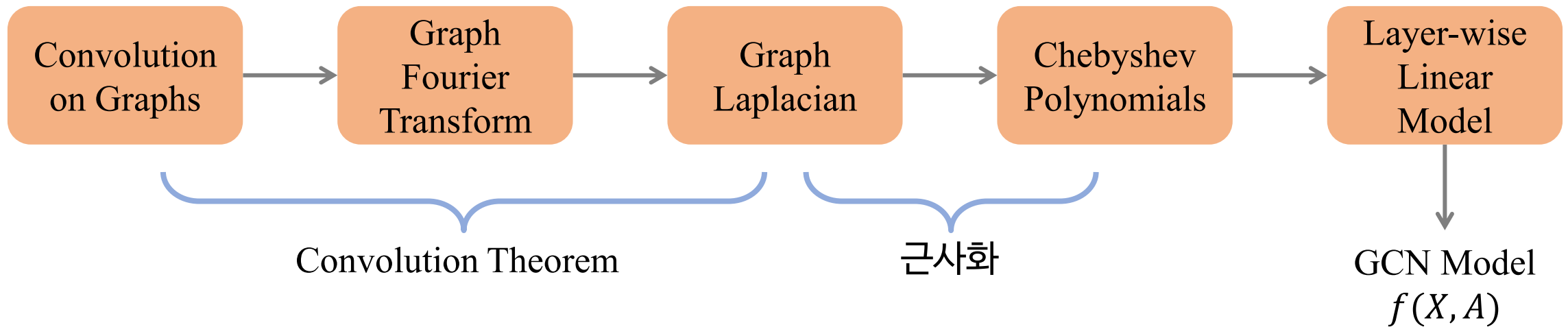
Renormalization

$$\tilde{L} = \frac{2}{\lambda_{\max}} L - I_N = L - I_N$$

$$L = I_N - D^{-1/2} A D^{-1/2}$$

$$\theta = \theta'_0 = -\theta'_1$$

### Summary





# Graph Convolutional Networks (GCN)

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

Layer 1

$$Z = f(X, A) = \text{softmax} \left( \hat{A} \text{ReLU} \left( \hat{A} X W^{(0)} \right) W^{(1)} \right)$$

Layer 2

→ Two-layer convolutional neural network

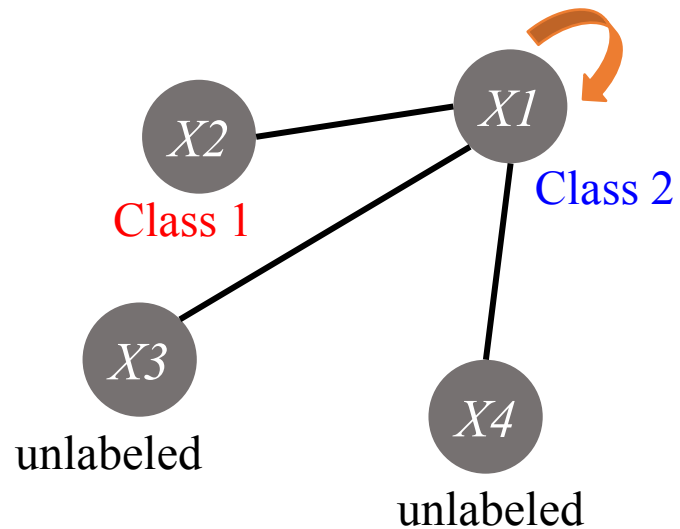
**Loss function**

$$\mathcal{L} = - \sum_{l \in \mathcal{Y}_L} \sum_{f=1}^F Y_{lf} \ln Z_{lf}$$

- Cross-entropy error는 Labeled example에 대하여 진행
- $W^{(0)}, W^{(1)}$ 은 Gradient descent를 사용하여 훈련됨
- Full batch gradient descent 사용

## Graph Convolutional Networks (GCN)

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



$$A(4 \times 4)$$

0	1	1	1
1	0	0	0
1	0	0	0
1	0	0	0

$$I(4 \times 4)$$

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

self connections

$$\tilde{A}(4 \times 4)$$

1	1	1	1
1	1	0	0
1	0	1	0
1	0	0	1

$$D(4 \times 4)$$

3	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

$$\tilde{D}(4 \times 4)$$

4	0	0	0
0	2	0	0
0	0	2	0
0	0	0	2



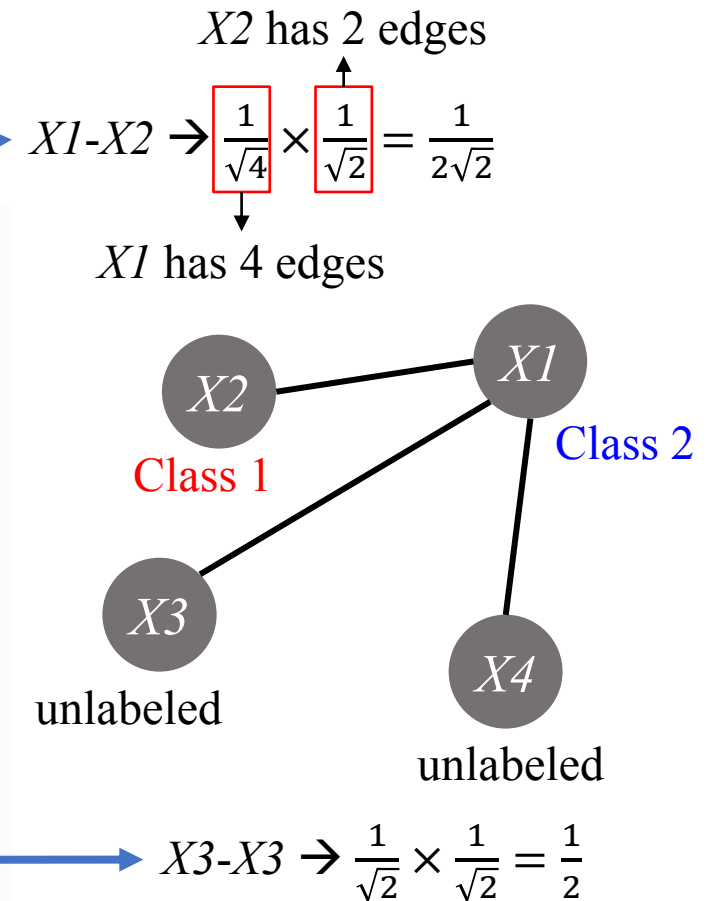
# Graph Convolutional Networks (GCN)

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

$$\tilde{D}^{-\frac{1}{2}} A \tilde{D}^{-\frac{1}{2}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

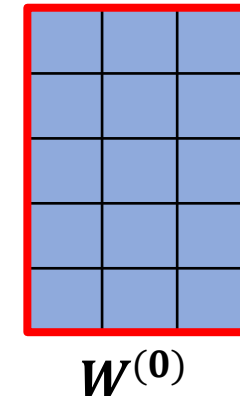
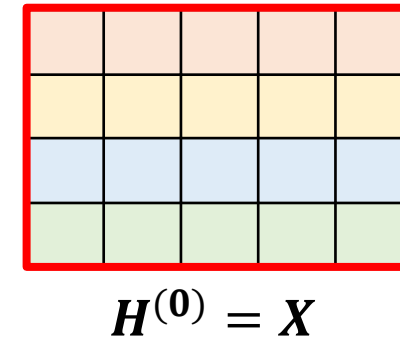
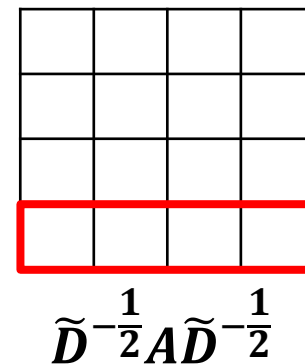
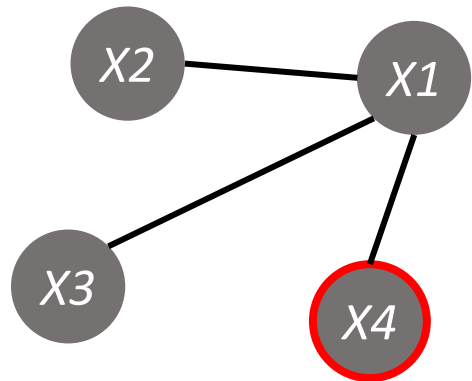
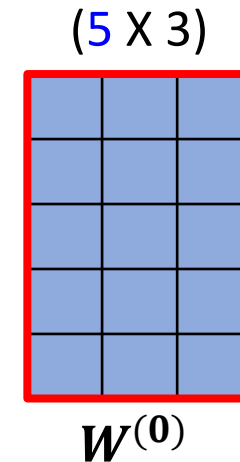
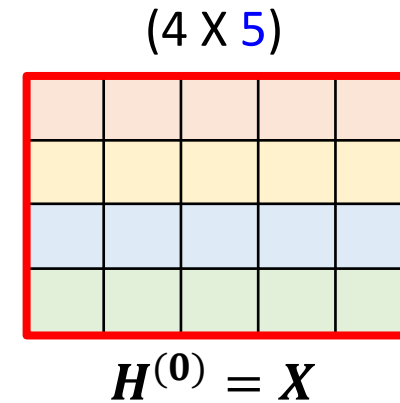
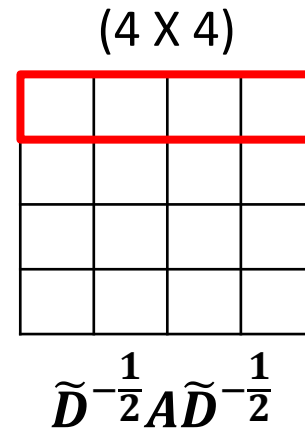
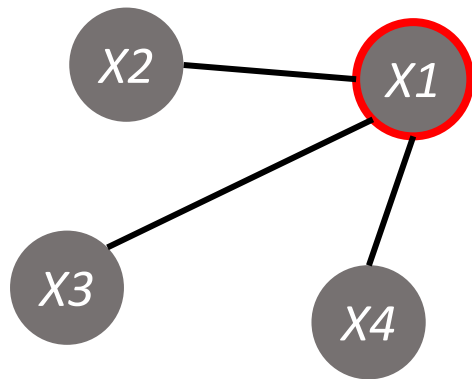
$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{1}{4} & \frac{1}{4} & 0 & 0 \\ \frac{1}{4} & 0 & \frac{1}{4} & 0 \\ \frac{1}{4} & 0 & 0 & \frac{1}{4} \end{bmatrix}$$

Handwritten matrices and labels for nodes  $x_1, x_2, x_3, x_4$  are shown. Red circles highlight the values  $\frac{1}{4}$  in the matrix corresponding to the  $x_1-x_2$  and  $x_3-x_3$  edges.



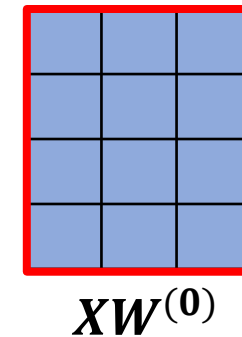
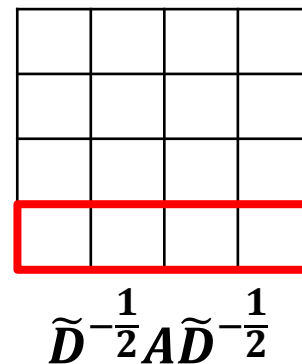
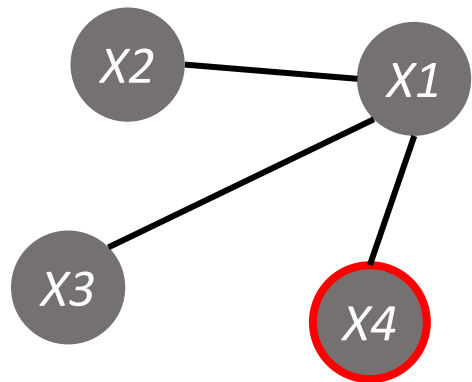
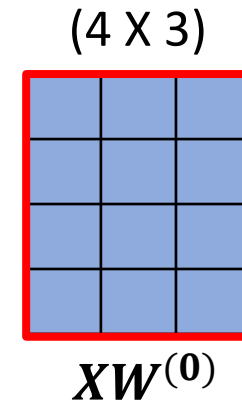
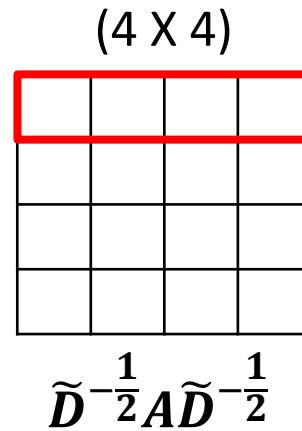
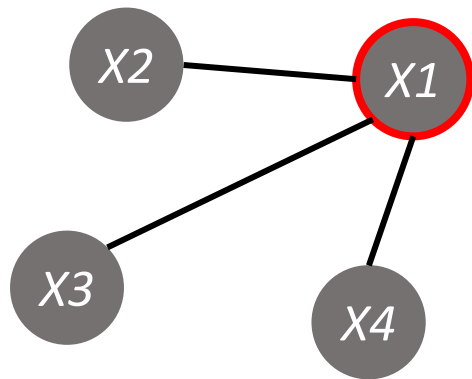
# Graph Convolutional Networks (GCN)

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



# Graph Convolutional Networks (GCN)

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



## Two-layer GCN

Layer 1

$$Z = f(X, A) = \text{softmax}\left(\hat{A} \text{ReLU}\left(\hat{A}XW^{(0)}\right)W^{(1)}\right)$$

$$\begin{aligned} H^{(1)} &= \sigma(\tilde{D}^{-\frac{1}{2}}A\tilde{D}^{-\frac{1}{2}}H^{(0)}W^{(0)}) \\ &= \text{ReLU}(\tilde{D}^{-\frac{1}{2}}A\tilde{D}^{-\frac{1}{2}}H^{(0)}W^{(0)}) \\ &= \text{ReLU}(\hat{A}XW^{(0)}) \end{aligned}$$

$$H^{(1)} = \text{ReLU} \left( \begin{array}{c} \begin{array}{|c|c|c|c|} \hline & & & \\ \hline & & & \\ \hline & & & \\ \hline & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|} \hline \text{orange} & \text{orange} & \text{orange} & \text{orange} & \text{orange} \\ \hline \text{yellow} & \text{yellow} & \text{yellow} & \text{yellow} & \text{yellow} \\ \hline \text{light blue} & \text{light blue} & \text{light blue} & \text{light blue} & \text{light blue} \\ \hline \text{green} & \text{green} & \text{green} & \text{green} & \text{green} \\ \hline \end{array} & \begin{array}{|c|c|c|} \hline \text{blue} & \text{blue} & \text{blue} \\ \hline \text{blue} & \text{blue} & \text{blue} \\ \hline \text{blue} & \text{blue} & \text{blue} \\ \hline \text{blue} & \text{blue} & \text{blue} \\ \hline \text{blue} & \text{blue} & \text{blue} \\ \hline \text{blue} & \text{blue} & \text{blue} \\ \hline \end{array} \end{array} \right) = \begin{array}{|c|c|c|} \hline \text{orange} & \text{orange} & \text{orange} \\ \hline \text{yellow} & \text{yellow} & \text{yellow} \\ \hline \text{light blue} & \text{light blue} & \text{light blue} \\ \hline \text{green} & \text{green} & \text{green} \\ \hline \end{array}$$

$\tilde{D}^{-\frac{1}{2}}A\tilde{D}^{-\frac{1}{2}}$ 
 $H^{(0)} = X$ 
 $W^{(0)}$

## Two-layer GCN

Layer 2

$$Z = f(X, A) = \text{softmax}\left(\hat{A} \text{ReLU}\left(\hat{A}XW^{(0)}\right)W^{(1)}\right)$$

$$\begin{aligned} Z &= f(X, A) \\ &= \text{softmax}(A^{\wedge} \text{ReLU}(A^{\wedge}XW^{(0)})W^{(1)}) \\ &= \text{softmax}(A^{\wedge}H^{(1)}W^{(1)}) \end{aligned}$$

$$Z = \text{softmax} \left( \begin{array}{c} \begin{array}{|c|c|c|c|} \hline & & & \\ \hline & & & \\ \hline & & & \\ \hline & & & \\ \hline \end{array} & \begin{array}{|c|c|c|} \hline \text{orange} & \text{orange} & \text{orange} \\ \hline \text{yellow} & \text{yellow} & \text{yellow} \\ \hline \text{blue} & \text{blue} & \text{blue} \\ \hline \text{green} & \text{green} & \text{green} \\ \hline \end{array} & \begin{array}{|c|c|} \hline \text{blue} & \text{blue} \\ \hline \text{blue} & \text{blue} \\ \hline \text{blue} & \text{blue} \\ \hline \end{array} \end{array} \right) = \begin{array}{|c|c|} \hline \text{orange} & \text{orange} \\ \hline \text{yellow} & \text{yellow} \\ \hline \text{blue} & \text{blue} \\ \hline \text{green} & \text{green} \\ \hline \end{array} \begin{array}{l} \rightarrow \text{Class 1} \\ \rightarrow \text{Class 2} \end{array}$$

$\tilde{D}^{-\frac{1}{2}}A\tilde{D}^{-\frac{1}{2}}$ 
 $H^{(1)}$ 
 $W^{(1)}$

## 4 EXPERIMENTS

### Datasets

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Dataset	Type	Nodes	Edges	Classes	Features	Label rate
Citeseer	Citation network	3,327	4,732	6	3,703	0.036
Cora	Citation network	2,708	5,429	7	1,433	0.052
Pubmed	Citation network	19,717	44,338	3	500	0.003
NELL	Knowledge graph	65,755	266,144	210	5,414	0.001

Node: Documents

Edge: Citation Links

Label rate: training nodes / entire node

Node feature: sparse bag of words



# Set-up and Baselines

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- Set-up
  - ✓ Two-layer GCN (10-layer GCN in appendix)
  - ✓ A test set of 1,000 labeled examples
  - ✓ Train all models for 200 epochs using Adam
  - ✓ A learning rate of 0.01
  - ✓ Initialize weights using the initialization in Glorot & Bengio (2010)
- Baselines
  - ✓ Label propagation(LP)
  - ✓ Semi-supervised embedding (SemiEmb)
  - ✓ Manifold regularization (ManiReg)
  - ✓ Skip-gram based graph embeddings (DeepWalk)
  - ✓ Iterative classification algorithm (ICA)
  - ✓ Planetoid (Planetoid)

## Semi-Supervised Node Classification

- Mean accuracy of 100 runs with random weight initialization
- Hyperparameters
  - Citeseer, Cora and Pubmed: 0.5 (dropout rate),  $5 \cdot 10^{-4}$  (L2 regularization) and 16 (number of hidden units)
  - NELL: 0.1 (dropout rate),  $1 \cdot 10^{-5}$  (L2 regularization) and 64 (number of hidden units)

Method	Citeseer	Cora	Pubmed	NELL	
ManiReg [3]	60.1	59.5	70.7	21.8	
SemiEmb [28]	59.6	59.0	71.1	26.7	
LP [32]	45.3	68.0	63.0	26.5	
DeepWalk [22]	43.2	67.2	65.3	58.1	
ICA [18]	69.1	75.1	73.9	23.1	
Planetoid* [29]	64.7 (26s)	75.7 (13s)	77.2 (25s)	61.9 (185s)	
<b>GCN (this paper)</b>	<b>70.3 (7s)</b>	<b>81.5 (4s)</b>	<b>79.0 (38s)</b>	<b>66.0 (48s)</b>	Classification accuracy
GCN (rand. splits)	67.9 $\pm$ 0.5	80.1 $\pm$ 0.5	78.9 $\pm$ 0.7	58.4 $\pm$ 1.7	Training time until convergence

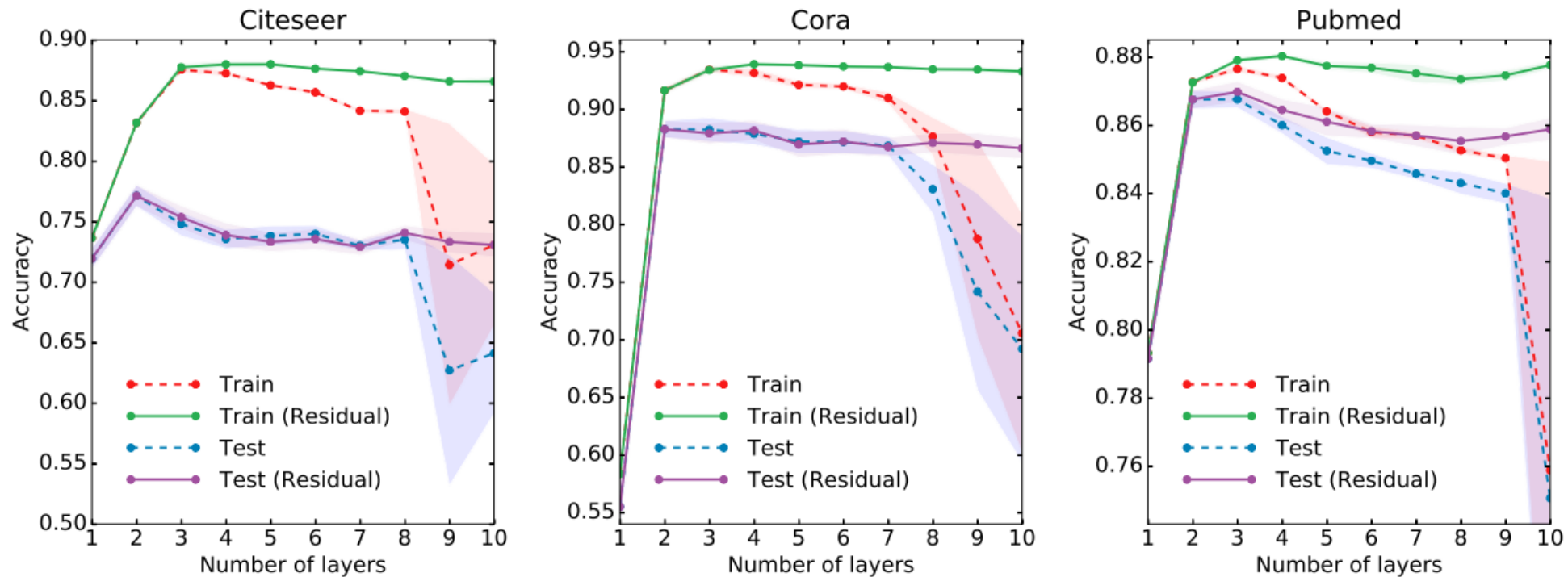
## Evaluation of Propagation Model

- Compare different variants of our proposed per-layer propagation model on the citation network datasets

Description	Propagation model	Citeseer	Cora	Pubmed	
Chebyshev filter (Eq. 5)	$K = 3$	69.8	79.5	74.4	
	$K = 2$	69.6	81.2	73.8	
1 <sup>st</sup> -order model (Eq. 6)	$X\Theta_0 + D^{-\frac{1}{2}}AD^{-\frac{1}{2}}X\Theta_1$	68.3	80.0	77.5	
Single parameter (Eq. 7)	$(I_N + D^{-\frac{1}{2}}AD^{-\frac{1}{2}})X\Theta$	69.3	79.2	77.4	
<b>Renormalization trick (Eq. 8)</b>	$\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}X\Theta$	<b>70.3</b>	<b>81.5</b>	<b>79.0</b>	original model
1 <sup>st</sup> -order term only	$D^{-\frac{1}{2}}AD^{-\frac{1}{2}}X\Theta$	68.7	80.5	77.8	
Multi-layer perceptron	$X\Theta$	46.5	55.1	71.4	

# Experiments on Model Depth

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



# Conclusions and Limitations

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- GCN model for semi-supervised classification on graph-structured data
  - Spectral graph convolutions
  - Layer-wise linear model
  
- Memory requirement
  - Full-batch gradient descent → Memory requirement grows
  - Mini-batch stochastic gradient descent
  
- Directed edges and edge features
  - Limited to undirected graphs (weighted or unweighted)
  
- Limiting assumptions
  - Equal importance of self-connections vs. edges to neighboring nodes

# References

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- [발표자료] Semi-supervised Classification with Graph Convolutional Networks, 윤훈상, 고려대학교.
- [발표자료] Spectral-based Graph Convolutional Networks, 최종현, 고려대학교.
- [발표자료] Graph Convolution Networks, 이민정, 고려대학교.
- Convolution, <https://en.wikipedia.org/wiki/Convolution>
- Semi-supervised learning, [https://en.wikipedia.org/wiki/Semi-supervised\\_learning](https://en.wikipedia.org/wiki/Semi-supervised_learning)