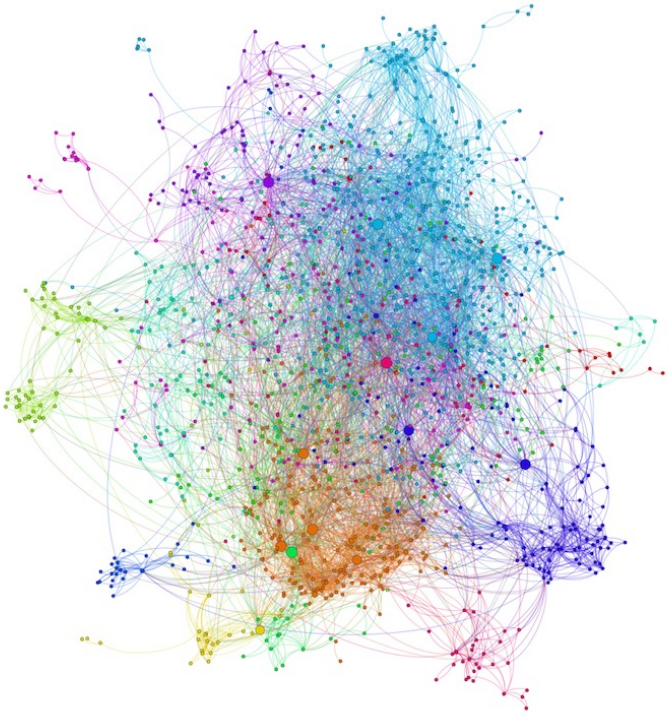
CUAI GNN 스터디

2022.04.05

발표자 : 배병현



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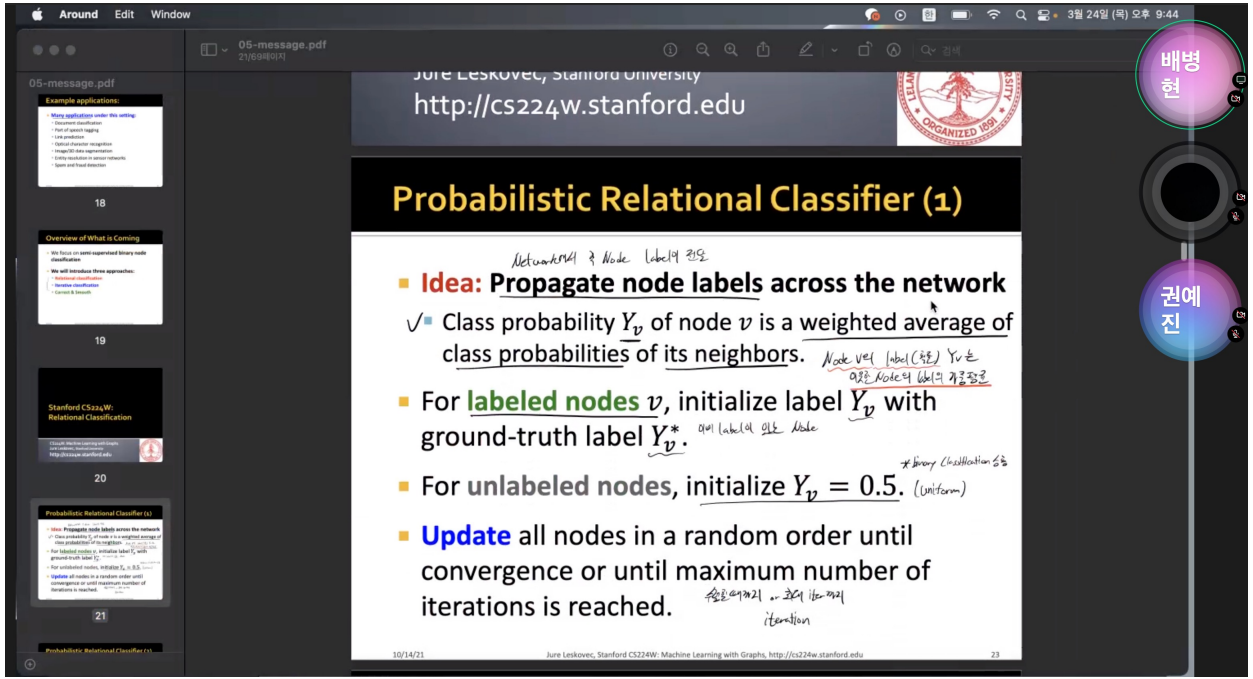
   - The Over-smoothing Problem in GNN

스터디 인증

세번째 미팅: 22.03.24

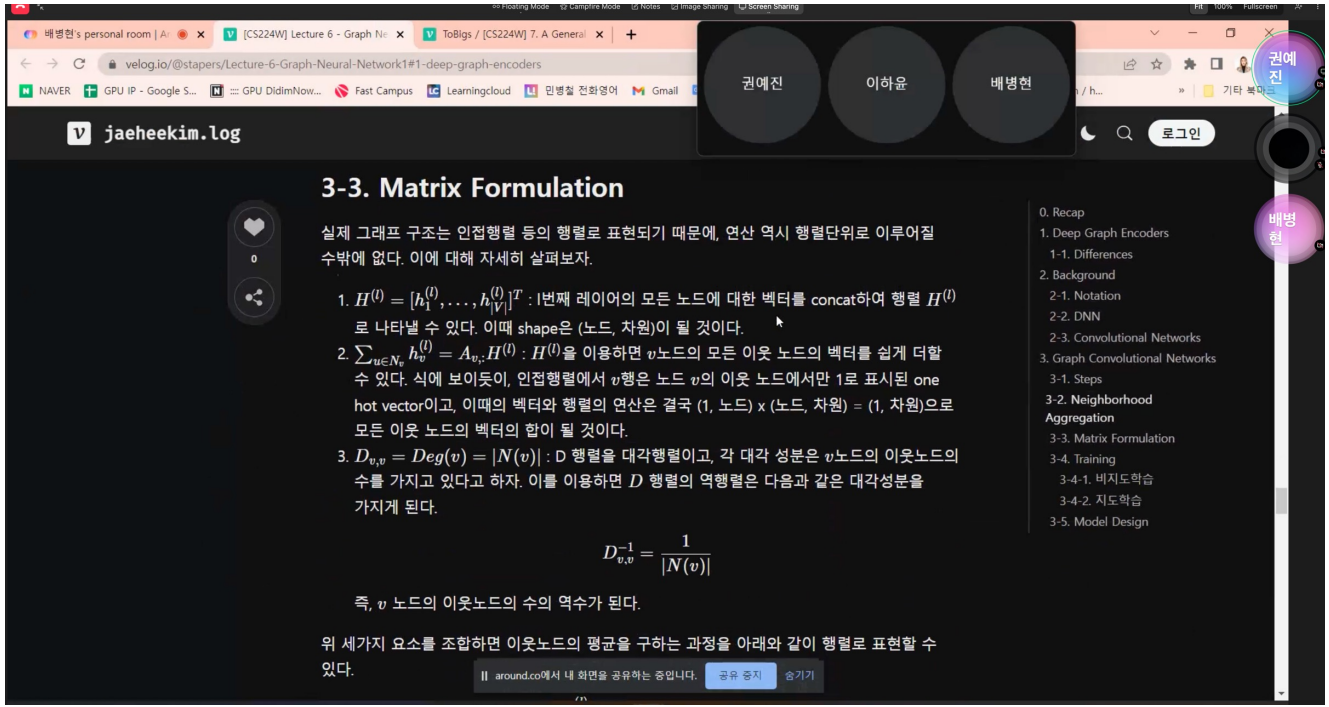
4. Link Analysis: PageRank 5. Label Propagation for Node Classification



스터디 인증

네번째 미팅: 22.03.31

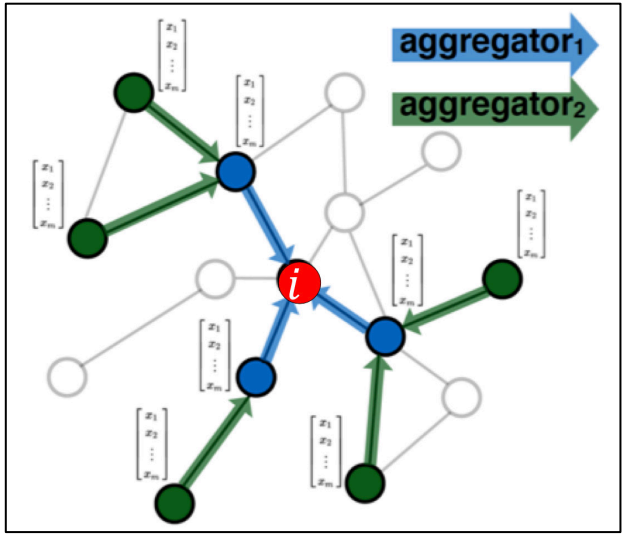
6. Graph Neural Networks 1: GNN Model 7. Graph Neural Networks 2: Design Space

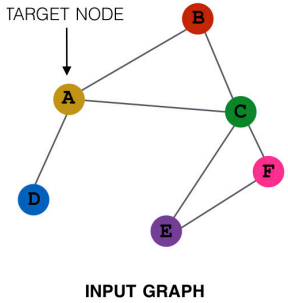


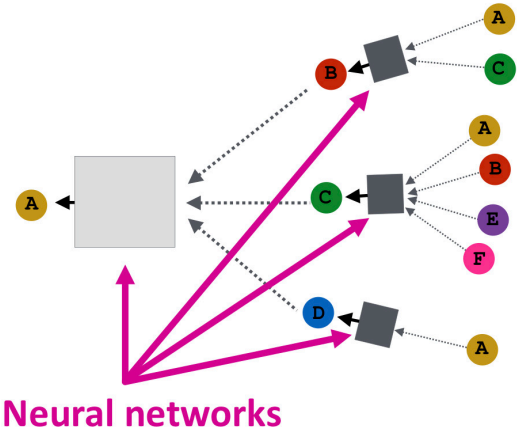
스터디 내용 공유: The Over-smoothing Problem in GNN

GNN: Aggregate from Neighbors

- Propagate and transform information





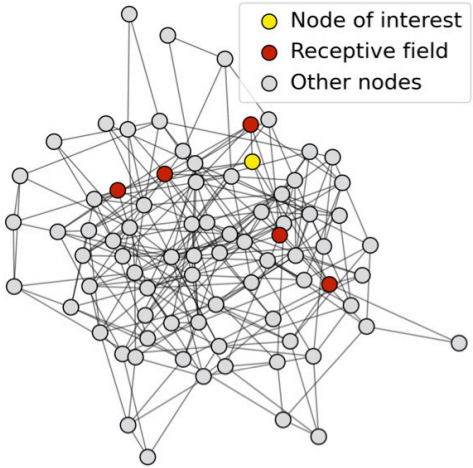


스터디 내용 공유: The Over-smoothing Problem in GNN

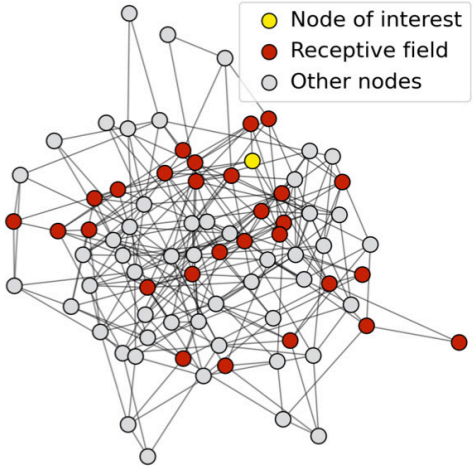
The Issue of stacking many GNN layers

- Receptive fields: 특정한 Node의 embedding을 결정하는 Node의 set

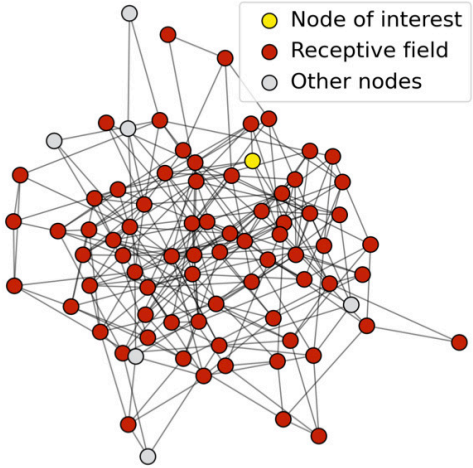
Receptive field for 1-layer GNN



Receptive field for 2-layer GNN



Receptive field for 3-layer GNN

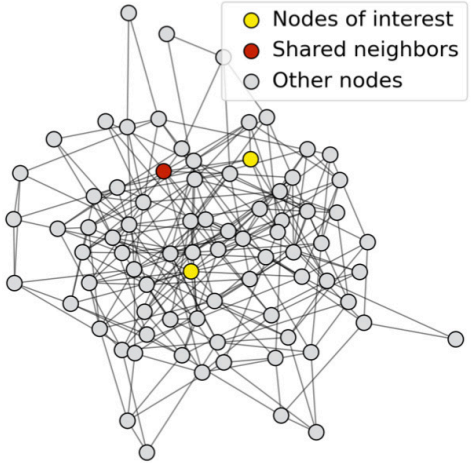


스터디 내용 공유: The Over-smoothing Problem in GNN

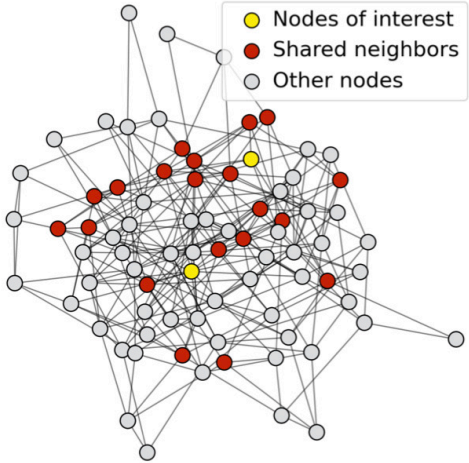
The Issue of stacking many GNN layers

- Layer를 많이 통과할수록 Node의 receptive fields가 겹치게 됨

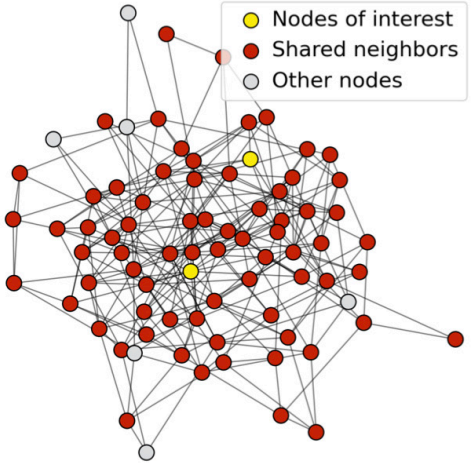
1-hop neighbor overlap
Only 1 node →



2-hop neighbor overlap
About 20 nodes →



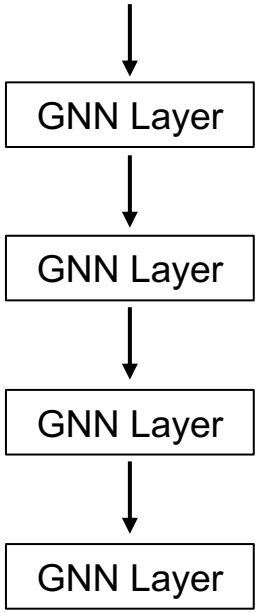
3-hop neighbor overlap
Almost all the nodes!



스터디 내용 공유: The Over-smoothing Problem in GNN

The Issue of stacking many GNN layers

- The Over-smoothing Problem: 많은 layers를 쌓으면서 node의 embedding vector가 같은 값으로 수렴하는 문제



어떻게 over-smoothing problem을 해결할 수 있을까?

1. 각 layer의 expressive power 높이기
2. Message를 pass하지 않는 layers 추가
3. Skip connection 추가

그 전에 풀고자 하는 문제에 대해 receptive field가 어느 정도가 적당한지 먼저 분석하는 것도 방법!

스터디 내용 공유: The Over-smoothing Problem in GNN

Overcoming over-smoothing problem

1. 각 layer의 expressive power 높이기

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

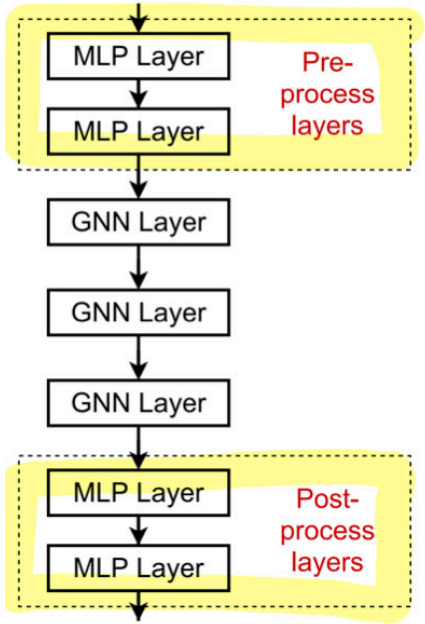
One layer perceptron

⇩

MLP로 변경

* Universal approximation theorem

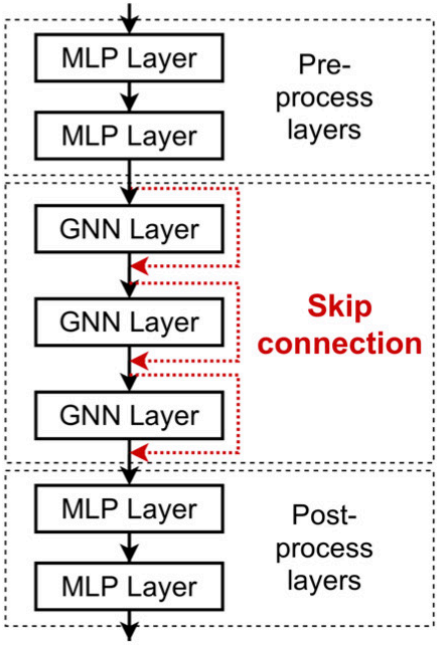
2. Message를 pass하지 않는 layers 추가

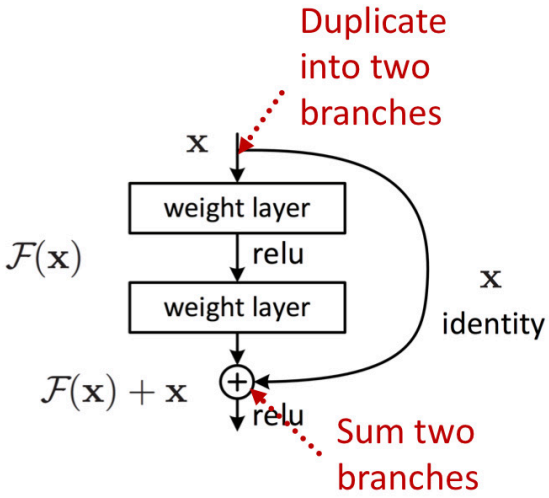


스터디 내용 공유: The Over-smoothing Problem in GNN

Overcoming over-smoothing problem

3. Skip connection 추가





Idea of skip connections:

Before adding shortcuts:

$$\boldsymbol{F}(\mathbf{x})$$

After adding shortcuts:

$$\boldsymbol{F}(\mathbf{x}) + \mathbf{x}$$

THANK YOU
FOR YOUR
ATTENTION