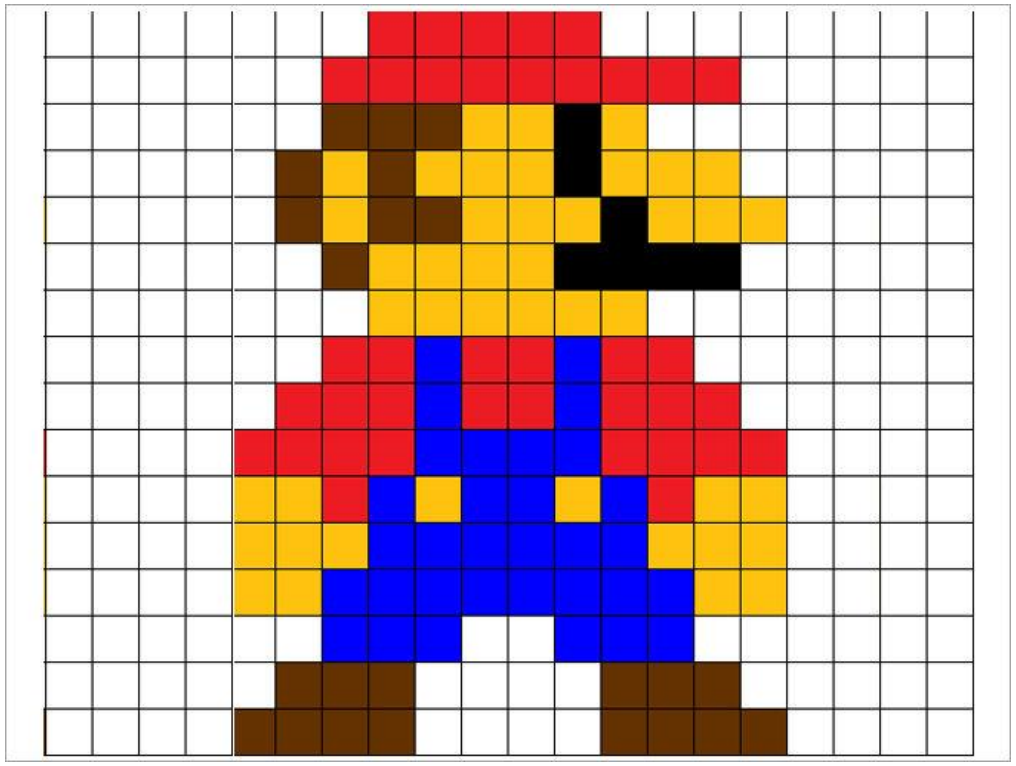
What is Graph?

Data Representation – Image and Sentence

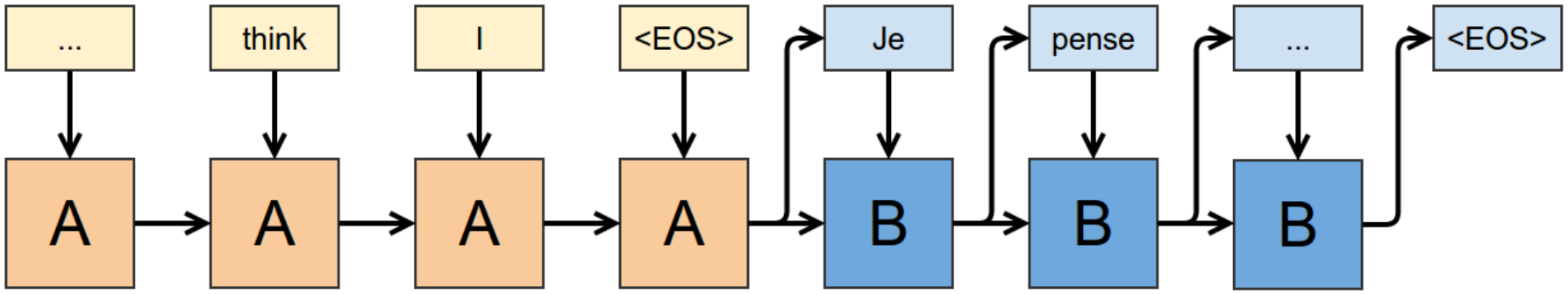
Image



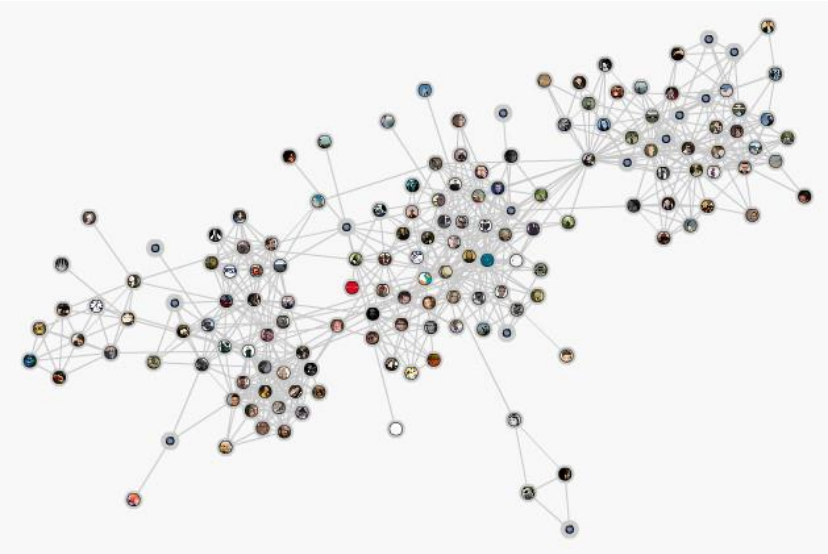
Images are represented with values on each pixel

Sentences are represented with character values

Sentence

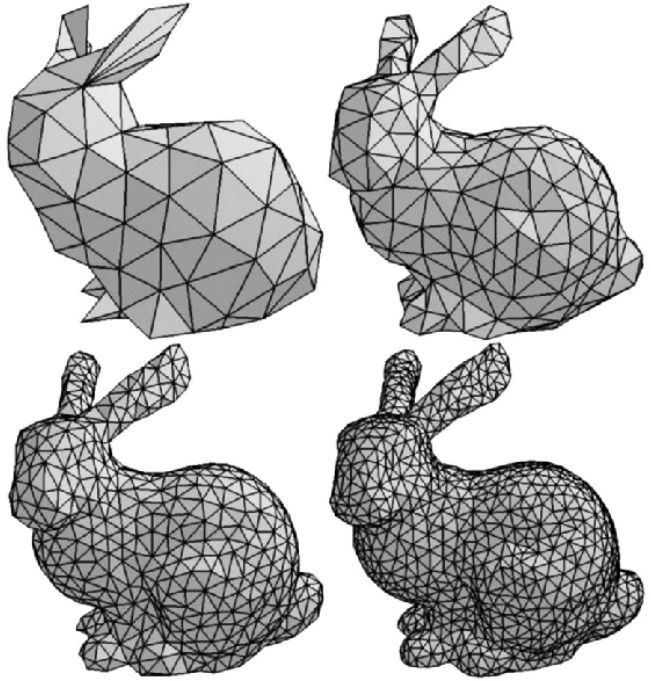


Data Representation – Graph

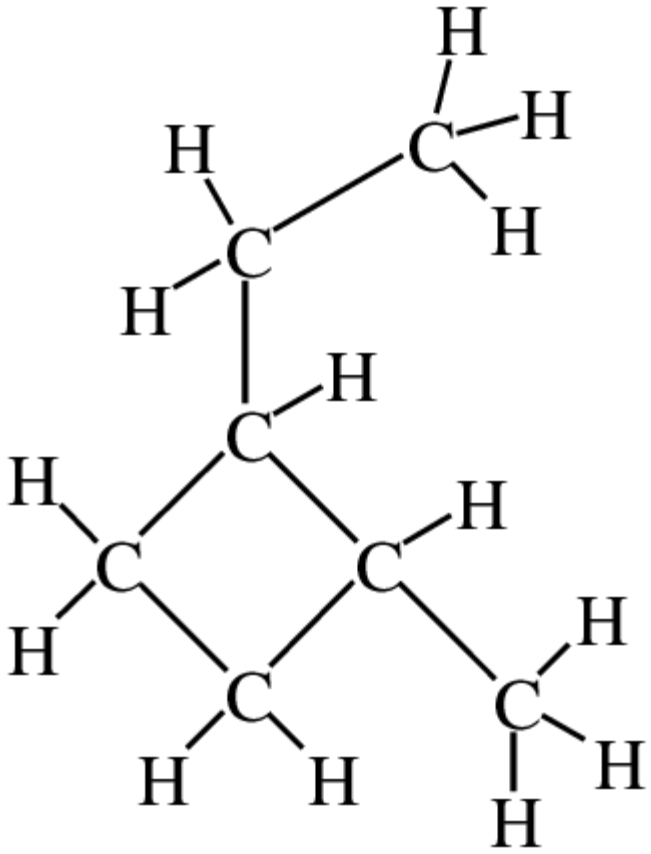


Social Graph : 사람들간의 관계

ex.) facebook



3D Mesh



Molecular Graph

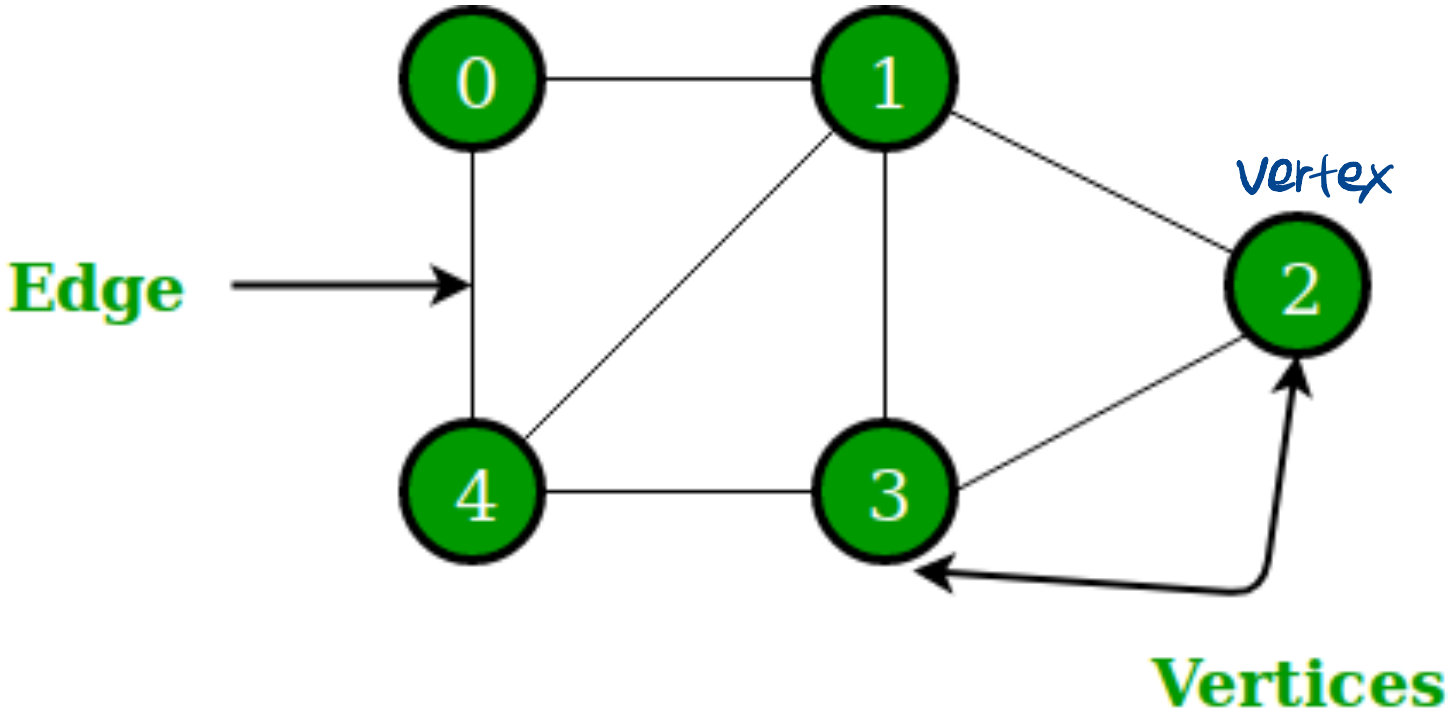
분자

Graph Structure

Directed graph

Undirected graph

weighted unweighted



Vertex (Node)

ex) User (gender, age ···)

Edge

ex) relationship(intimacy, ···)

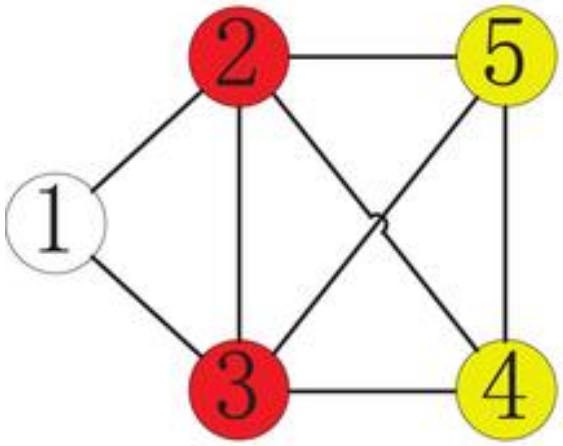
Graph Structure

Vertex (Node)
Node Feature Matrix

Edge
Adjacency Matrix

node n개

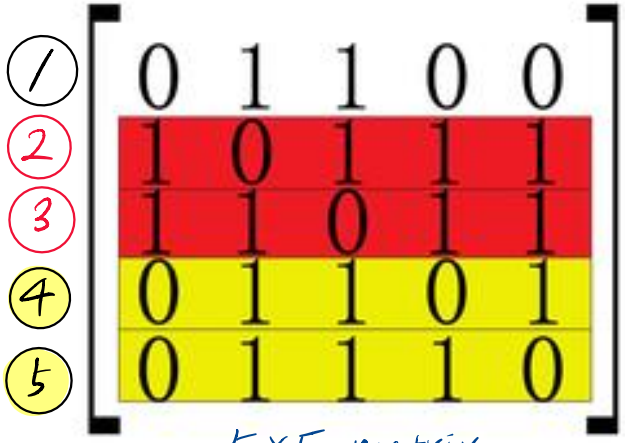
Network



5 nodes

n x n matrix

Adjacency matrix A



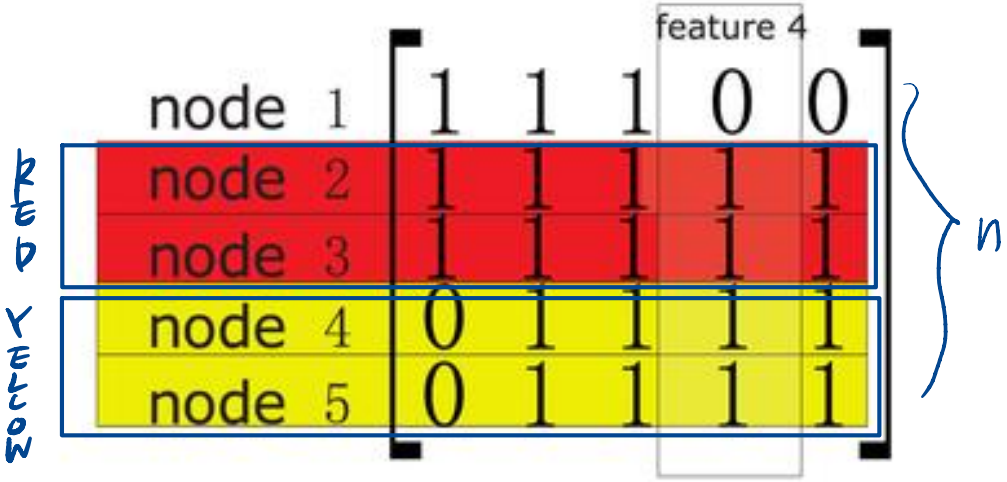
5 x 5 matrix

A_{ij} = i번째 node와 j번째 node가 연결되어있는냐 (edge의 유무)

n x f matrix

feature 개수 : f

Feature matrix A+I

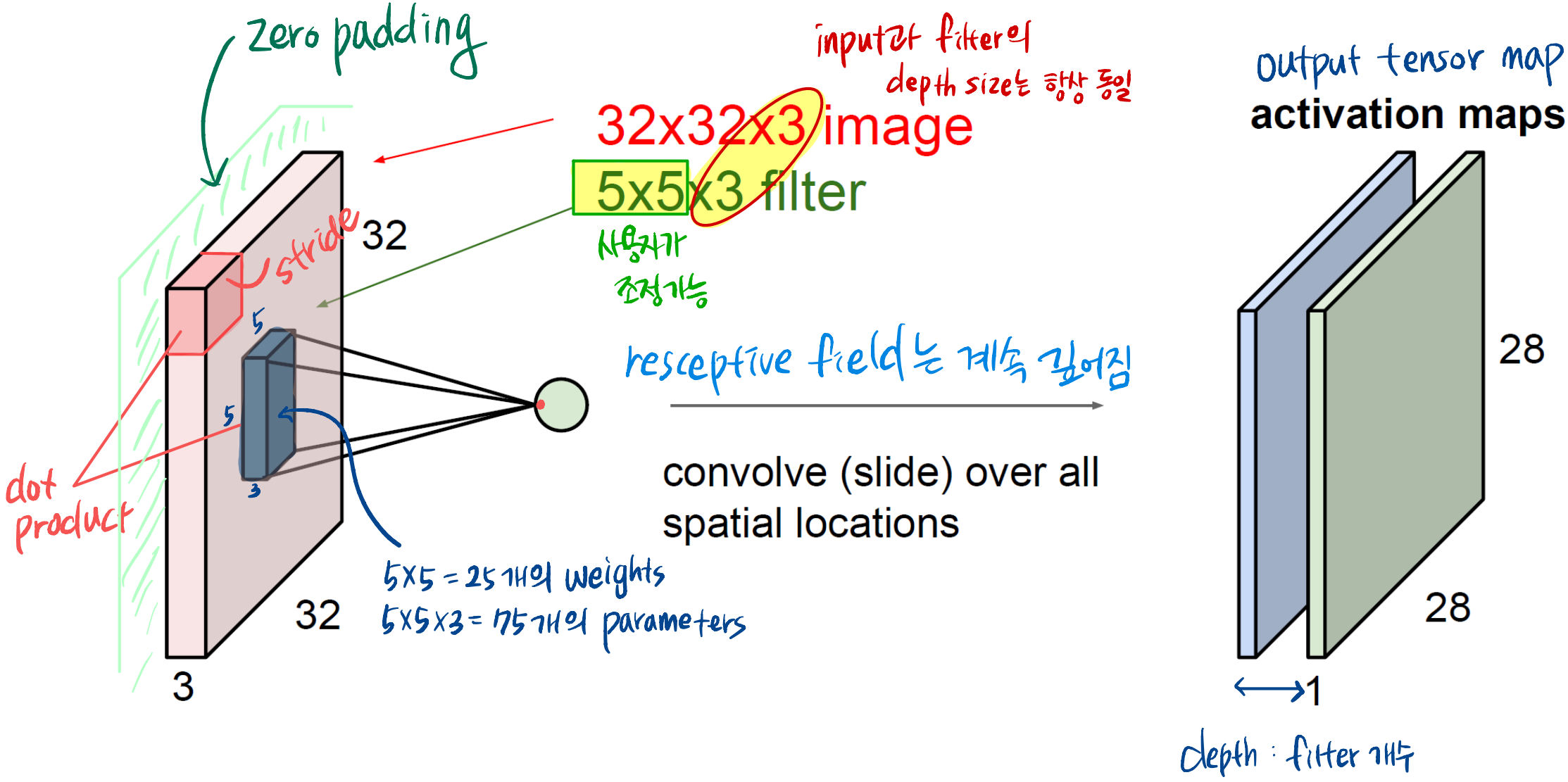


X_{ij} = i번째 노드의 j번째 feature

node가 가진 정보 : 색깔

Graph Convolution Network

Convolution Layer
: Preserve the spatial structure



Weight sharing

Reduce the number of parameters (같은 filter)
–〉 less overfitting, low computational cost

Learn local features 

Translation invariance (이미지가 달라져도 값이 비슷하게 나옴)

What should we update?

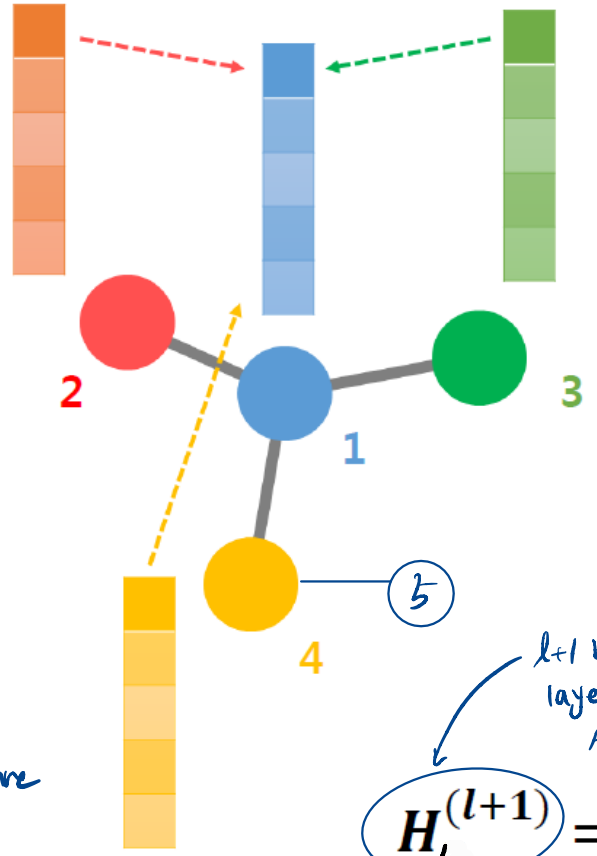
CNN updates values in activation map in each layer.
Values of activation map determine the state of image.

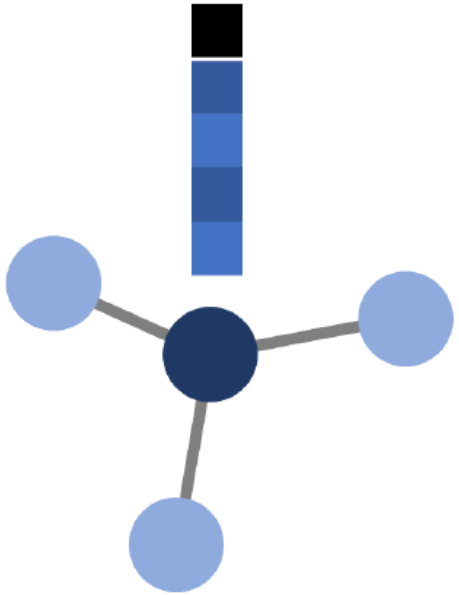
Values of each node feature determine the state of graph.

–〉 Make each layer of network update values of each node feature

How to update hidden states in GCN

① weight sharing





$H_i^{(l)}$ $W^{(l)}$

n: node f: feature

feature map n×f

$l+1$ 번째 layer을 통과한 H_i의 정보

l번째 layer의 weight

(local) node i와 연결되어있는 node들

$$H_i^{(l+1)} = \sigma\left(H_1^{(l)}W^{(l)} + H_2^{(l)}W^{(l)} + H_3^{(l)}W^{(l)} + H_4^{(l)}W^{(l)} + b^{(l)}\right)$$

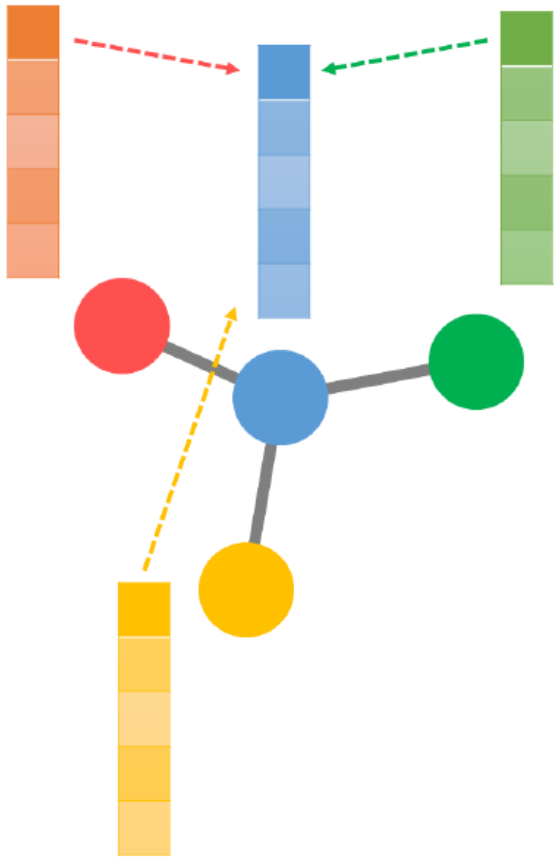
1st node

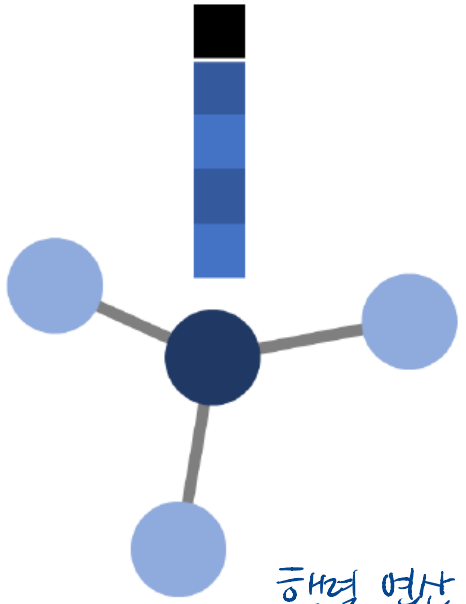
$$H_i^{(l+1)} = \sigma\left(\sum_{j\in N(i)} H_j^{(l)}W^{(l)} + b^{(l)}\right)$$

Hidden state (node - feature matrix)

weight sharing → general한 특성을 추출

How to update hidden states in GCN





행렬 연산 이용

$$H^{(l+1)} = \sigma\left(AH^{(l)}W^{(l)} + b^{(l)}\right)$$

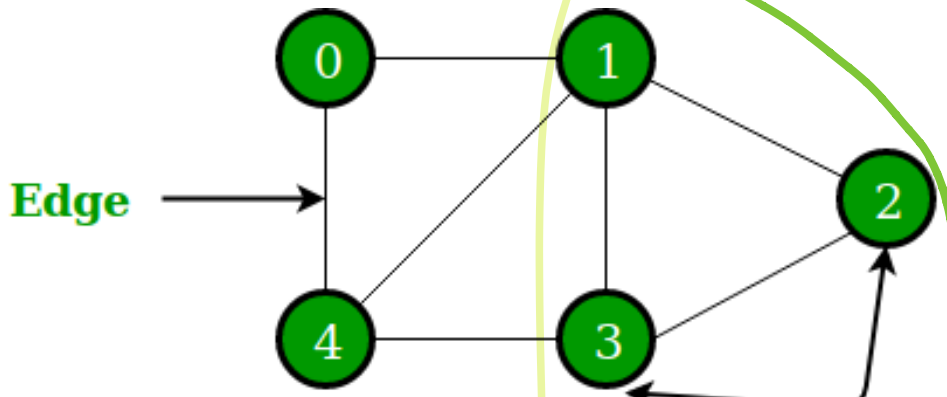
learnable parameters are shared

How to update hidden states in GCN

$$H^{(l+1)} = \sigma(AH^{(l)}W^{(l)} + b^{(l)})$$

filter의 역할

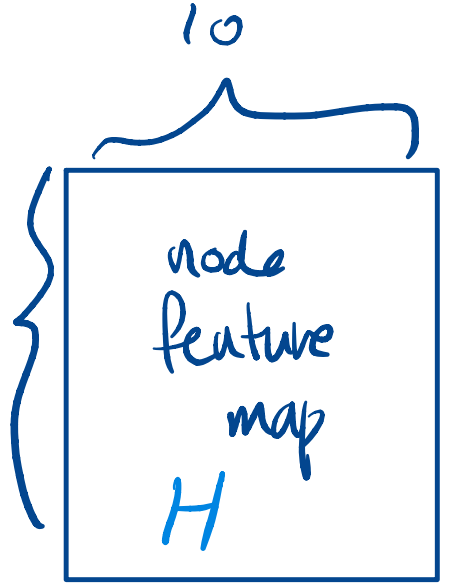
본인의 이전 정보를 받기 위해 1을 채워넣음

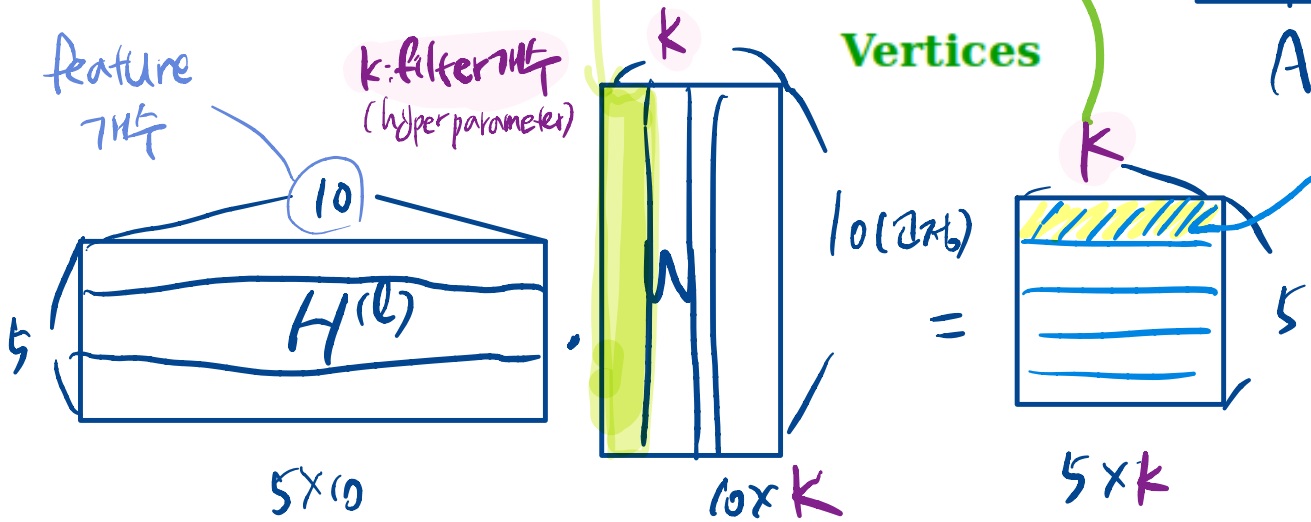


A

	0	1	2	3	4
0	1	1	0	0	1
1	1	1	1	1	1
2	0	1	1	1	0
3	0	1	1	1	1
4	1	1	0	1	1

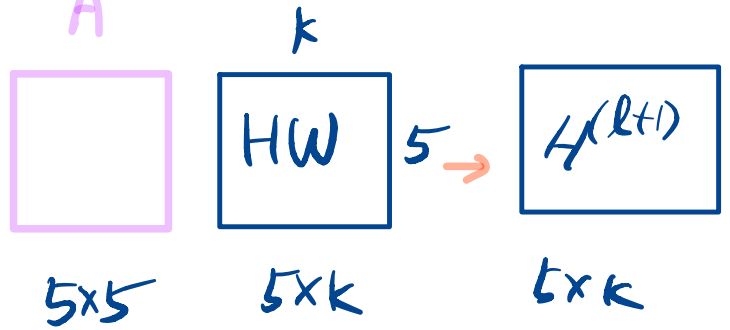
Adjacency matrix 5×5



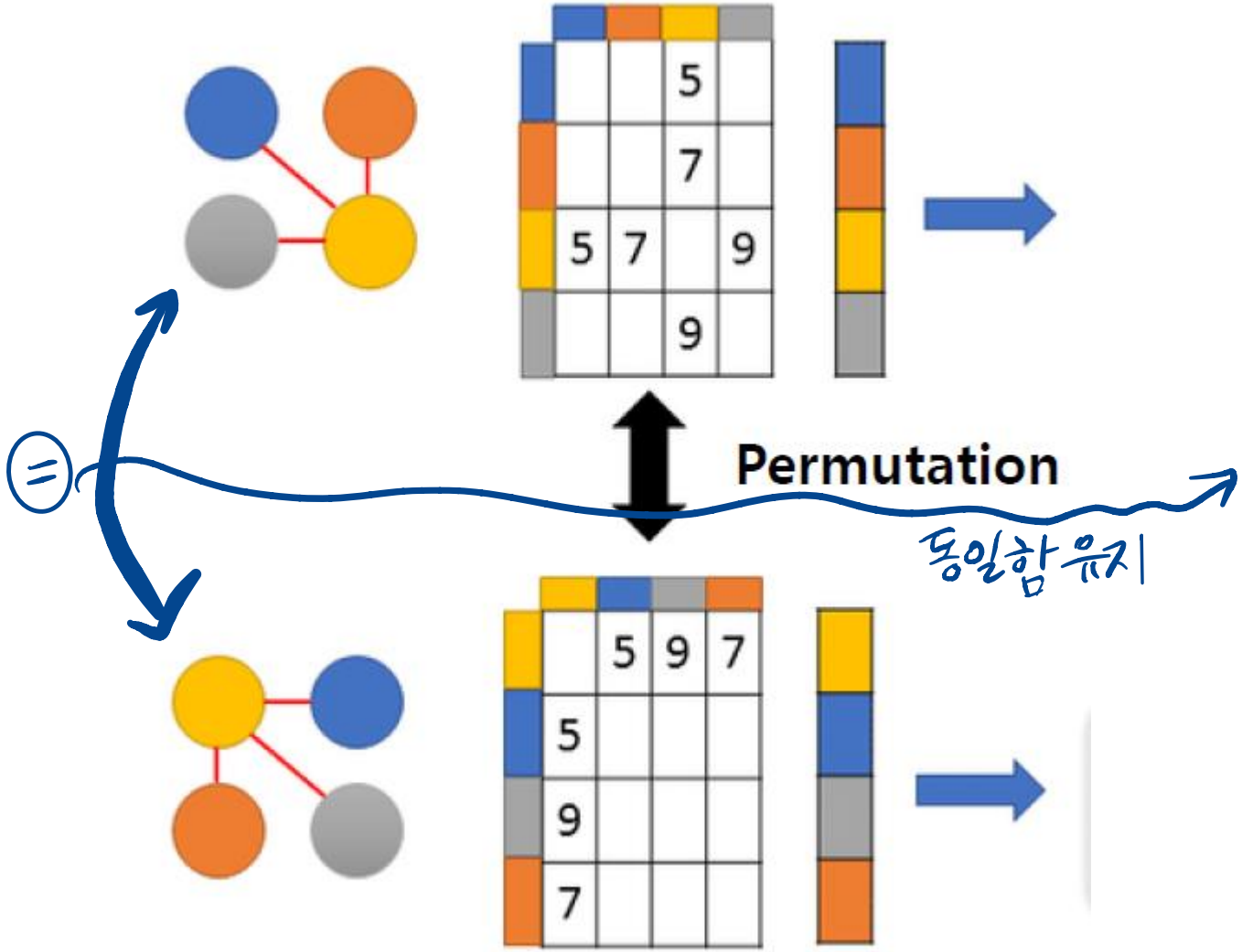


첫번째 node의 더 고차원적인 정보를 담음

글자에 있는 정보만 받아들임



Readout – Permutation Invariance



Node-wise summation

$$z_G = \tau\left(\sum_{i \in G} MLP\left(H_i^{(L)}\right)\right)$$

$MLP = \varphi(W^T x + b)$

Overall Structure of GCN