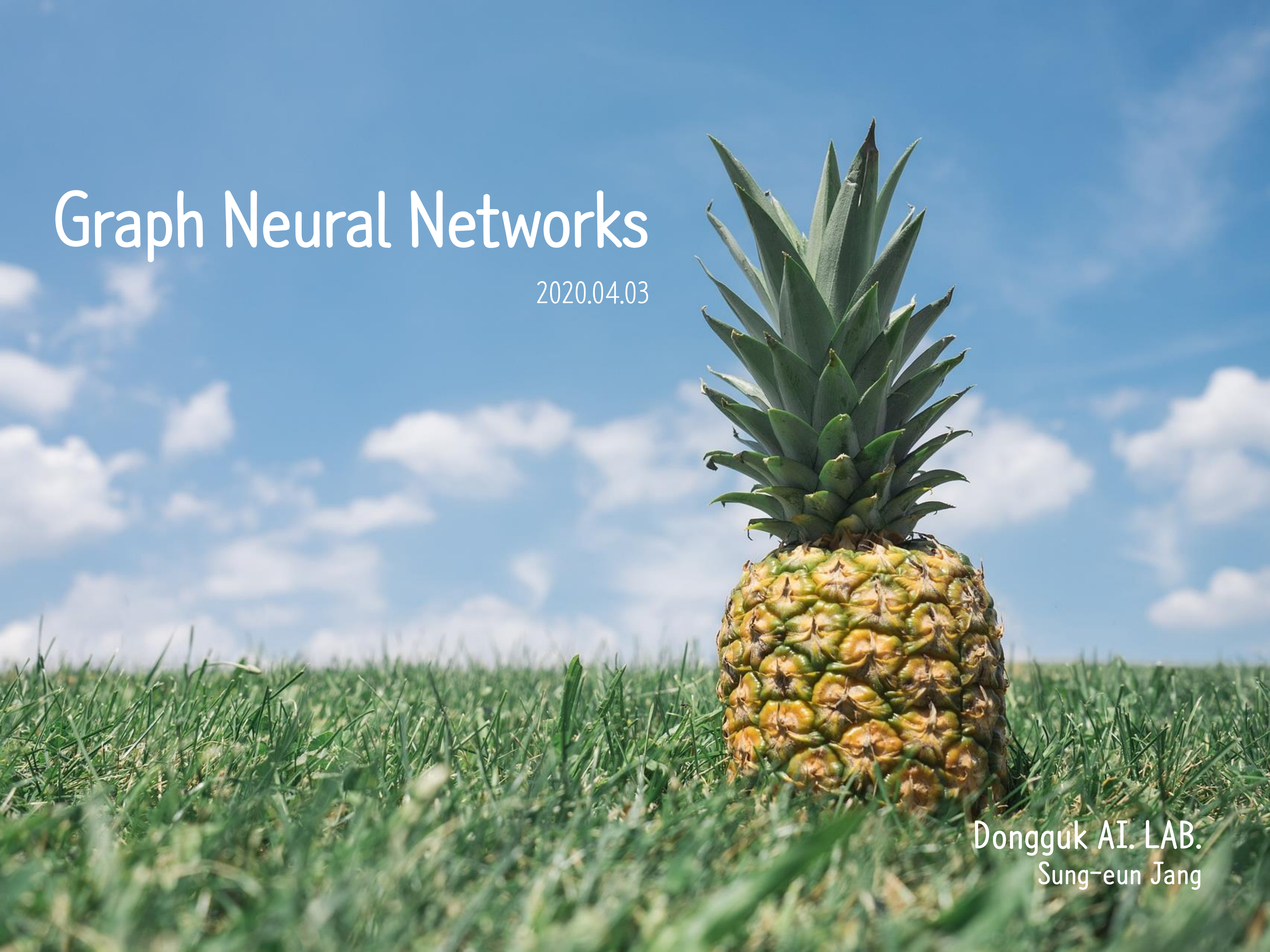


Graph Neural Networks

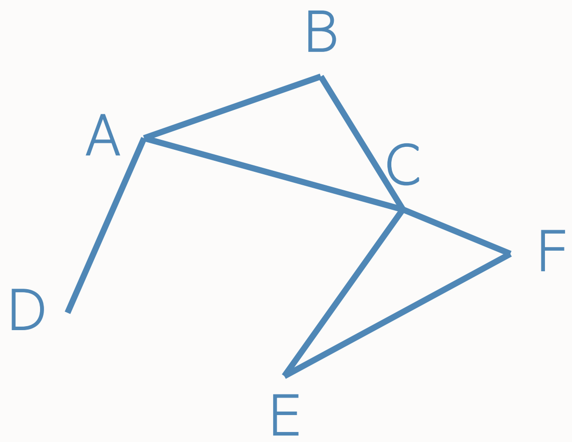
2020.04.03

Dongguk AI. LAB.
Sung-eun Jang

Graph

Definition of Graph

- Graph
  - A collection of objects where some pairs of objects are connected by links

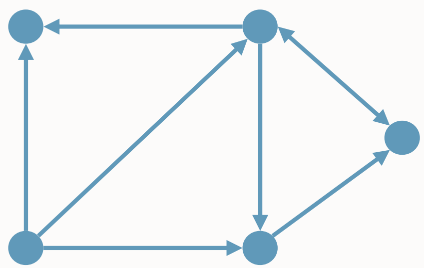


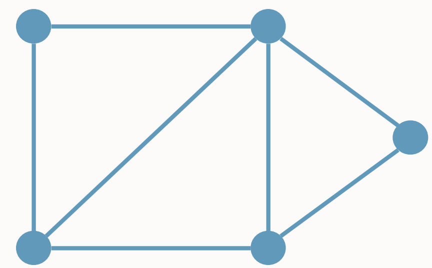
- Components of a Graph
  - Objects nodes, vertices N
  - Interactions links, edges E
  - System network, graph $G(N,E)$

Graph

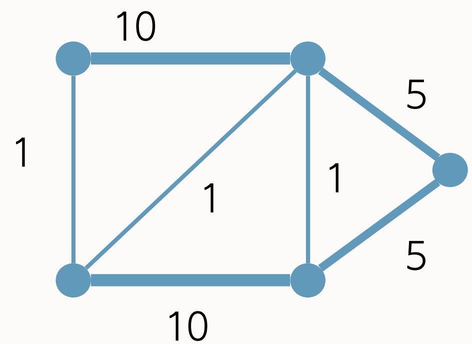
Structure of Graph

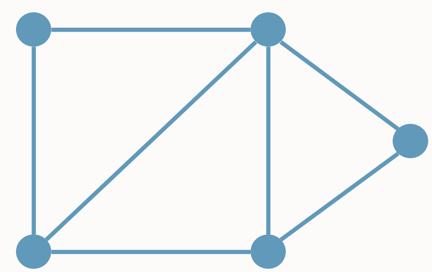
- Directed / Undirected





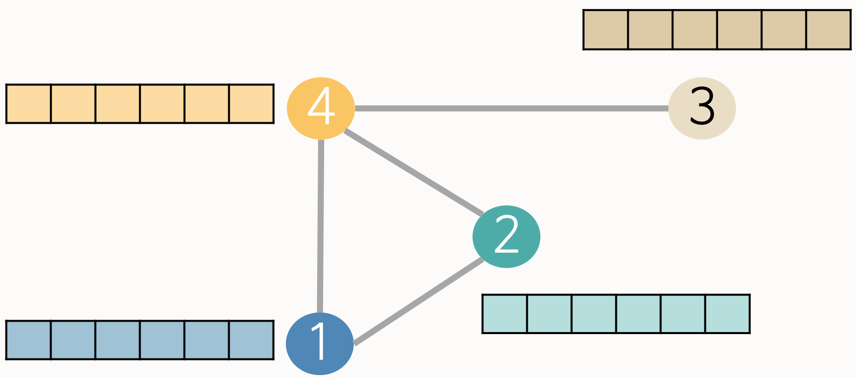
- Weighted / Unweighted



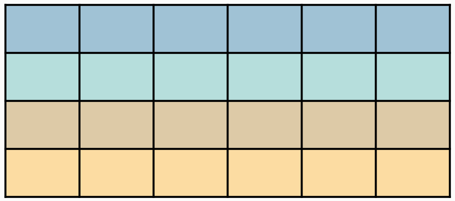


Graph

Graph Representation



Node-feature matrix



Adjacency matrix

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

$$A = \begin{cases} A_{ij} = 1 \; if \; there \; is \; edge \\ A_{ij} = 0 \; if \; there \; is \; no \; edge \end{cases}$$

Degree matrix

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

$$D_{ii} = \sum_{i \sim j} A_{ij}$$

Laplacian matrix

2	−1	0	−1
1	2	0	−1
0	0	3	−1
−1	−1	−1	2

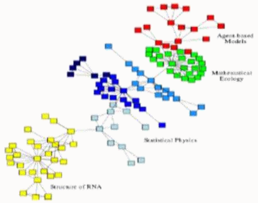
$$L = A - D$$

Graph

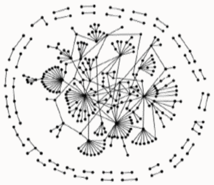
Why Graph?

- Universal Language for describing complex data
- Shared vocabulary between fields
- Data availability & computational challenges

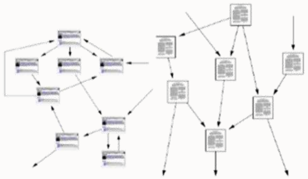
Social networks



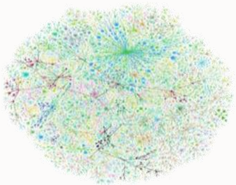
Economic networks



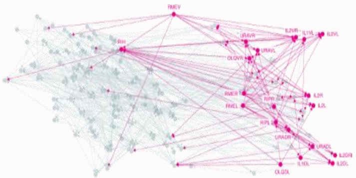
Communication networks



Information networks:
Web & citations



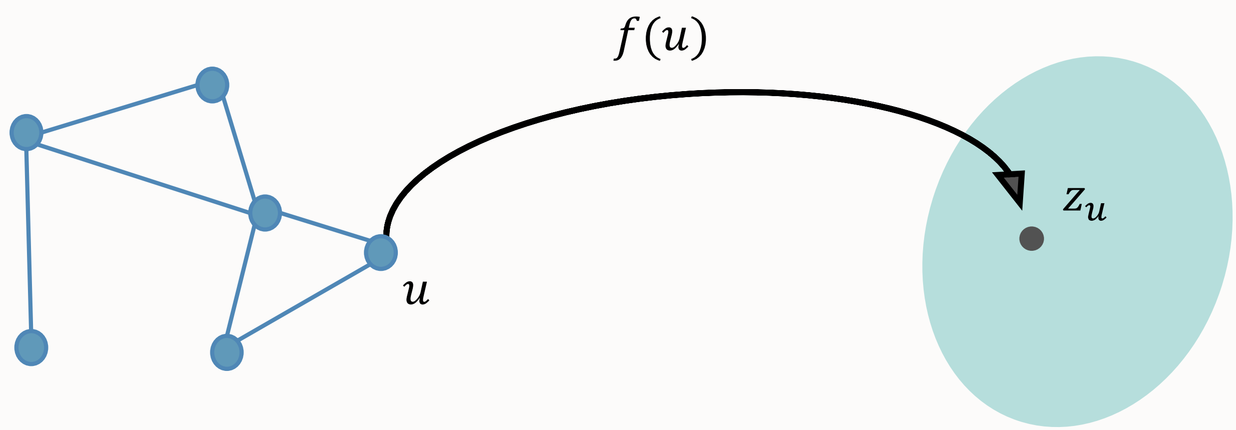
Internet



Networks of neurons

Node Embeddings

Definition.



- Node embedding function (f) map each node in a graph into a low-dimensional space
- similarity in the embedding space approximates similarity in the graph
- Could be helpful with tasks such as…

  ➔ node classification, graph classification, link prediction…

Node Embeddings

Shallow Encoders

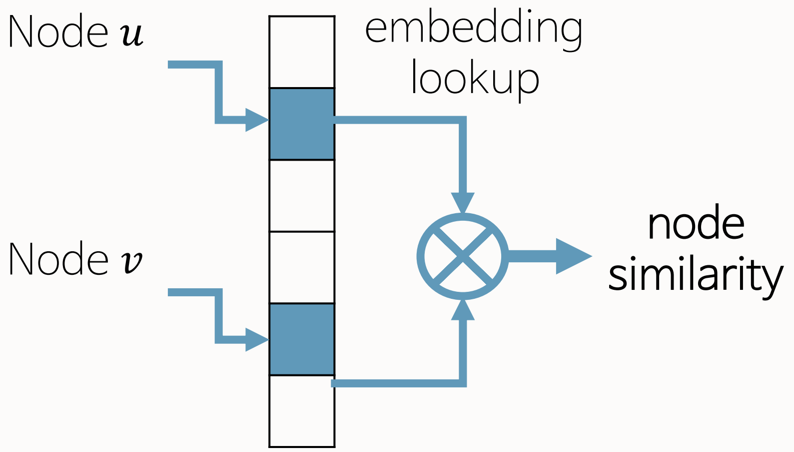
- Use a lookup table consisting of unique embedding of every nodes in graph

- Limitations

  - O(|V|) parameters are needed

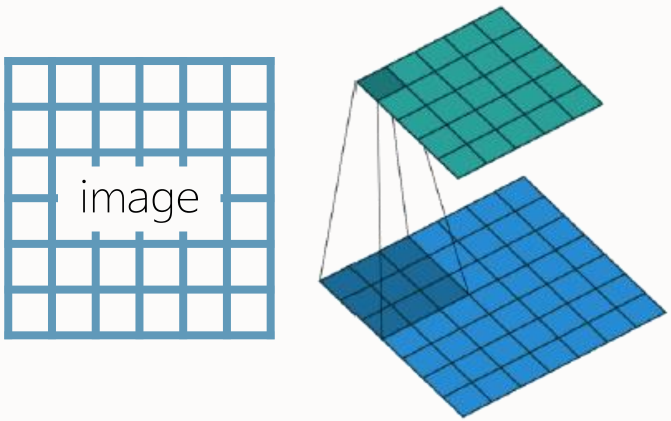
  - Inherently Transductive

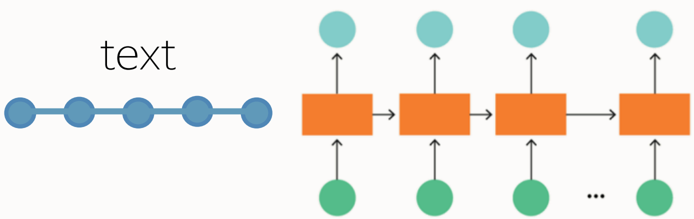
  - Do not incorporate node features



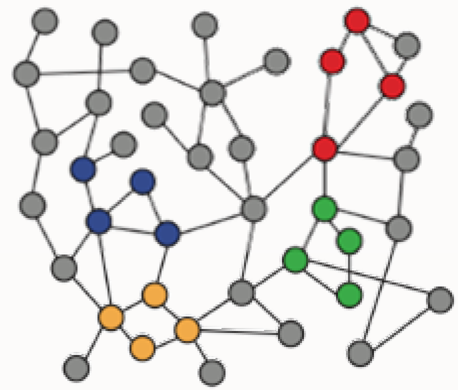
Node Embeddings

Graph and Modern Deep Learning





graph

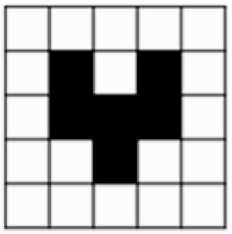


- Arbitrary size
- Complex topological structure
- No fixed node ordering
- Dynamic and multimodal features

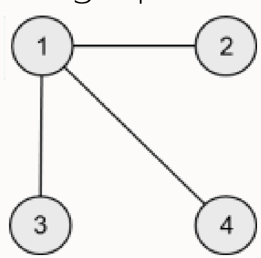
Graph Convolutional Network

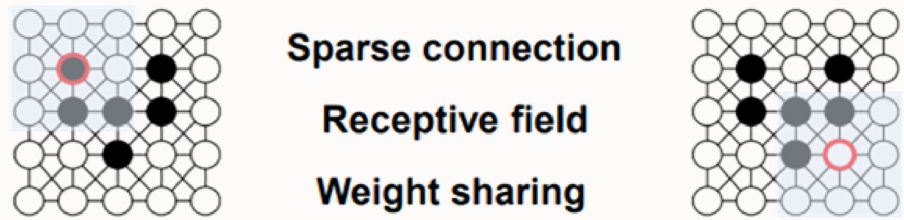
From Image to Graph

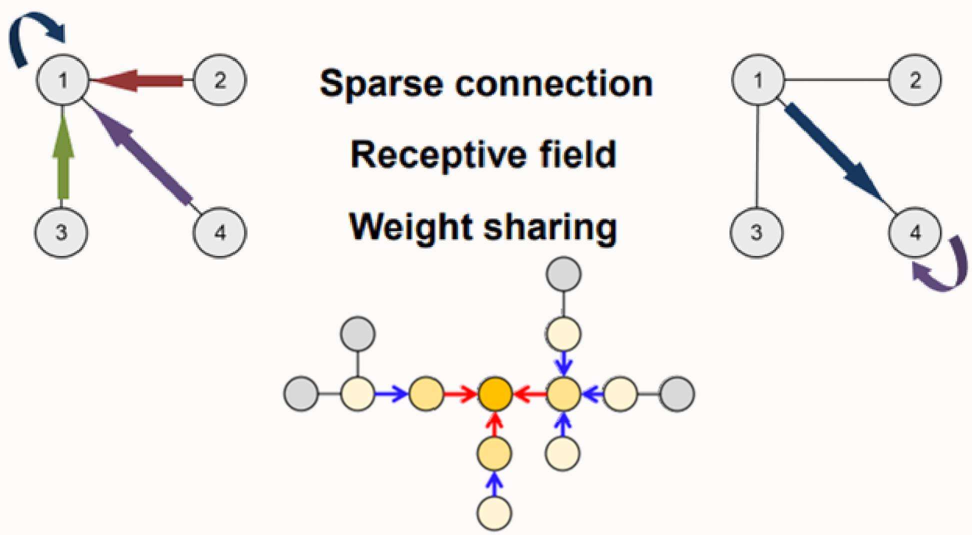
image



graph



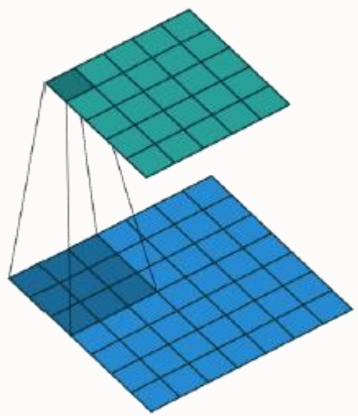




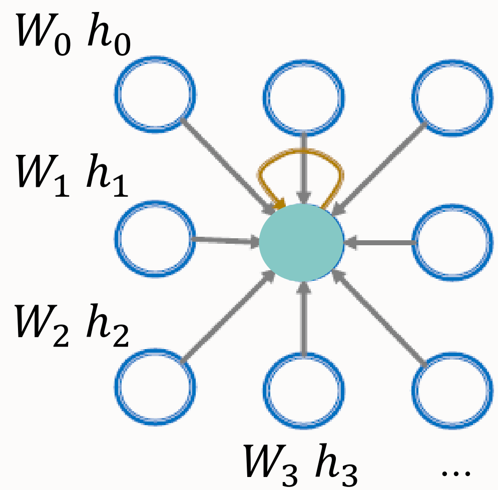
Graph Convolutional Network

GCN

image



graph



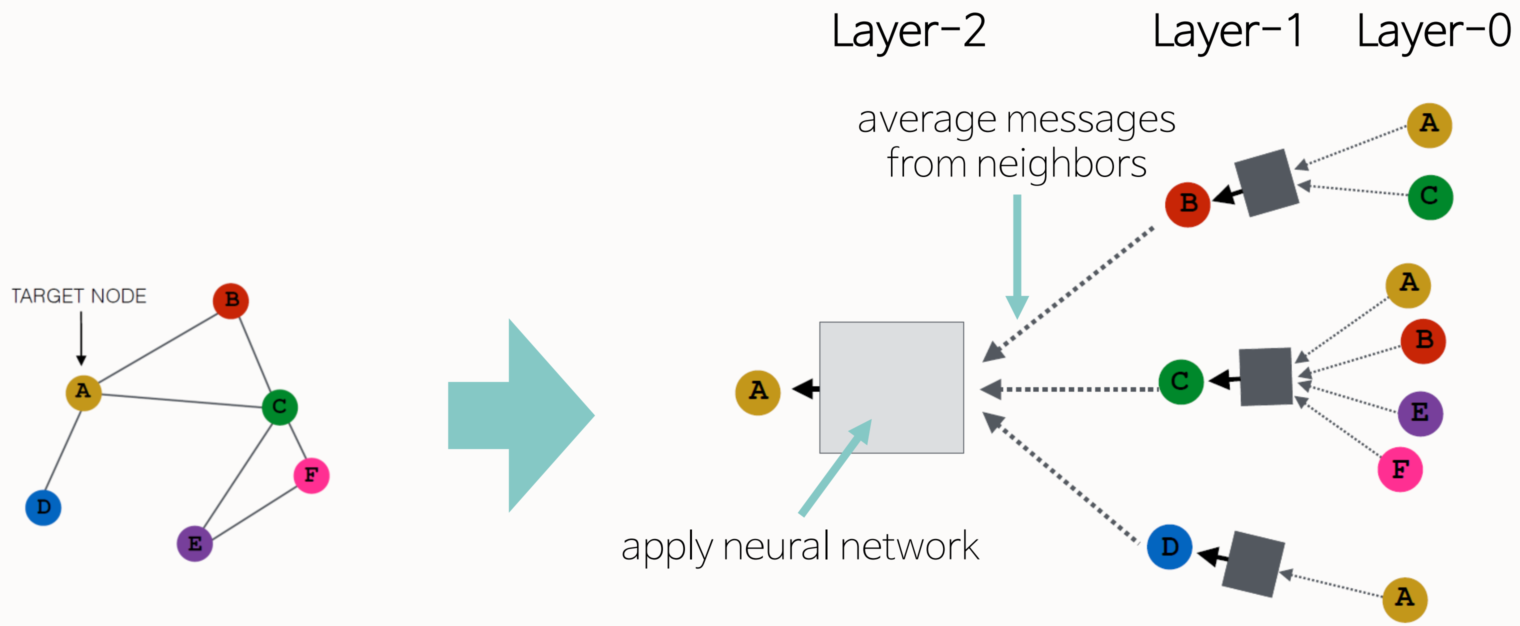
$$\sum_i W_i\ h_i$$

- Transform information at the neighbors and combine it

  1) Transform "messages" h_i from neighbors:
  2) Add them up

Graph Convolutional Network

Compute Node Features

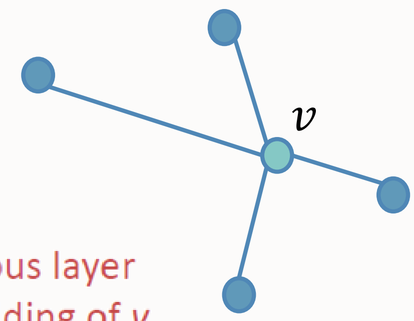


- Generate node embeddings based on local network neighborhoods

- Nodes have embeddings at each layer, repeating combine messages from their neighbor using neural networks

Graph Convolutional Network

Compute Node Features



Initial 0-th layer embeddings are equal to node features

$$\boxed{\mathbf{h}_v^0 = \mathbf{x}_v}$$

Previous layer embedding of *v*

$$\mathbf{h}_v^k = \boxed{\sigma}\left(\mathbf{W}_k \boxed{\sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|}} + \mathbf{B}_k \boxed{\mathbf{h}_v^{k-1}}\right), \quad \forall k \in \{1, \ldots, K\}$$

$$\boxed{\mathbf{z}_v} = \mathbf{h}_v^K$$

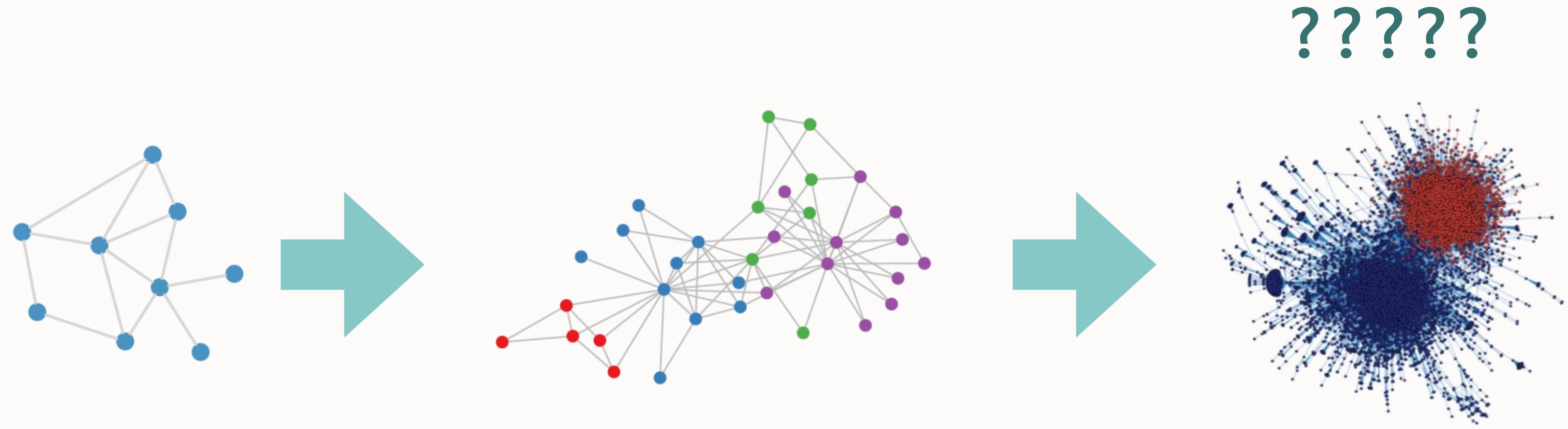
Average of neighbor's previous layer embeddings

Embedding after K layers of neighborhood aggregation

Non-linearity (e.g., ReLU)

Graph Convolutional Network

Limitation of GCN



- For training of the embeddings, model requires that all nodes in the graph are present during training time

- As the number of nodes increases, the matrix becomes larger and computational cost increases accordingly.

GraphSAGE

Definition

- GraphSAGE (**SA**mple and aggre**G**at**E**)

  - Instead of training individual embeddings for each node, generates embeddings by **sampling** features from neighborhoods

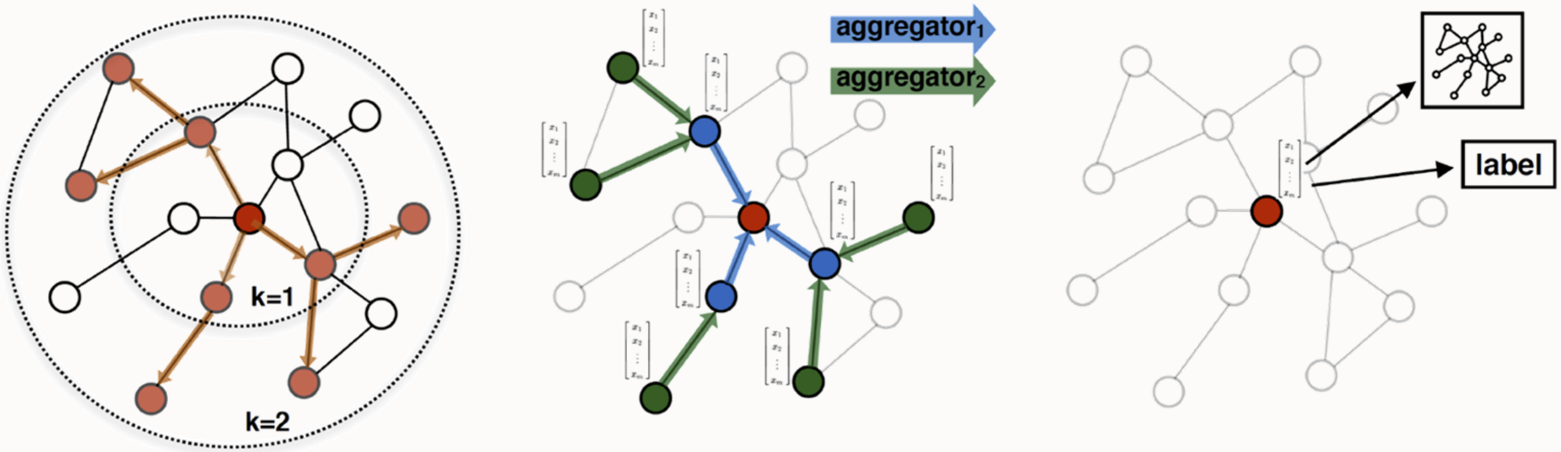
  ➔ **mini batch**

  - Train a set of aggregator functions that learn to **aggregate** feature information a node's local neighborhood

  ➔ **aggregating**

GraphSAGE

Mini batch



1. Sample neighborhood

2. Aggregate feature information from neighbors

3. Predict graph context and label using aggregated information

GraphSAGE

Aggregating

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|} + \mathbf{B}_k \mathbf{h}_v^{k-1}\right)$$

Concatenate neighbor embedding and self embedding

$$\mathbf{h}_v^k = \sigma\left(\left[\mathbf{W}_k \cdot \boxed{\mathrm{AGG}\left(\{\mathbf{h}_u^{k-1}, \forall u \in N(v)\}\right)}, \mathbf{B}_k \mathbf{h}_v^{k-1}\right]\right)$$

Generalized aggregation

GraphSAGE

Aggregating

- Mean

$$\text{AGG} = \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|}$$

- Pool

Element-wise mean/max

$$\text{AGG} = \boxed{\gamma}\left(\{\mathbf{Q}\mathbf{h}_u^{k-1}, \forall u \in N(v)\}\right)$$

- LSTM

$$\text{AGG} = \text{LSTM}\left([\mathbf{h}_u^{k-1}, \forall u \in \pi(N(v))]\right)$$

GraphSAGE

Algorithm

Algorithm 1: GraphSAGE embedding generation (i.e., forward propagation) algorithm

---

Input : Graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$; input features $\{\mathbf{x}_v, \forall v \in \mathcal{V}\}$; depth K; weight matrices $\mathbf{W}^k, \forall k \in \{1, ..., K\}$; non-linearity σ; differentiable aggregator functions $\text{AGGREGATE}_k, \forall k \in \{1, ..., K\}$; neighborhood function $\mathcal{N} : v \to 2^{\mathcal{V}}$

Output : Vector representations $\mathbf{z}_v$ for all $v \in \mathcal{V}$

$\mathbf{h}_v^0 \leftarrow \mathbf{x}_v, \forall v \in \mathcal{V}$;
for $k = 1...K$ **do**
  for $v \in \mathcal{V}$ **do**
    $\mathbf{h}_{\mathcal{N}(v)}^k \leftarrow \text{AGGREGATE}_k(\{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}(v)\})$;
    $\mathbf{h}_v^k \leftarrow \sigma\left(\mathbf{W}^k \cdot \text{CONCAT}(\mathbf{h}_v^{k-1}, \mathbf{h}_{\mathcal{N}(v)}^k)\right)$
  end
  $\mathbf{h}_v^k \leftarrow \mathbf{h}_v^k / \|\mathbf{h}_v^k\|_2, \forall v \in \mathcal{V}$
end
$\mathbf{z}_v \leftarrow \mathbf{h}_v^K, \forall v \in \mathcal{V}$

GraphSAGE

Weighting factor in GraphSAGE

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v)} \boxed{\frac{\mathbf{h}_u^{k-1}}{|N(v)|}} + \mathbf{B}_k \mathbf{h}_v^{k-1}\right)$$

Weighting factor

$$\alpha_{vu} = \frac{1}{|N(v)|}$$

- α_{vu} (importance) is defined explicitly based on the structure properties of graph
- All neighbors $u \in N(v)$ are equally important to node v

Graph Attention Network

Idea

- Specify arbitrary importances to different neighbors of each node in the graph

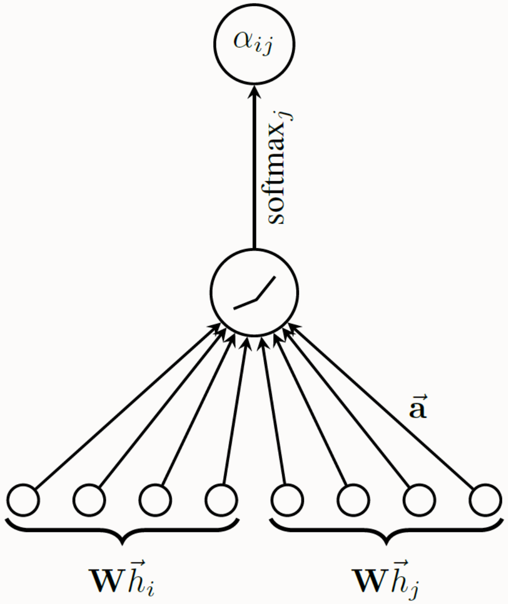
- Compute embedding h_v^k of each node in the graph following an **attention strategy**:

➔ Nodes attend over their neighborhoods' message

➔ Implicitly specifying different weights to different nodes

Graph Attention Network

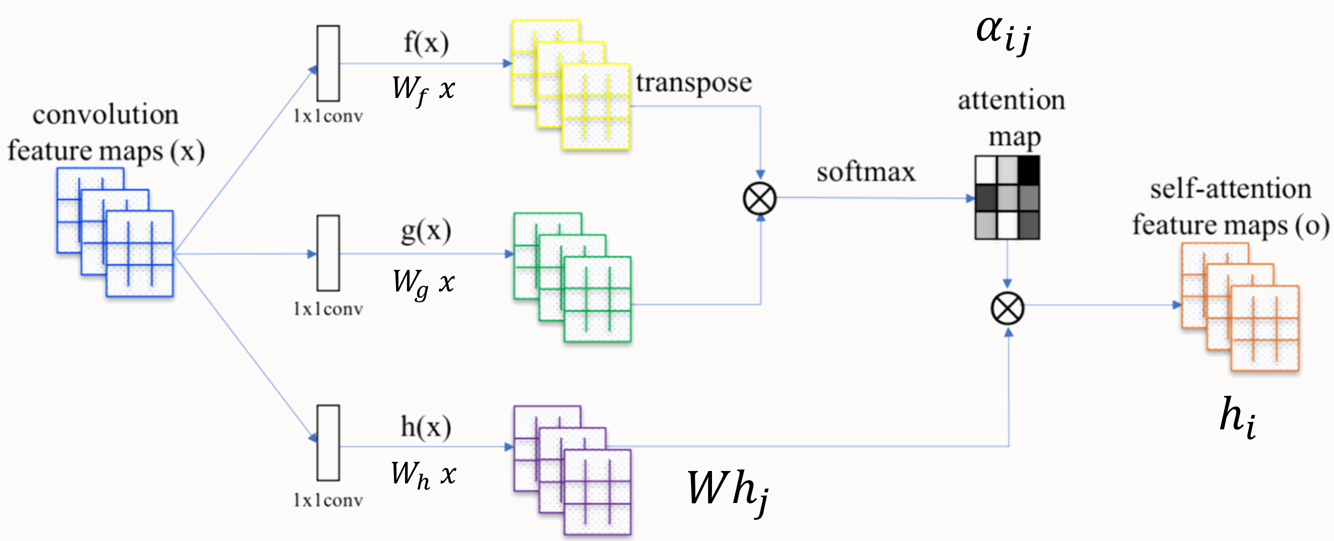
Attention



$$\vec{h}'_i = \sigma\left(\sum_{j \in \mathcal{N}_i} \alpha_{ij} \mathbf{W} \vec{h}_j\right)$$

Graph Attention Network

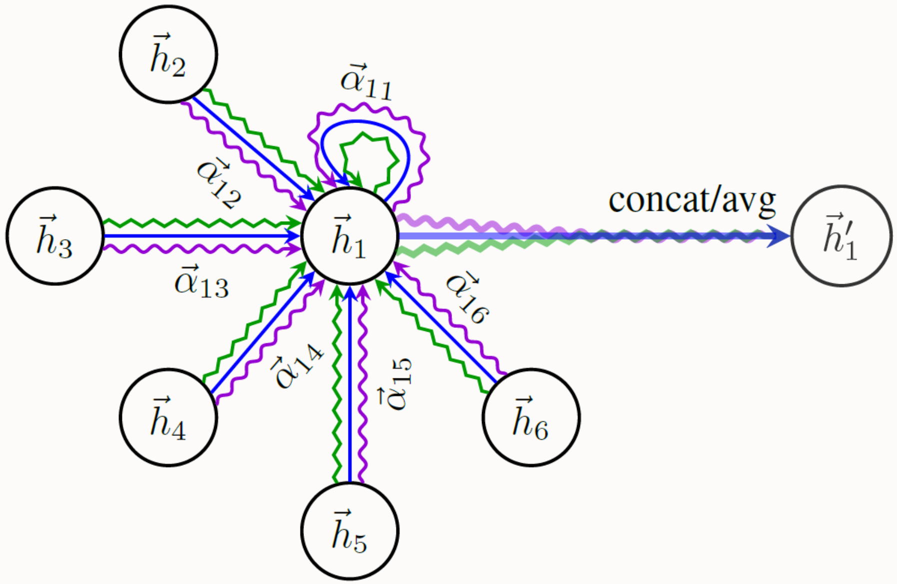
Self attention



$$\vec{h}'_i = \sigma\left(\sum_{j\in\mathcal{N}_i} \alpha_{ij}\mathbf{W}\vec{h}_j\right)$$

Graph Attention Network

Multi-head attention.



$$\vec{h}'_i = \Big\Vert_{k=1}^{K} \sigma\left(\sum_{j\in\mathcal{N}_i} \alpha_{ij}^k \mathbf{W}^k \vec{h}_j\right)$$

$$\vec{h}'_i = \sigma\left(\frac{1}{K}\sum_{k=1}^{K}\sum_{j\in\mathcal{N}_i} \alpha_{ij}^k \mathbf{W}^k \vec{h}_j\right)$$

Graph Attention Network

Result

Table 2: Summary of results in terms of classification accuracies, for Cora, Citeseer and Pubmed. GCN-64* corresponds to the best GCN result computing 64 hidden features (using ReLU or ELU).

Transductive

Method	Cora	Citeseer	Pubmed
MLP	55.1%	46.5%	71.4%
ManiReg (Belkin et al., 2006)	59.5%	60.1%	70.7%
SemiEmb (Weston et al., 2012)	59.0%	59.6%	71.7%
LP (Zhu et al., 2003)	68.0%	45.3%	63.0%
DeepWalk (Perozzi et al., 2014)	67.2%	43.2%	65.3%
ICA (Lu & Getoor, 2003)	75.1%	69.1%	73.9%
Planetoid (Yang et al., 2016)	75.7%	64.7%	77.2%
Chebyshev (Defferrard et al., 2016)	81.2%	69.8%	74.4%
GCN (Kipf & Welling, 2017)	81.5%	70.3%	**79.0%**
MoNet (Monti et al., 2016)	$81.7 \pm 0.5\%$	—	$78.8 \pm 0.3\%$
GCN-64*	$81.4 \pm 0.5\%$	$70.9 \pm 0.5\%$	$\mathbf{79.0} \pm 0.3\%$
GAT (ours)	$\mathbf{83.0} \pm 0.7\%$	$\mathbf{72.5} \pm 0.7\%$	$\mathbf{79.0} \pm 0.3\%$

Reference

Lorem Ipsum is simply dummy text of the printing and typesetting industry.

- Kipf, T. N., & Welling, M. (2016). Semi-supervised classification with graph convolutional networks. arXiv preprint arXiv:1609.02907.
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- https://www.cs.ubc.ca/~lsigal/532S_2018W2/Lecture18a.pdf

Thank You

제목을 입력하세요

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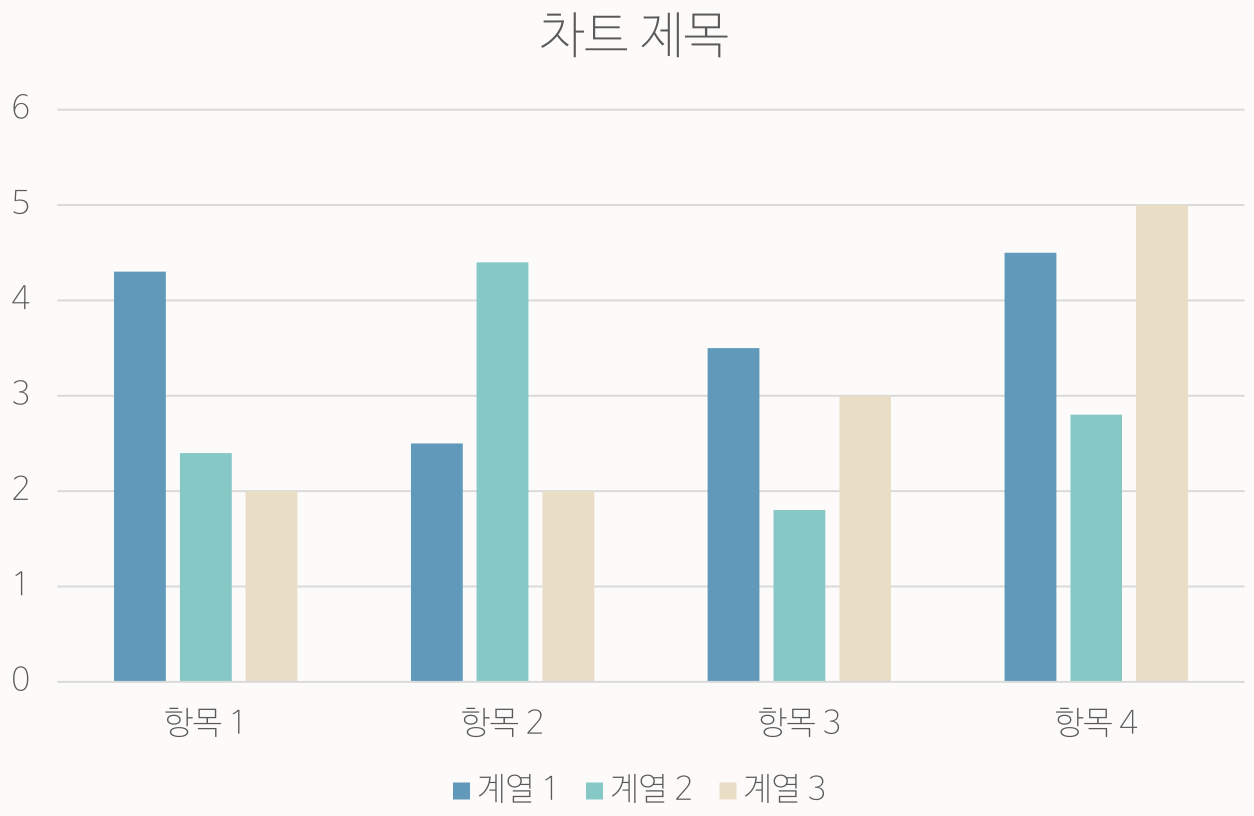

Graph Attention Network

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제목을 입력하세요

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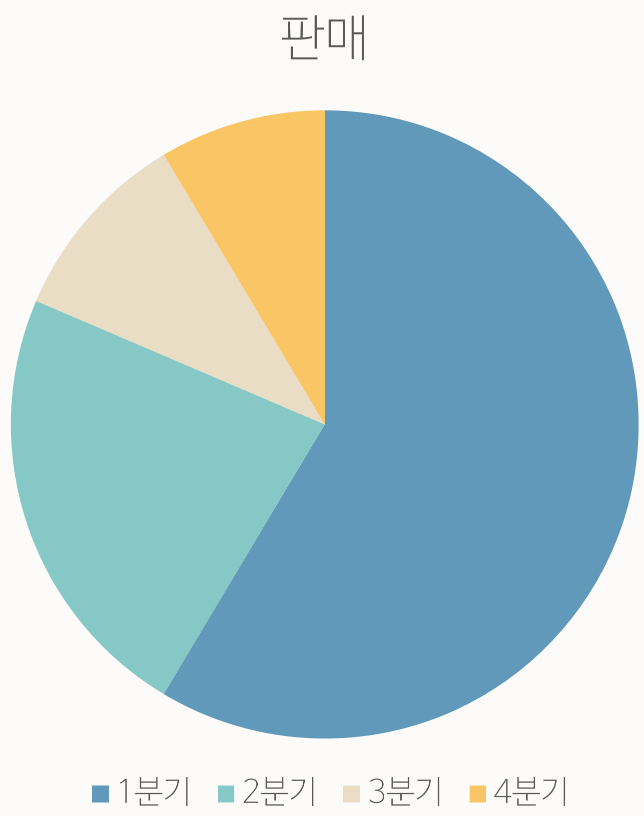

제목을 입력하세요

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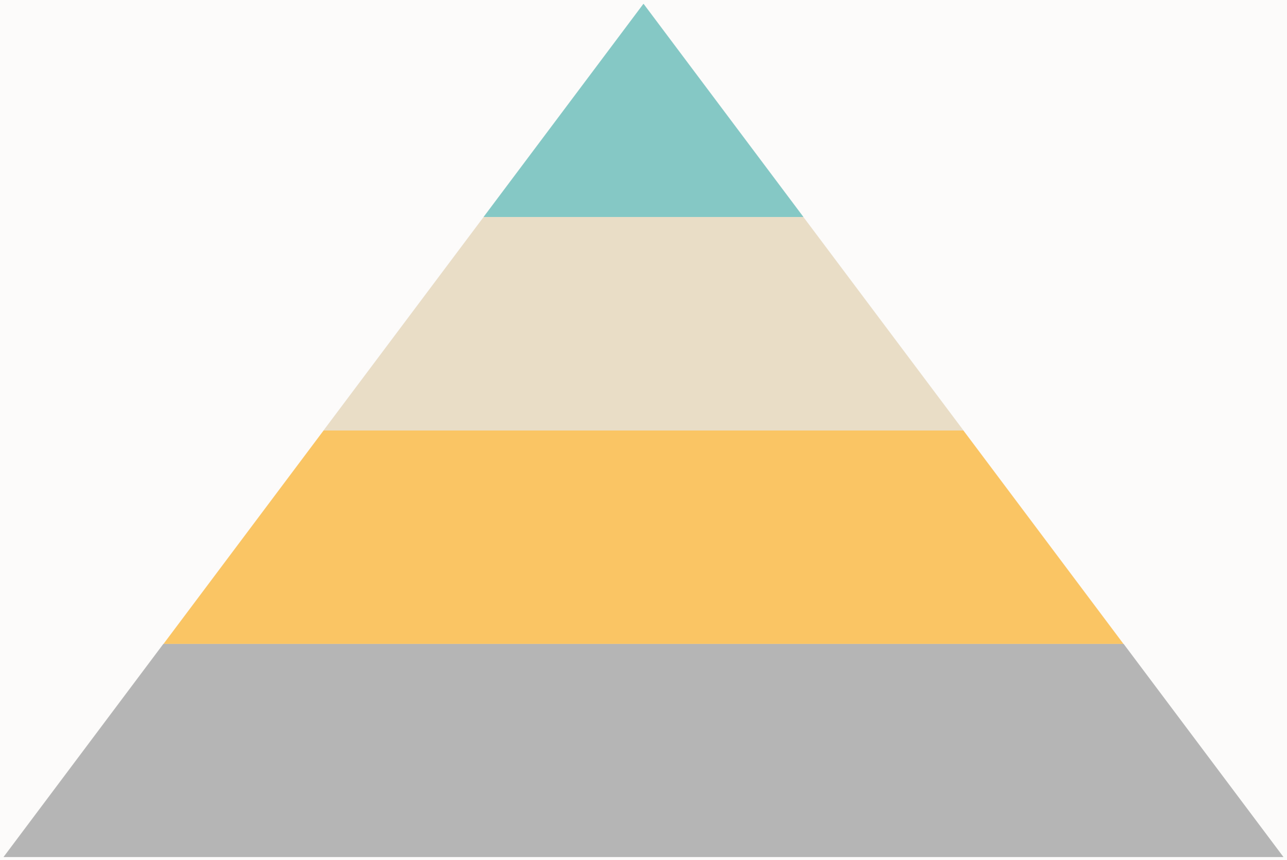
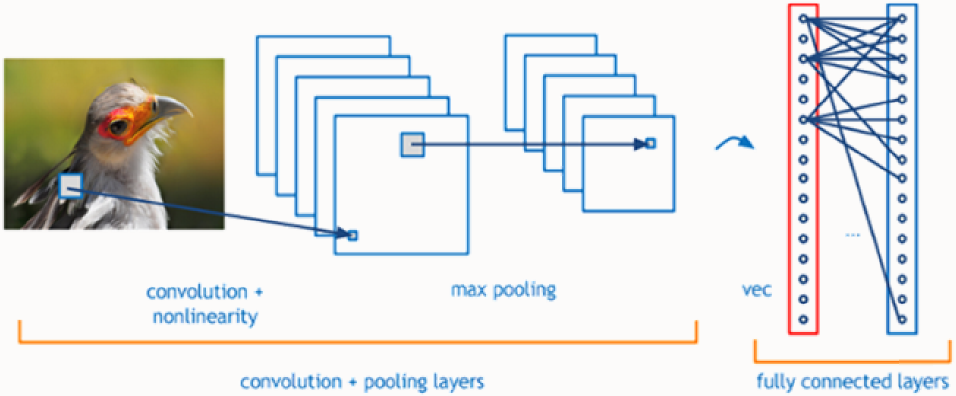
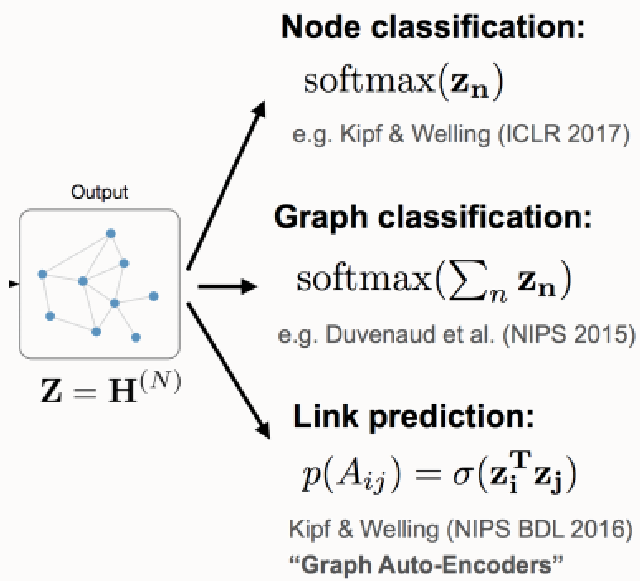




Sparse connection
Weight sharing
Receptive field



Graph Convolutional Network

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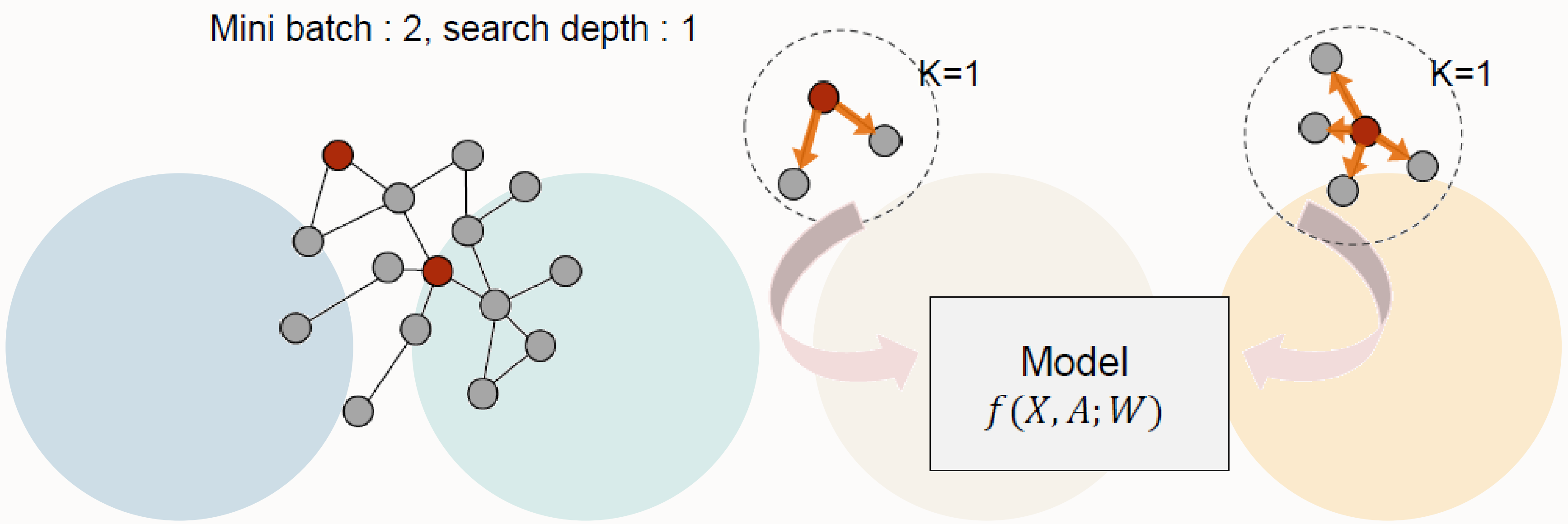

GraphSAGE

Mini batch

Mini batch : 2, search depth : 2