Scaling Up GNNs

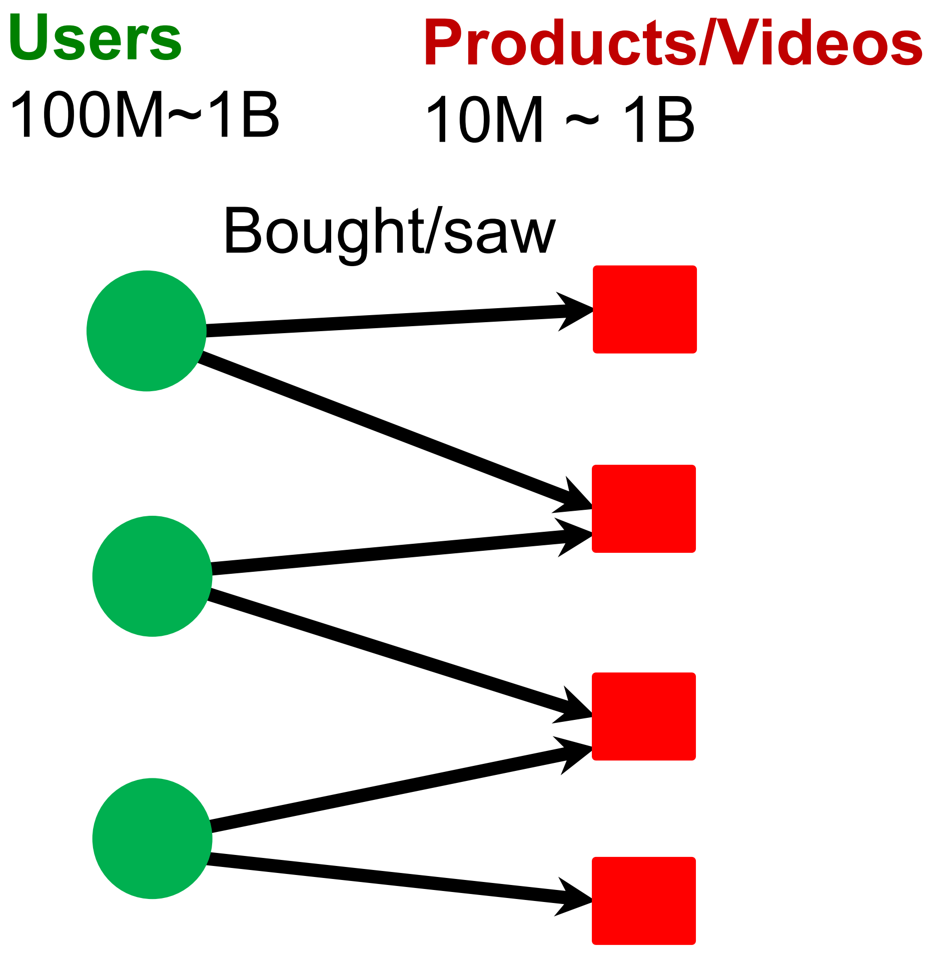
CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Announcements

- **Homework 3** due today
  - Late submissions accepted until end of day Monday, 11/20
- **Colab 5** released on course website
  - Due Tuesday, 12/05
- **Regrade request deadlines**
  - **Homework 2**: Saturday, 11/18
    - Solutions and statistics released on Ed
  - Regrade request policy update on Ed

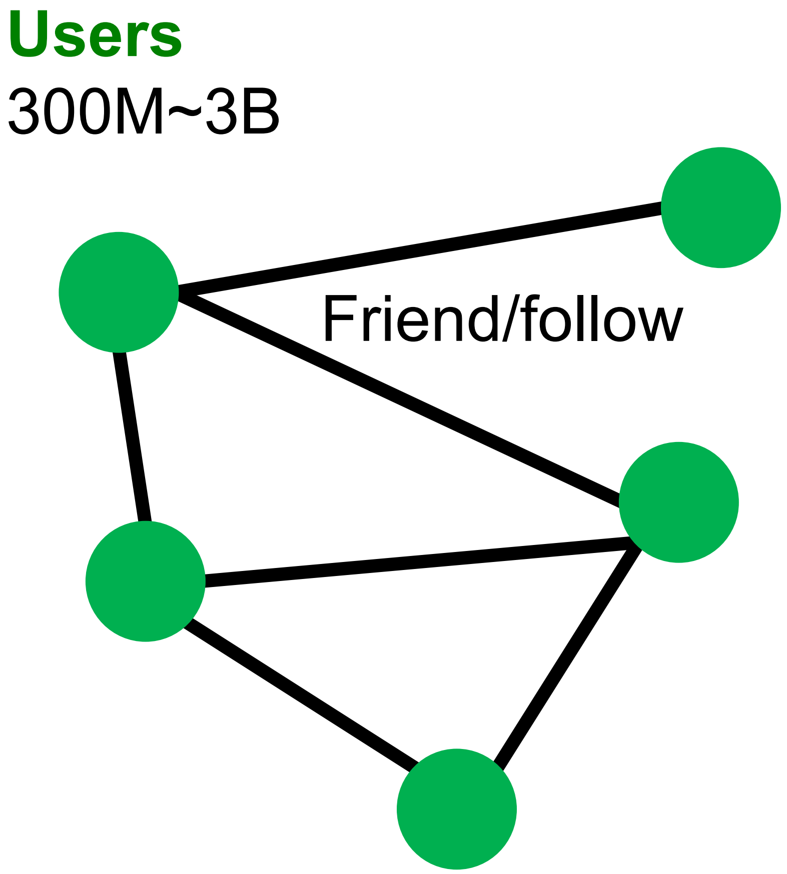
Graphs in Modern Applications

- **Recommender systems:**
  - Amazon
  - YouTube
  - Pinterest
  - Etc.
- **ML tasks:**
  - Recommend items
    (link prediction)
  - Classify users/items
    (node classification)



Graphs in Modern Applications

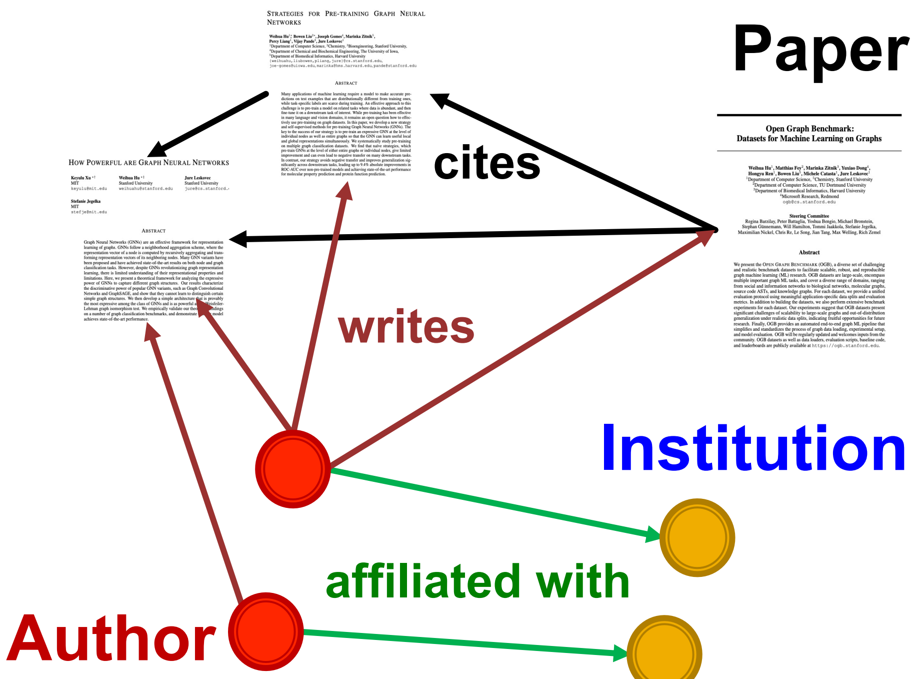
- **Social networks:**
  - Facebook
  - Twitter
  - Instagram
  - Etc.
- **ML tasks:**
  - Friend recommendation (link-level)
  - User property prediction (node-level)



Graphs in Modern Applications

- **Academic graph:**
  - Microsoft Academic Graph
- **ML tasks:**
  - Paper categorization (node classification)
  - Author collaboration recommendation
  - Paper citation recommendation (link prediction)

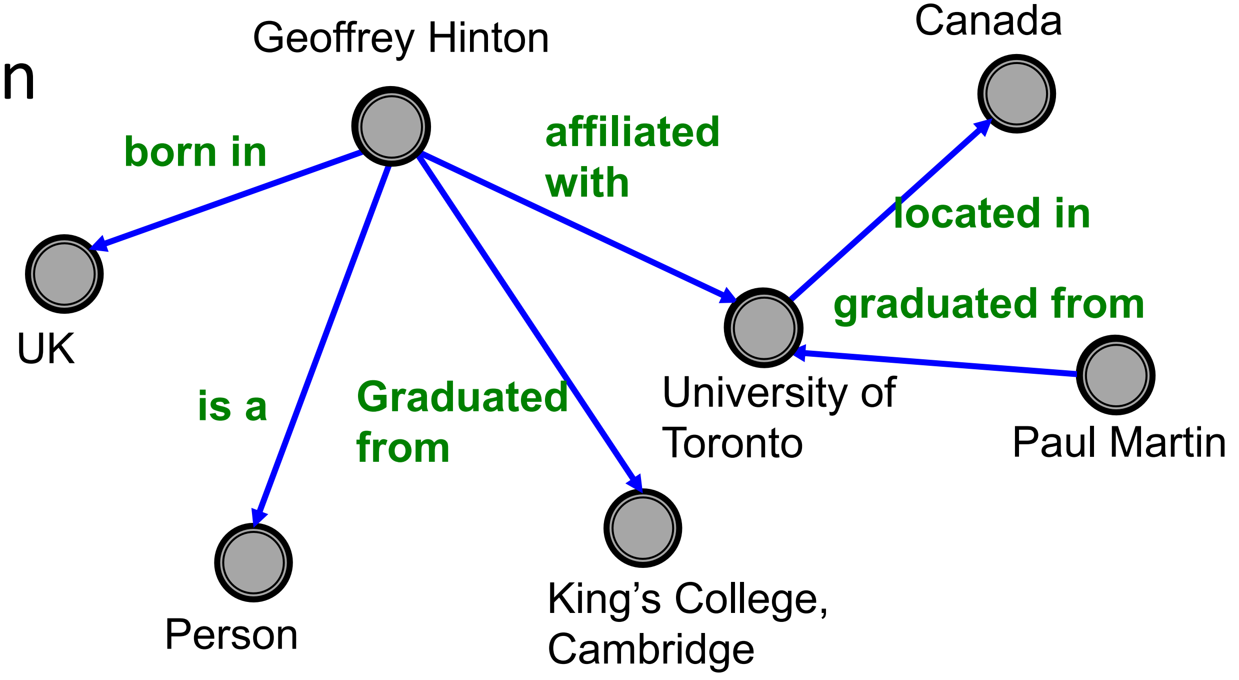
Papers	**Authors**
120M	120M



Graphs in Modern Applications

- **Knowledge Graphs (KGs):**
  - Wikidata
  - Freebase
- **ML tasks:**
  - KG completion
  - Reasoning

Entities
80M—90M



What is in Common?

- **Large-scale:**
  - #nodes ranges from 10M to 10B.
  - #edges ranges from 100M to 100B.
- **Tasks**
  - **Node-level**: User/item/paper classification.
  - **Link-level**: Recommendation, completion.
- **Todays' lecture**
  - **Scale up GNNs to large graphs!**

Why is it Hard?

- **Recall: How we usually train an ML model on large data (N = #data is large)**
- **Objective**: Minimize the averaged loss

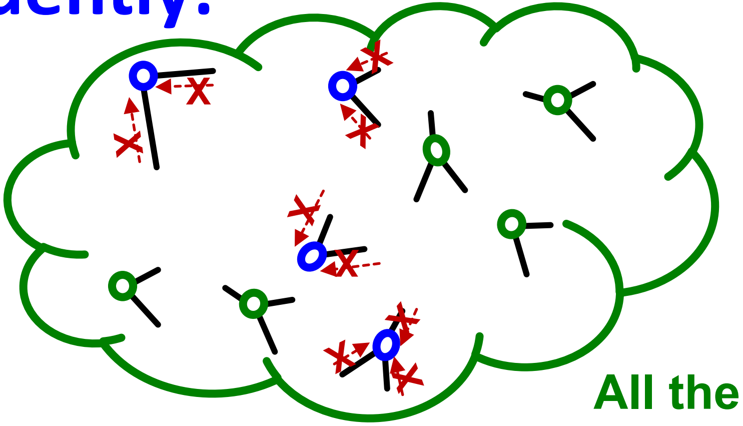
$$\ell(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=0}^{N-1} \ell_i(\boldsymbol{\theta})$$

  - $\boldsymbol{\theta}$: model parameters, $\ell_i(\boldsymbol{\theta})$: loss for i-th data point.
- We perform **Stochastic Gradient Descent (SGD)**.
  - Sample M ($\ll N$) data points (**mini-batches**).
  - Compute the $\ell_{sub}(\boldsymbol{\theta})$ over the M data points.
  - Perform SGD: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \nabla \ell_{sub}(\boldsymbol{\theta})$

Why is it Hard?

What if we were to use the standard SGD for GNN?

- **In mini-batch, we sample M ($\ll N$) nodes independently:**



  - **Sampled nodes will be be isolated from each other!**
  - GNN generates node embeddings by aggregating neighboring node features.
    - **GNN does not access to neighboring nodes within the mini-batch!**
- **Standard SGD cannot effectively train GNNs.**

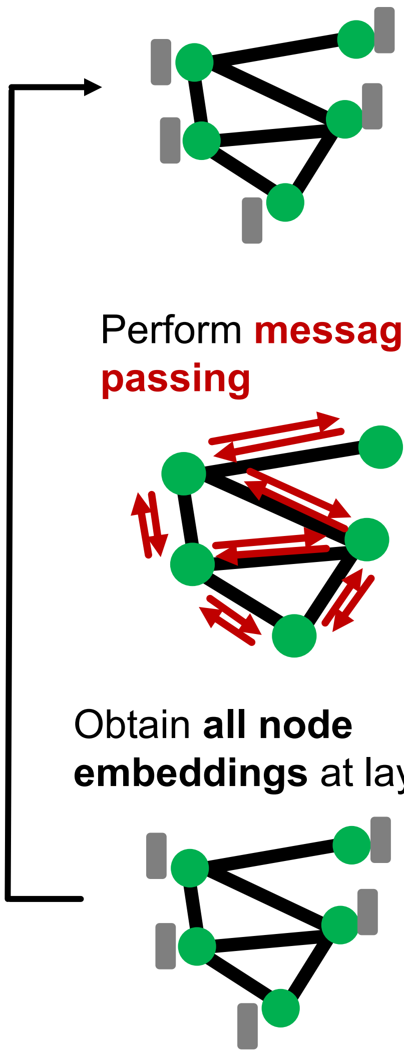
Why is it Hard?

- **Naïve full-batch implementation:** Generate embeddings of all the nodes **at the same time:**
  $H^{(k+1)} = \sigma(\tilde{A}H^{(k)}W_k^{\mathrm{T}} + H^{(k)}B_k^{\mathrm{T}})$
  - Load **the entire graph A and features X. Set $H^{(0)} = X$.**
  - **At each GNN layer: Compute embeddings of all nodes using all the node embeddings from the previous layer.**
  - Compute the loss
  - Perform gradient descent

Given **all node embeddings** at layer K

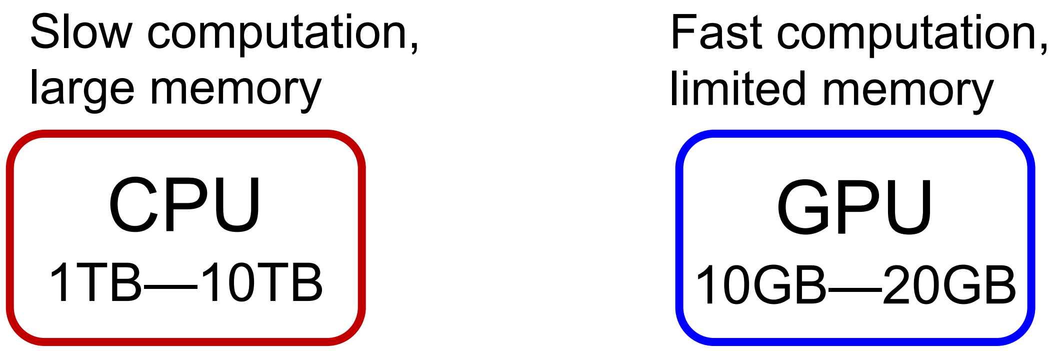
Perform **message-passing**

Obtain **all node embeddings** at layer K+1



Why is it Hard?

- However, **Full-batch** implementation is **not feasible** for a large graphs.
- **Why?**
  - Because we want to use GPU for fast training, but GPU memory is extremely limited (10GB-80GB).
  - **The entire graph and the features cannot be loaded on GPU.**


Slow computation, large memory
CPU
1TB—10TB
Fast computation, limited memory
GPU
10GB—20GB

Today's Lecture

We introduce **three methods for scaling up GNNs:**

- **Two** methods perform message-passing over **small subgraphs in each mini-batch**; only the subgraphs need to be loaded on a GPU at a time.
  - **Neighbor Sampling** [Hamilton et al. NeurIPS 2017]
  - **Cluster-GCN** [Chiang et al. KDD 2019]
- **One** method **simplifies a GNN into feature-preprocessing operation** (can be efficiently performed even on a CPU)
  - **Simplified GCN** [Wu et al. ICML 2019]

GraphSAGE Neighbor Sampling: Scaling up GNNs

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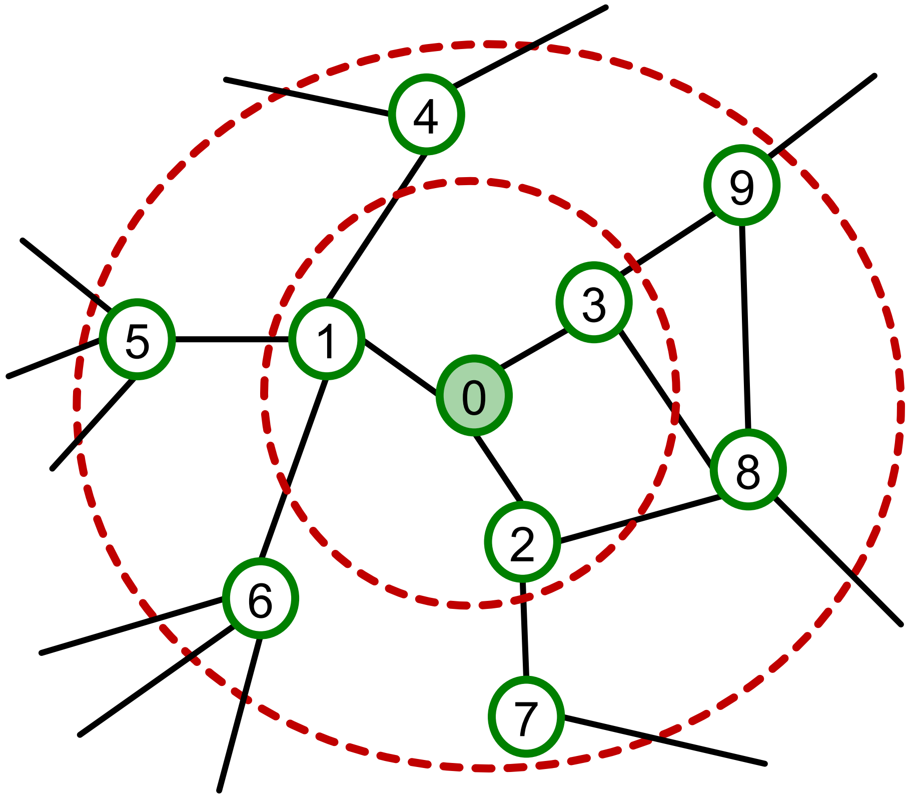
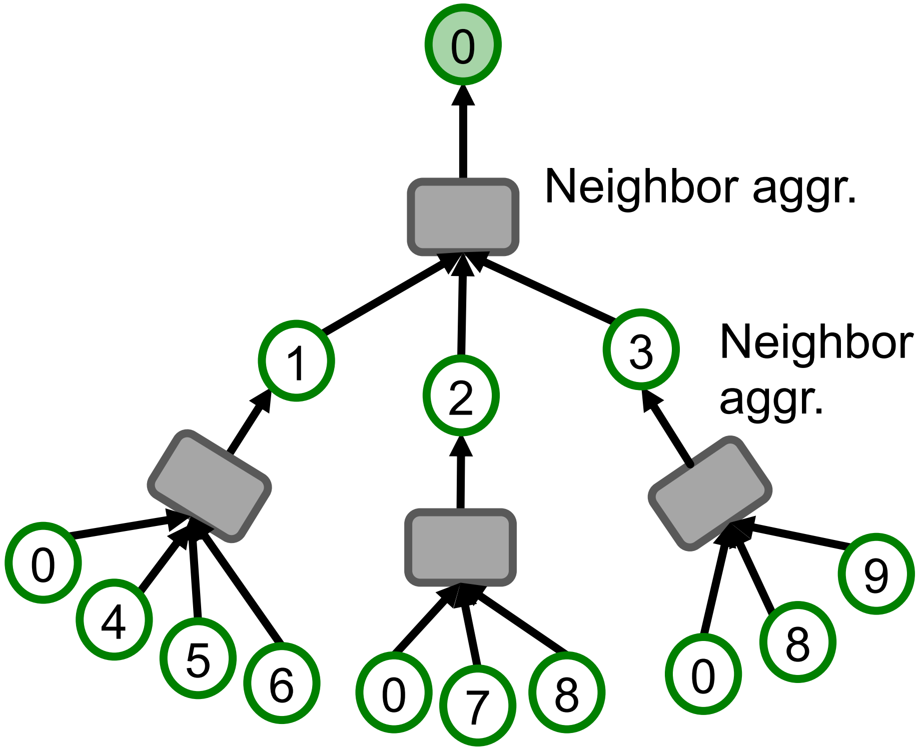
Recall: Computational Graph

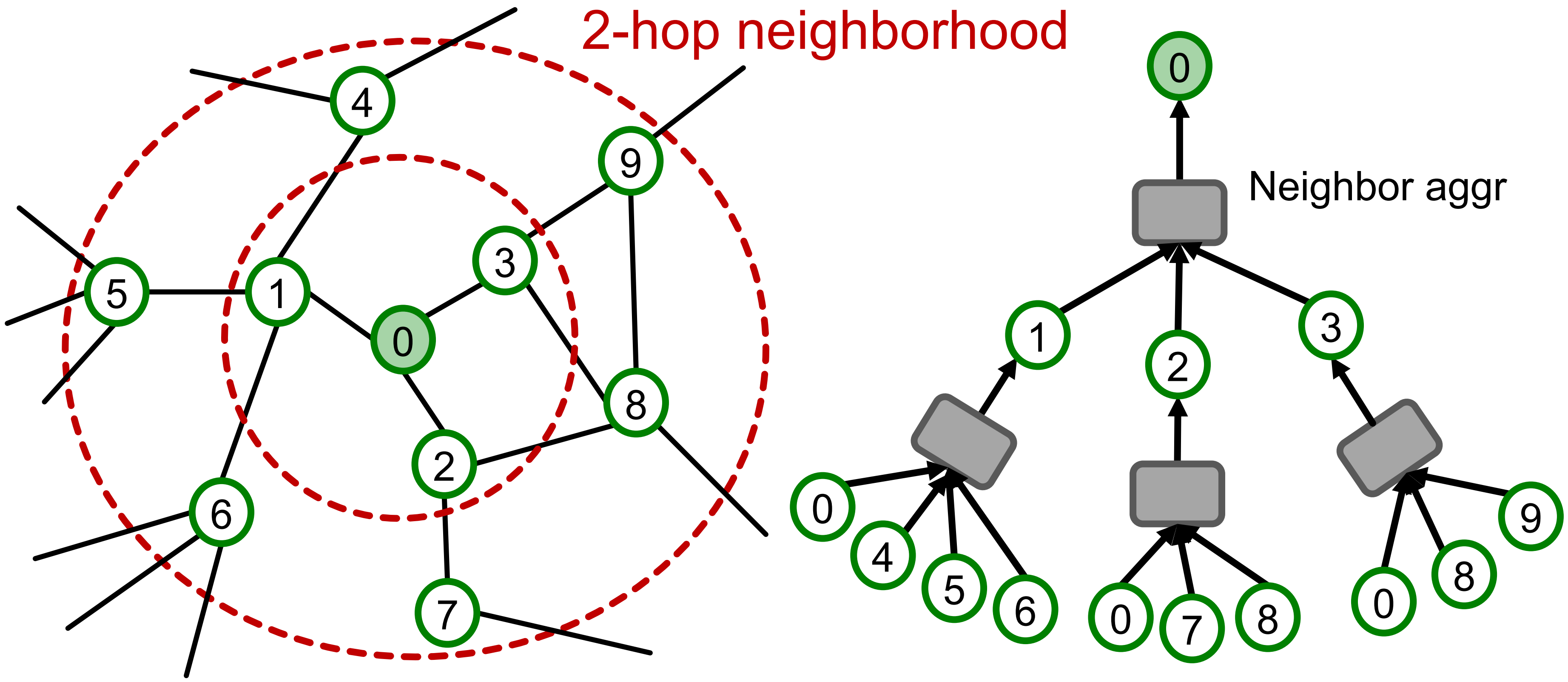
- **Recall**: GNNs generate node embeddings via neighbor aggregation.
  - Represented as a computational graph (right).





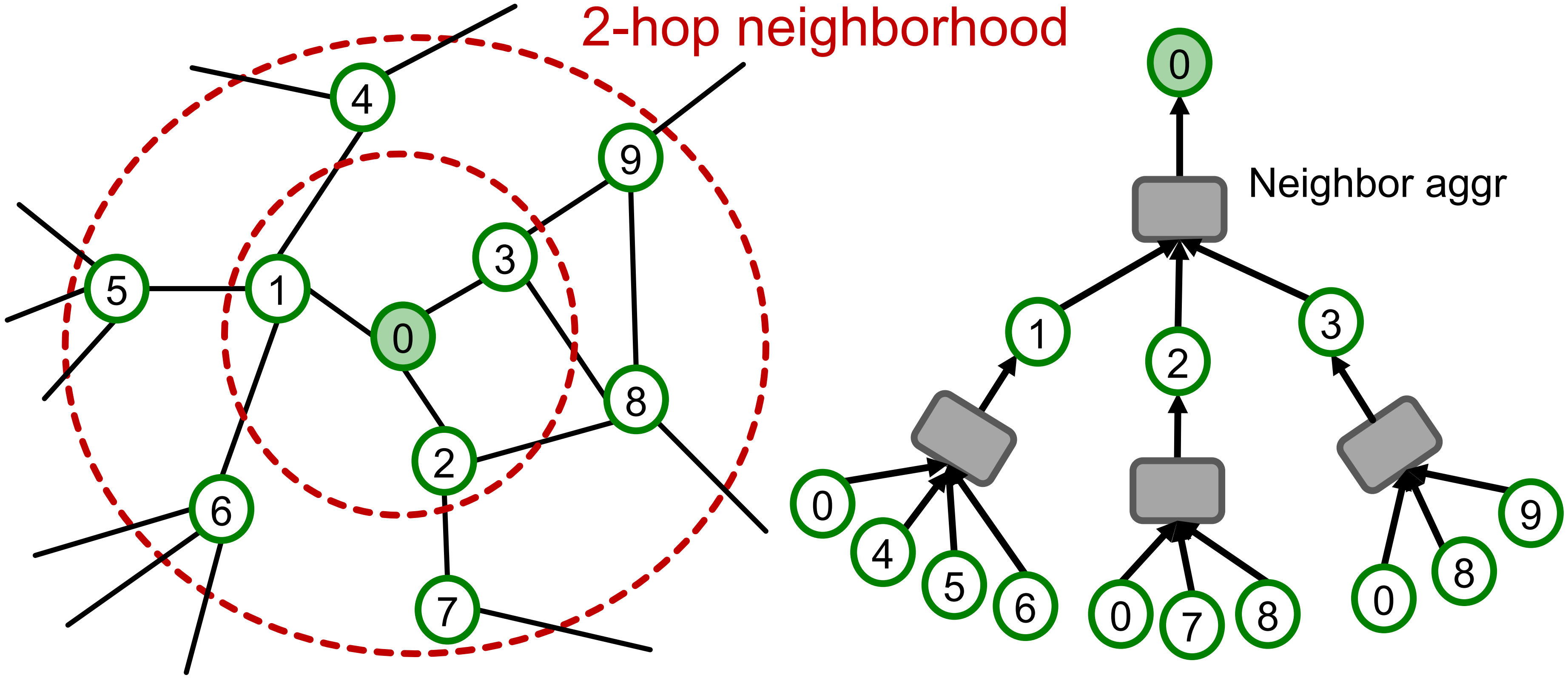
Recall: Computational Graph

- **Observation**: A 2-layer GNN generates embedding of node "0" using 2-hop neighborhood structure and features.



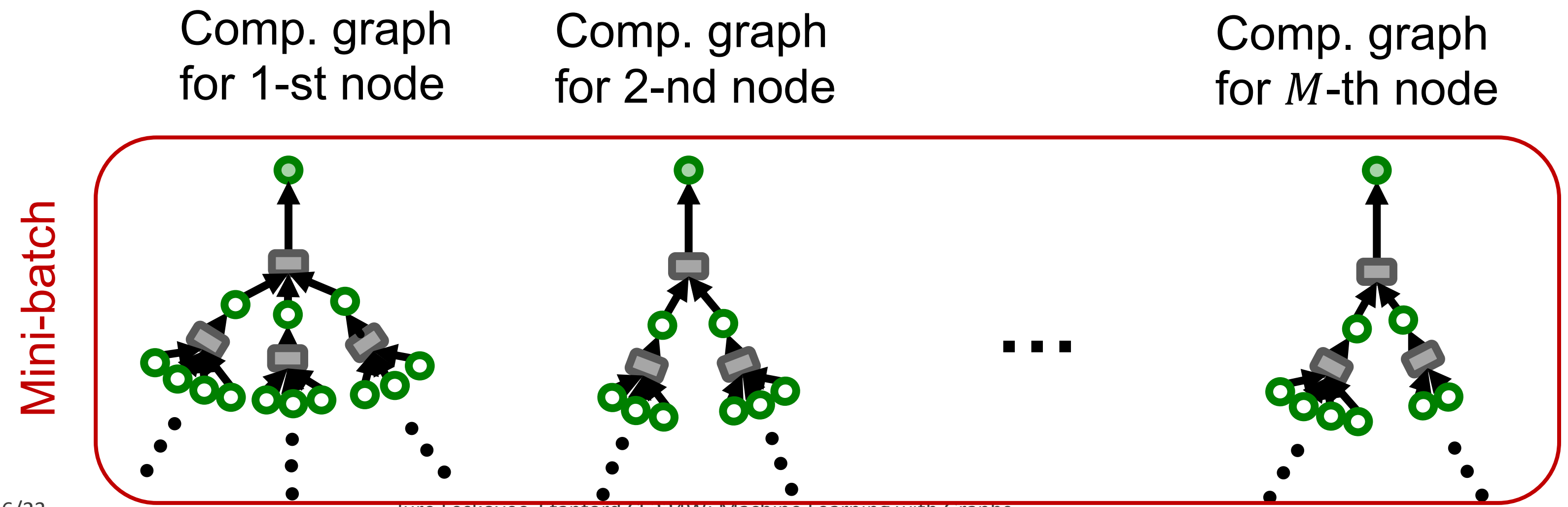
Recall: Computational Graph

- **Observation**: More generally, K-layer GNNs generate embedding of a node using K-hop neighborhood structure and features.



Computing Node Embeddings

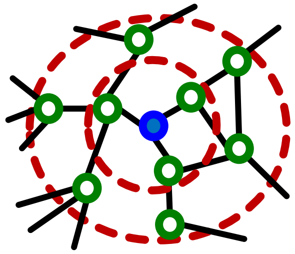
- **Key insight**: To compute embedding of a single node, all we need is **the K-hop neighborhood** (which defines the computation graph).
- Given a set of M different nodes in a **mini-batch**, we can generate their embeddings using M computational graphs. **Can be computed on GPU!**


Comp. graph for 1-st node
Comp. graph for 2-nd node
Comp. graph for M-th node
Mini-batch
…

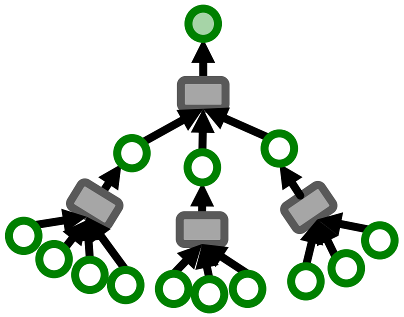
Stochastic Training of GNNs

- **We can now consider the following SGD strategy for training K-layer GNNs:**
  - Randomly sample M ($\ll N$) root nodes.
  - For each sampled root node v:
    - Get ***K*-hop neighborhood** and construct the **computation graph**.
    - Use the above to generate v's embedding.
  - Compute the loss $\ell_{sub}(\boldsymbol{\theta})$ averaged over the M nodes.
  - Perform SGD: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \nabla \ell_{sub}(\boldsymbol{\theta})$

K-hop neighborhood

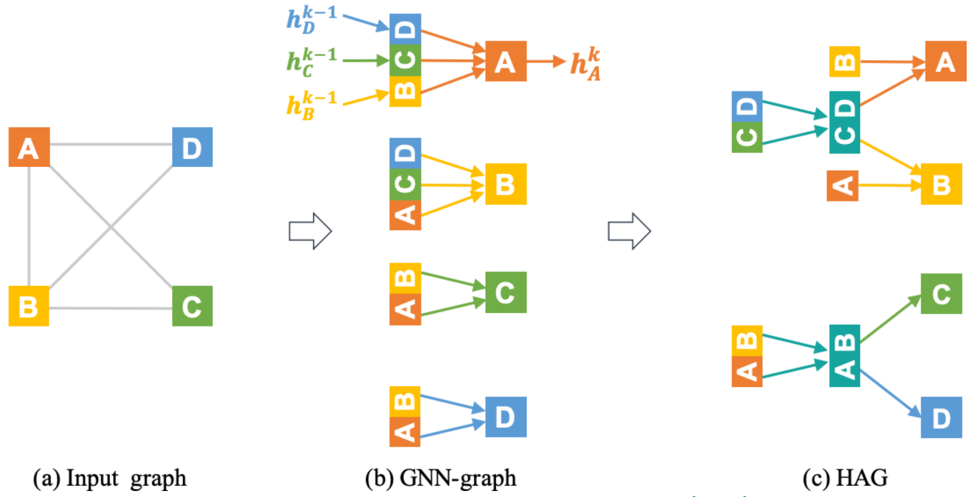


Computational graph



Issue with Stochastic Training (1)

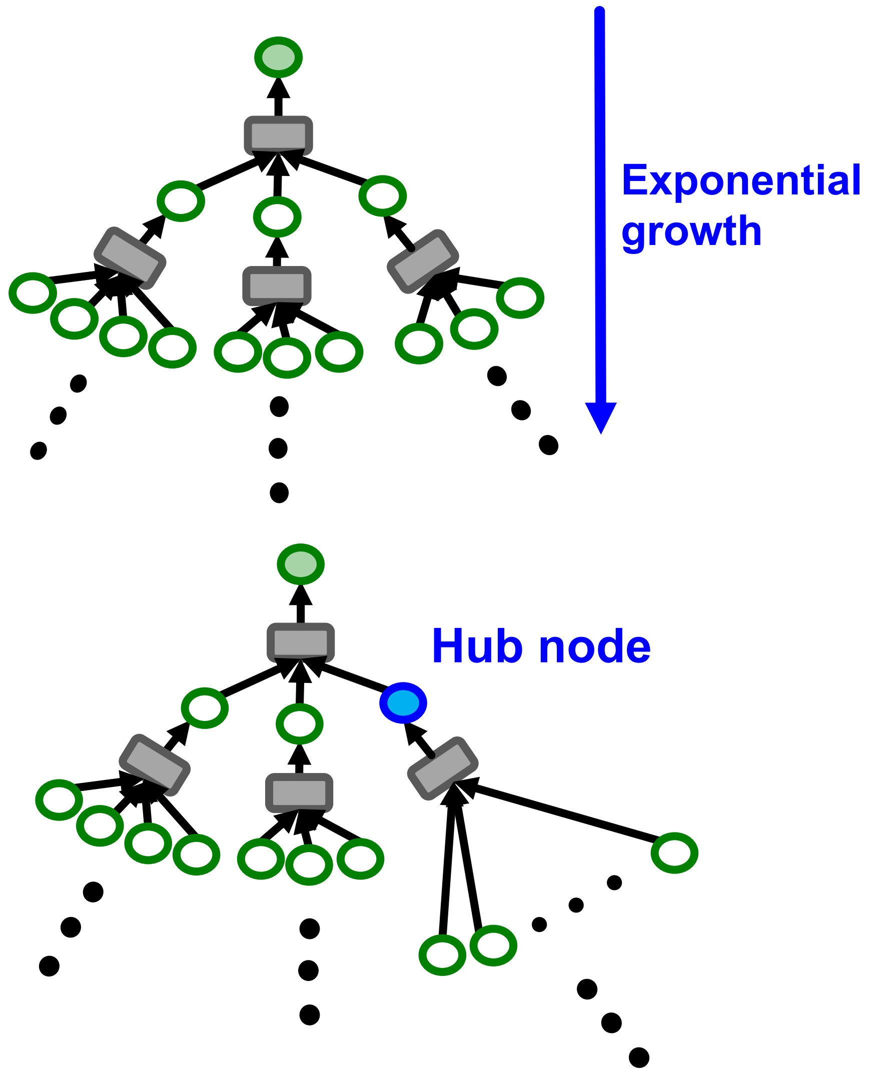
- **For each node**, we need to get **the entire K-hop neighborhood** and pass it through the computation graph.
- We need to aggregate lot of information just to compute one node embedding.
- **Some computational redundancy:**



Redundancy-Free Computation for Graph Neural Networks, KDD 202

Issue with Stochastic Training (2)

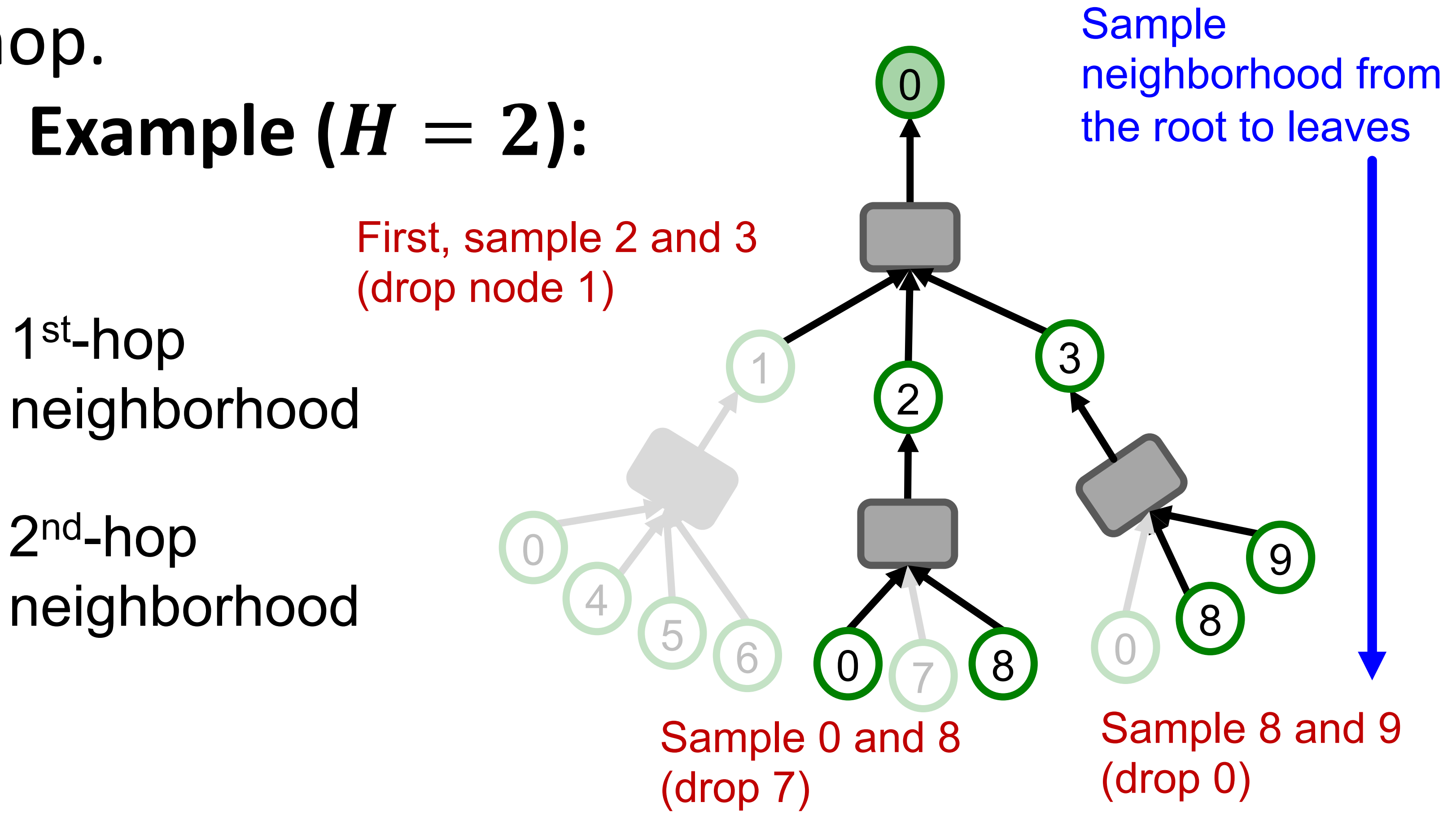
- **2nd issue:**
  - Computation graph becomes **exponentially large** with respect to the layer size K.
  - Computation graph explodes when it hits a **hub node** (high-degree node).
- **Next:** Make the comp. graph more compact!



Neighborhood Sampling

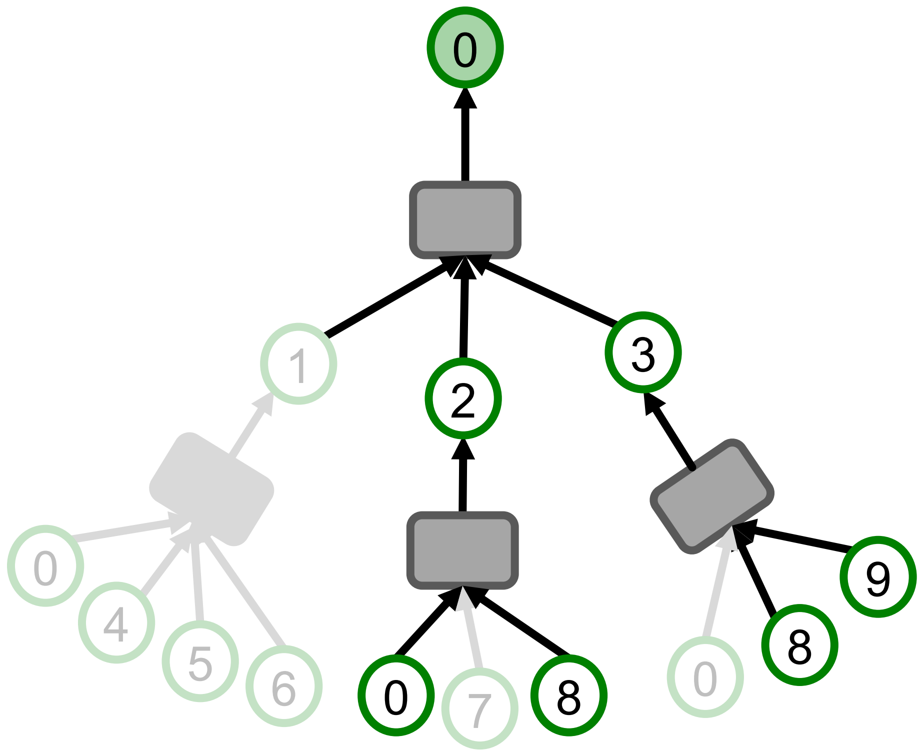
Key idea: **Construct the computational graph** by (randomly) sampling at most H neighbors at each hop.

- **Example ($H = 2$):**



Neighborhood Sampling

We can use the pruned computational graph to more efficiently compute node embeddings.

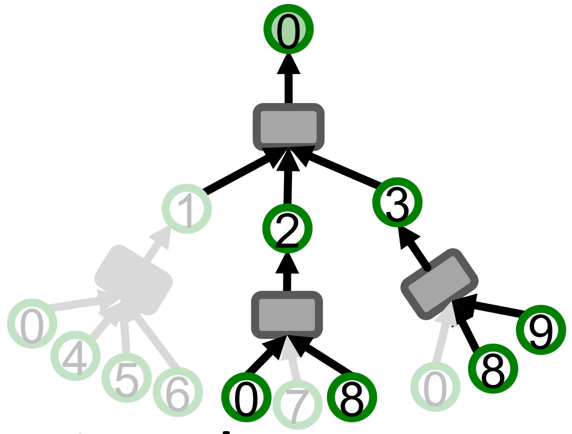


Neighborhood Sampling Algorithm

Neighbor sampling for K-layer GNN

- For $k = 1, 2, \ldots, K$:
  - For each node in k-hop neighborhood:
  - (Randomly) sample at most H_k neighbors:

1st-hop neighborhood	Sample $H_1 = 2$ neighbors
2nd-hop neighborhood	Sample $H_2 = 2$ neighbors



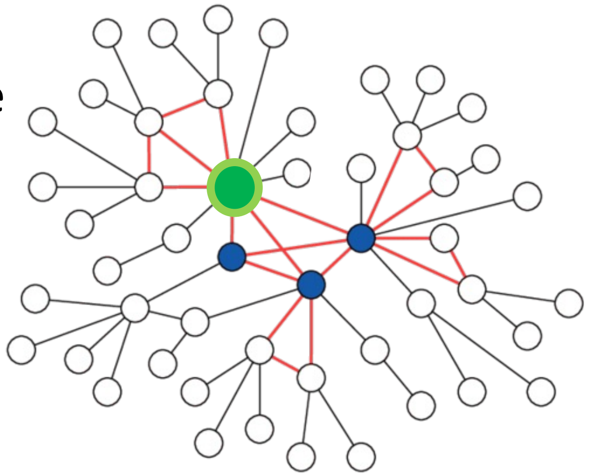
- K-layer GNN will at most involve $\prod_{k=1}^{K} H_k$ leaf nodes in comp. graph.

Remarks on Neighbor Sampling (1)

- **Remark 1: Trade-off in sampling number H**
  - Smaller H leads to more efficient neighbor aggregation, but results are less stable training **due to the larger variance** in neighbor aggregation.
- **Remark 2: Computational time**
  - Even with neighbor sampling, **the size of the computational graph is still exponential with respect to number of GNN layers K.**
  - Adding one GNN layer would make computation H times more expensive.

Remarks on Neighbor Sampling (2)

- **Remark 3: How to sample the nodes**
  - **Random sampling:** fast but many times not optimal (may sample many “unimportant” nodes)
  - **Random Walk with Restarts:**
    - Natural graphs are “scale free”, sampling random neighbors, samples many low degree “leaf” nodes.
    - Strategy to sample important nodes:
      - Compute Random Walk with Restarts score R_i starting at the **green** node
      - At each level sample H neighbors i with the highest R_i
    - This strategy works much better in practice.



Summary: Neighbor Sampling

- **A computational graph is constructed for each node in a mini-batch.**
- **In neighbor sampling, the comp. graph is pruned/sub-sampled to increase computational efficiency.**
- **The pruned comp. graph is used to generate a node embedding.**

- However, **computational graphs can still become large, especially for GNNs with many message-passing layers.**

Cluster-GCN: Scaling up GNNs

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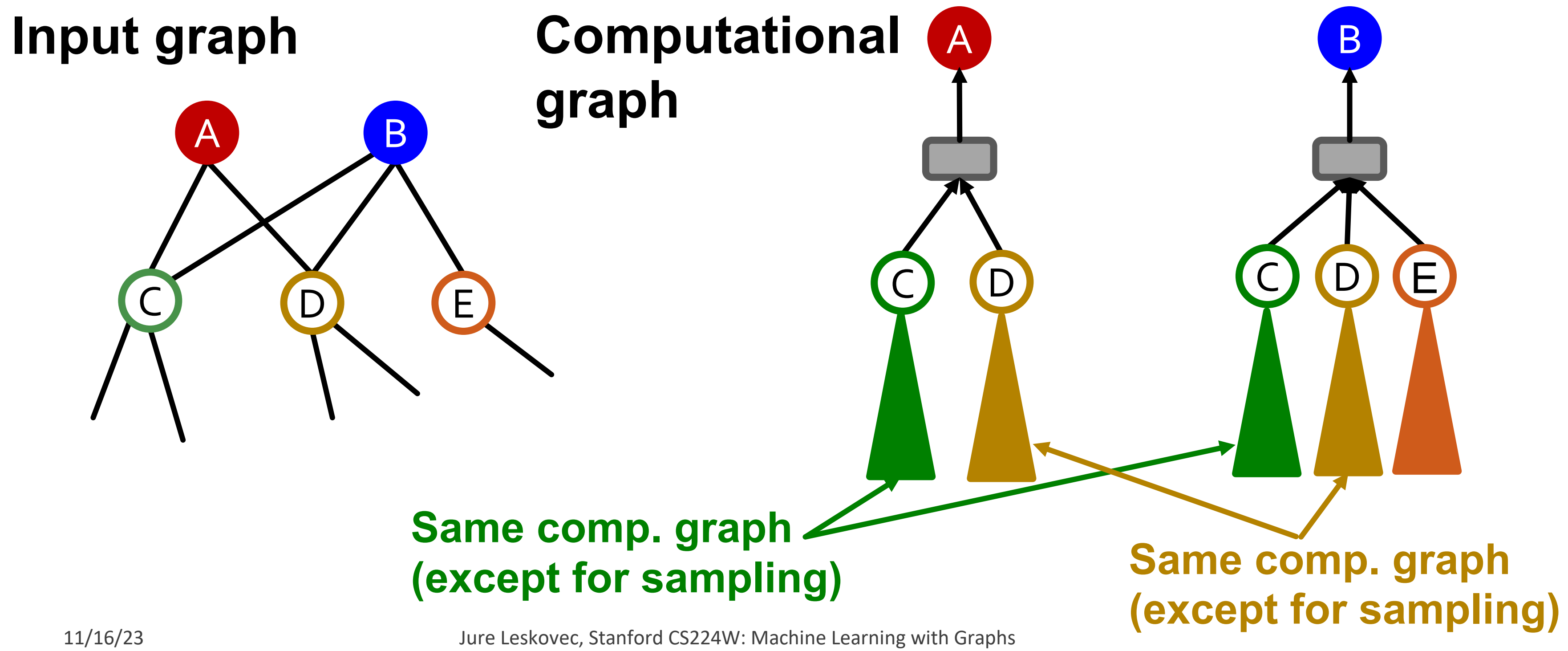
Issues with Neighbor Sampling

- **The size of computational graph becomes exponentially large w.r.t. the #GNN layers.**
- **Computation is redundant**, especially when nodes in a mini-batch share many neighbors.



Input graph
A
B
C
D
E
Computational graph
A
B
C
D
C
D
E
Same comp. graph (except for sampling)
Same comp. graph (except for sampling)

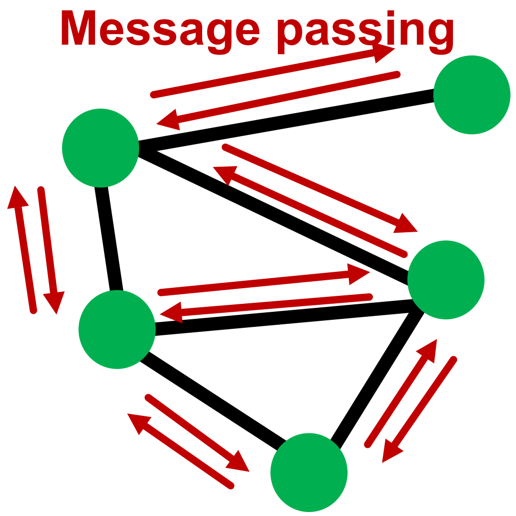
Recall: Full Batch GNN

- In full-batch GNN implementation, **all the node embeddings are updated together using embeddings of the previous layer.**

Update for all $v \in V$ **Message**

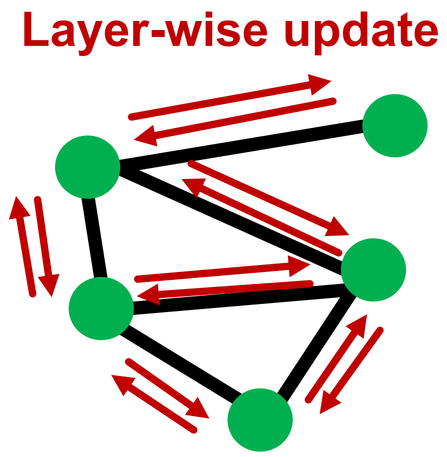
$$h_v^{(\ell)} = COMBINE\left(h_v^{(\ell-1)}, AGGR\left(\left\{\boldsymbol{h}_{\boldsymbol{u}}^{(\ell-1)}\right\}_{u \in N(v)}\right)\right)$$

- In each layer, only 2*#(edges) messages need to be computed.
- For K-layer GNN, only $2K$*#(edges) messages need to be computed.
- GNN's entire computation is only **linear** in #(edges) and #(GNN layers). **Fast!**



Insight from Full-batch GNN

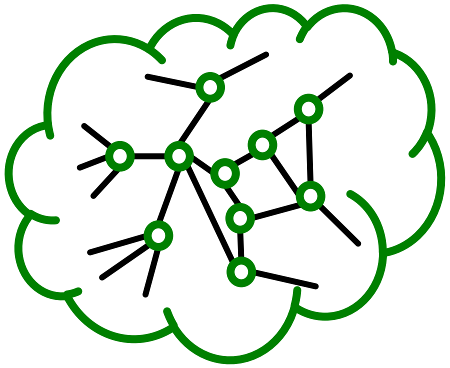
- The layer-wise node embedding update allows the re-use of embeddings from the previous layer.
- This significantly reduces the computational redundancy of neighbor sampling.
  - Of course, the layer-wise update is **not feasible** for a large graph due to **limited GPU memory**.
    - Requires putting the entire graph and features on GPU.



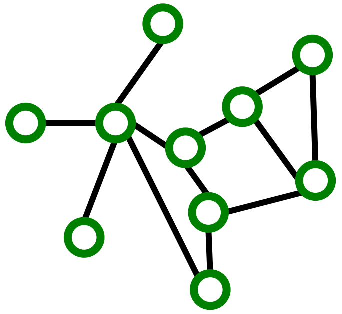
Subgraph Sampling

- **Key idea**: We can **sample a small subgraph of the large graph** and then perform the efficient **layer-wise** node embeddings update over the subgraph.

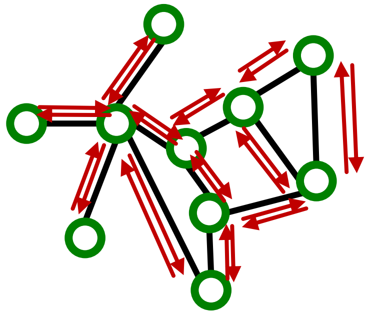
Large graph



Sampled subgraph
(small enough to
be put on a GPU)



**Layer-wise
node embeddings
update on the GPU**



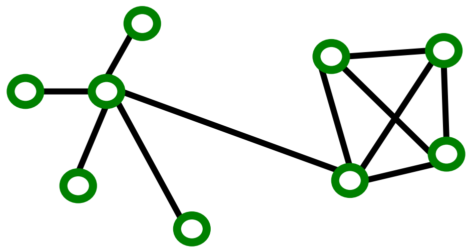
Subgraph Sampling

- Key question: **What subgraphs are good for training GNNs?**
  - **Recall: GNN performs node embedding by passing messages via the edges.**
    - Subgraphs **should retain edge connectivity structure of the original graph as much as possible.**
    - This way, the GNN over the subgraph generates embeddings closer to the GNN over the original graph.

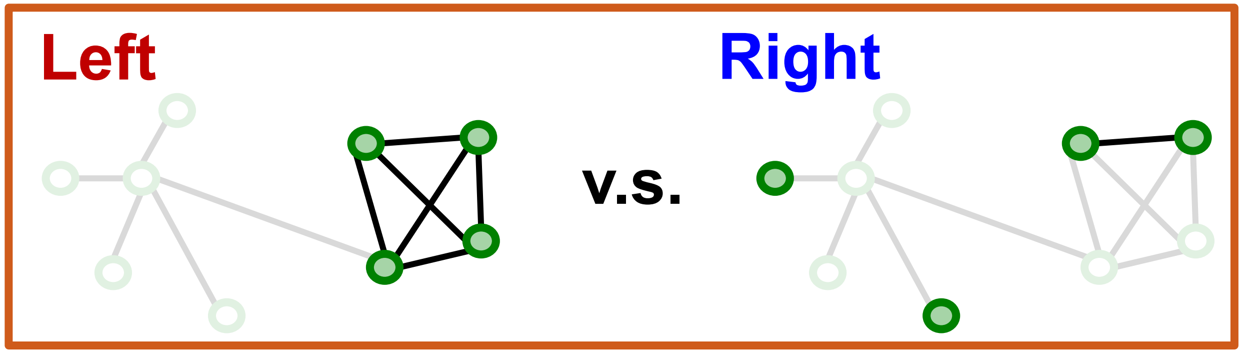
Subgraph Sampling: Case Study

- **Which subgraph is good for training GNN?**

Original graph



Subgraphs (both 4-node induced subgraph)



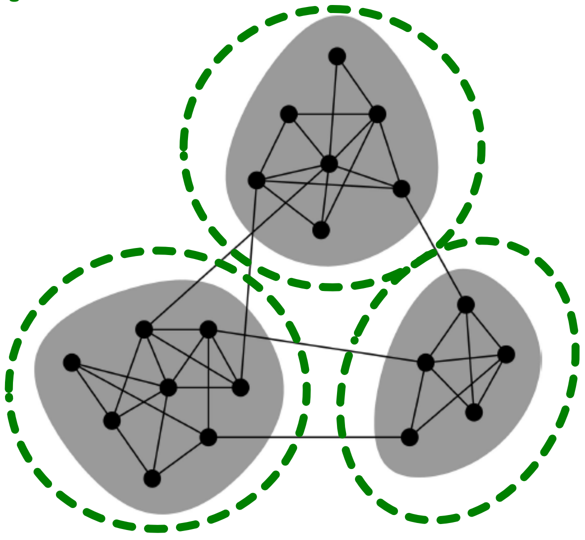
- **Left subgraph** retains the essential community structure among the 4 nodes → **Good**
- **Right subgraph** drops many connectivity patterns, even leading to isolated nodes → **Bad**

Exploiting Community Structure

Real-world graph exhibits community structure

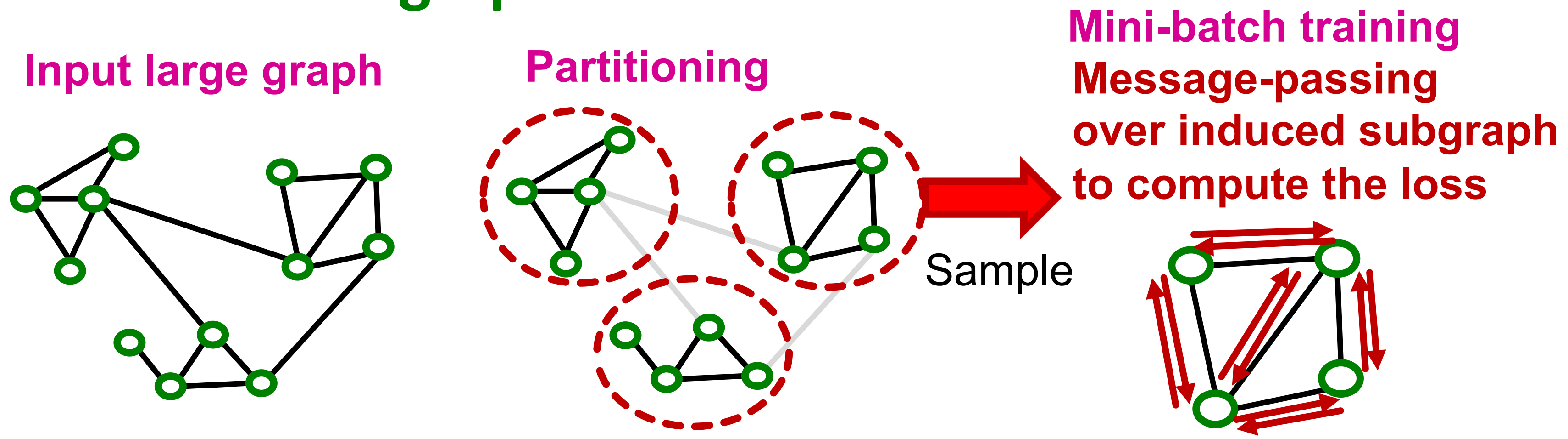
- A large graph can be decomposed into many small communities.

- **Key insight** [Chiang et al. KDD 2019]:
  Sample a community as a subgraph. Each subgraph retains essential local connectivity pattern of the original graph.



Cluster-GCN: Overview

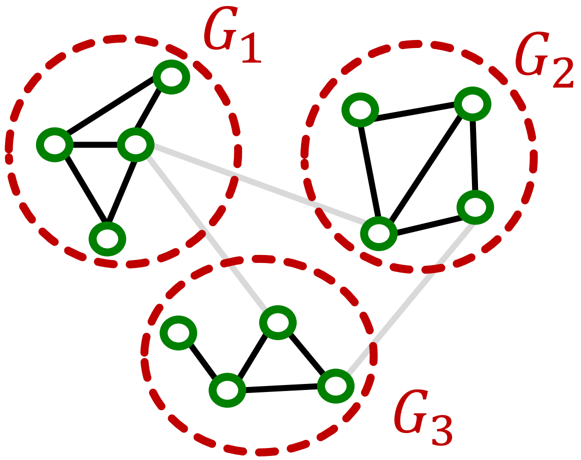
- **We first introduce "vanilla" Cluster-GCN.**
- **Cluster-GCN** consists of two steps:
  - **Pre-processing**: Given a large graph, partition it into groups of nodes (i.e., subgraphs).
  - **Mini-batch training**: Sample one node group at a time. Apply GNN's message passing over the **induced subgraph**.



Cluster-GCN: Pre-processing

- Given a large graph $G = (V, E)$, **partition its nodes V into C groups: $V_1, \dots, V_C$.**
  - We can use any scalable community detection methods, e.g., Louvain, METIS [Karypis et al. SIAM 1998].
- $V_1, \dots, V_C$ **induces** C subgraphs, $G_1, \dots, G_C$,
  - Recall: $G_c \equiv (V_c, E_c)$, where $E_c = \{(u, v) | u, v \in V_c\}$

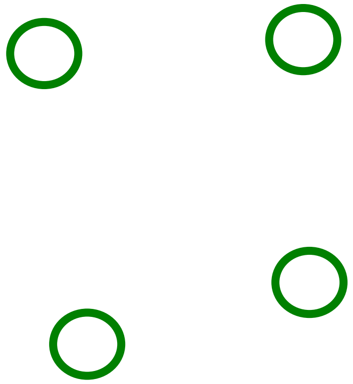
Notice: Between-group edges are *not* included in $G_1, \dots, G_C$.



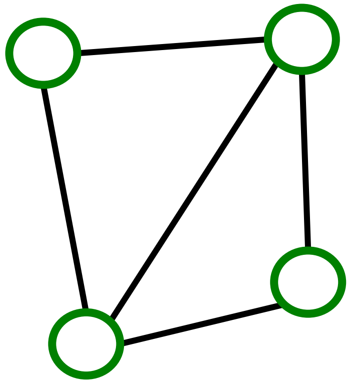
Cluster-GCN: Mini-batch Training

- For each mini-batch, **randomly sample a node group V_c**.
- Construct **induced subgraph $G_c = (V_c, E_c)$**

Sampled node group V_c

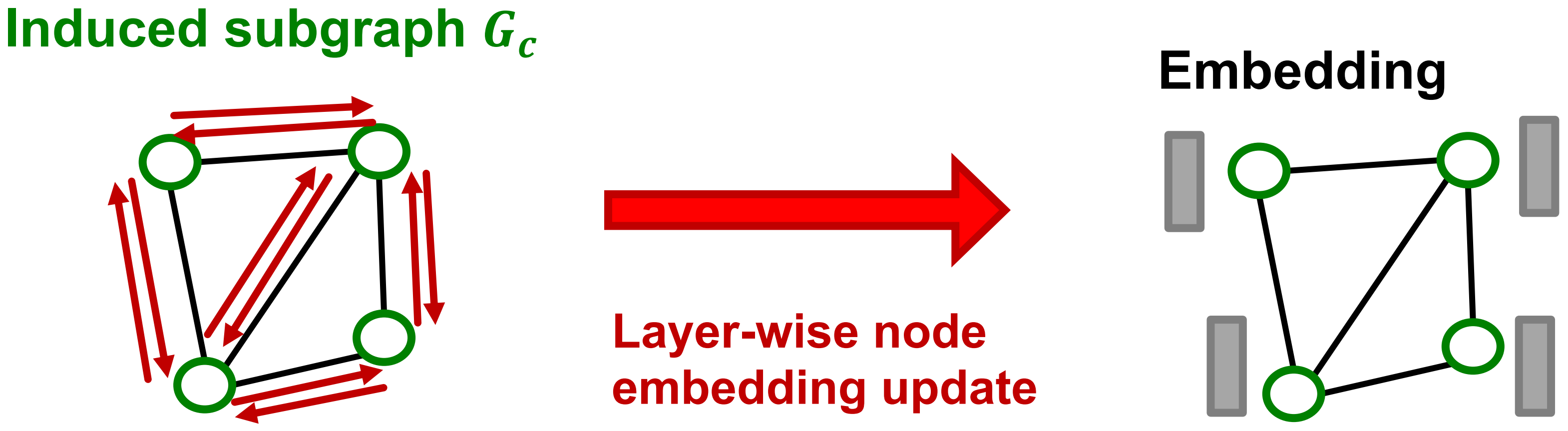


Induced subgraph G_c



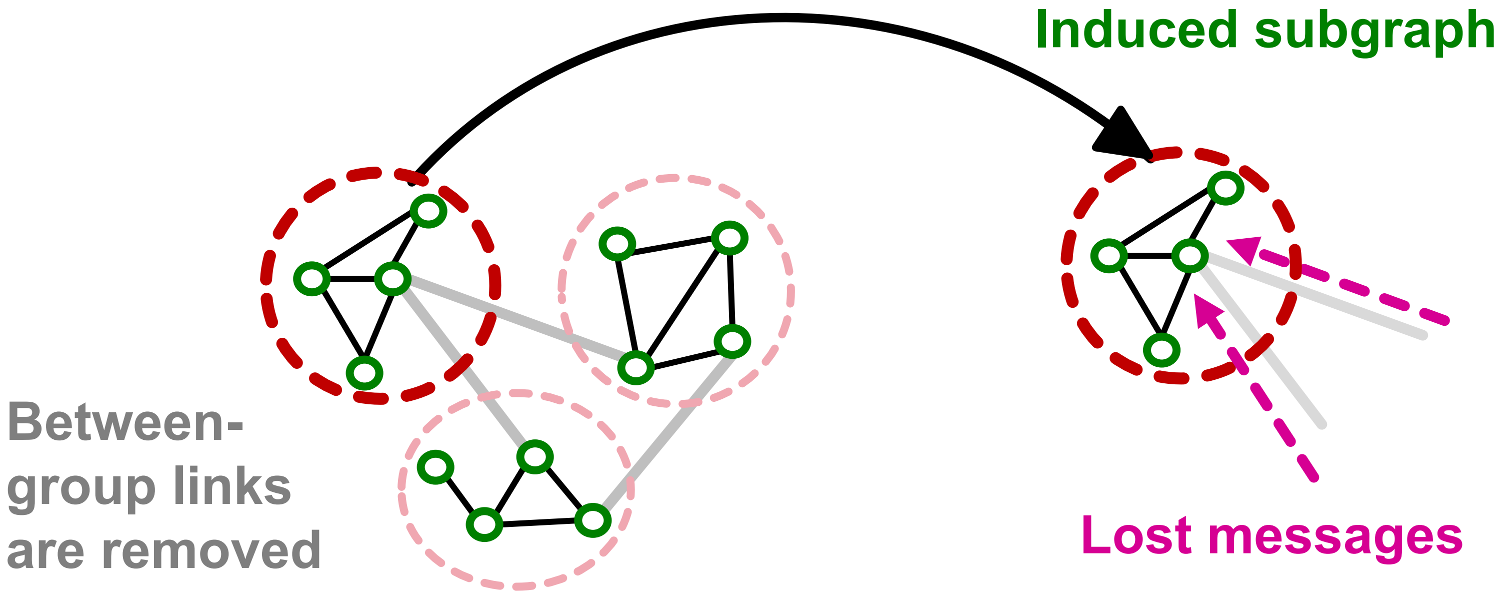
Cluster-GCN: Mini-batch Training

- Apply GNN's **layer-wise node update** over $\boldsymbol{G_c}$ to obtain embedding $\boldsymbol{h}_v$ for each node $v \in V_c$.
- Compute the loss for each node $v \in V_c$ and take average: $\ell_{sub}(\boldsymbol{\theta}) = (1/|V_c|) \cdot \sum_{v \in V_c} \ell_v(\boldsymbol{\theta})$
- Update params: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \nabla \ell_{sub}(\boldsymbol{\theta})$



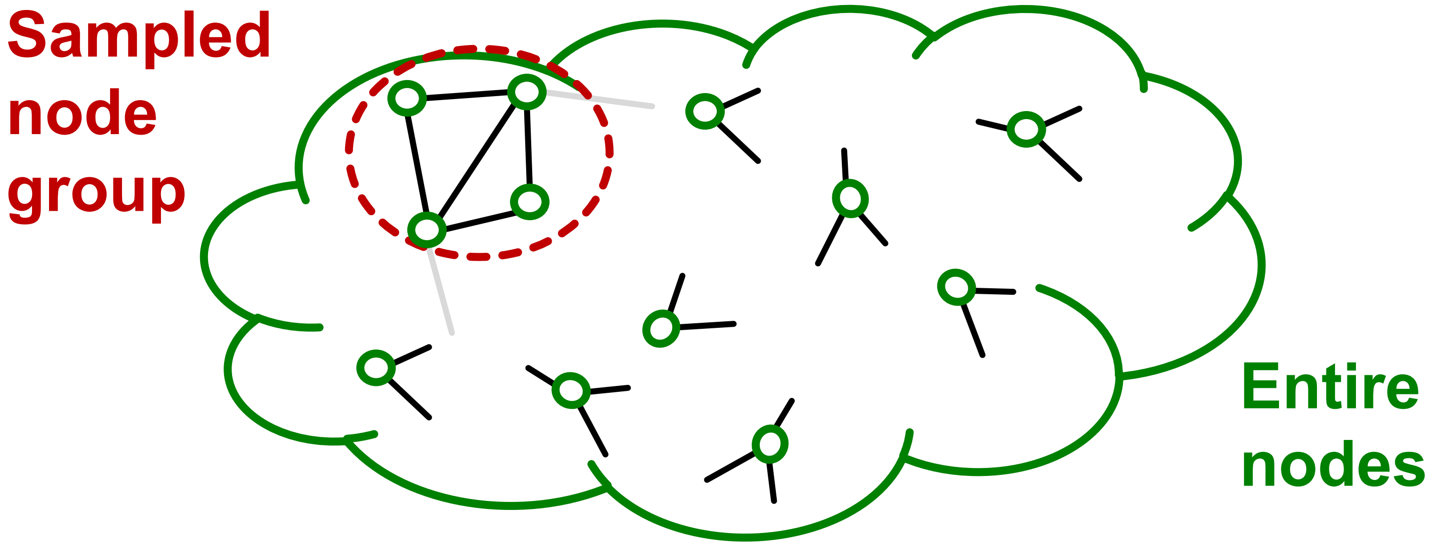
Issues with Cluster-GCN (1)

- **The induced subgraph removes between-group links.**
- As a result, ***messages from other groups will be lost during message passing*, which could hurt the GNN's performance.**



Issues with Cluster-GCN (2)

- Graph community detection algorithm **puts similar nodes together in the same group**.
- **Sampled node group** tends to only cover the small-concentrated portion of the **entire data**.



Issues with Cluster-GCN (3)

Sampled nodes are not diverse enough to be represent the entire graph structure:

- As a result, the gradient averaged over the sampled nodes, $\frac{1}{|V_c|}\sum_{v \in V_c} \ell_v(\boldsymbol{\theta})$, becomes unreliable.
  - **Fluctuates a lot from a node group to another.**
  - **In other words, the gradient has high variance.**
- **Leads to slow convergence of SGD**

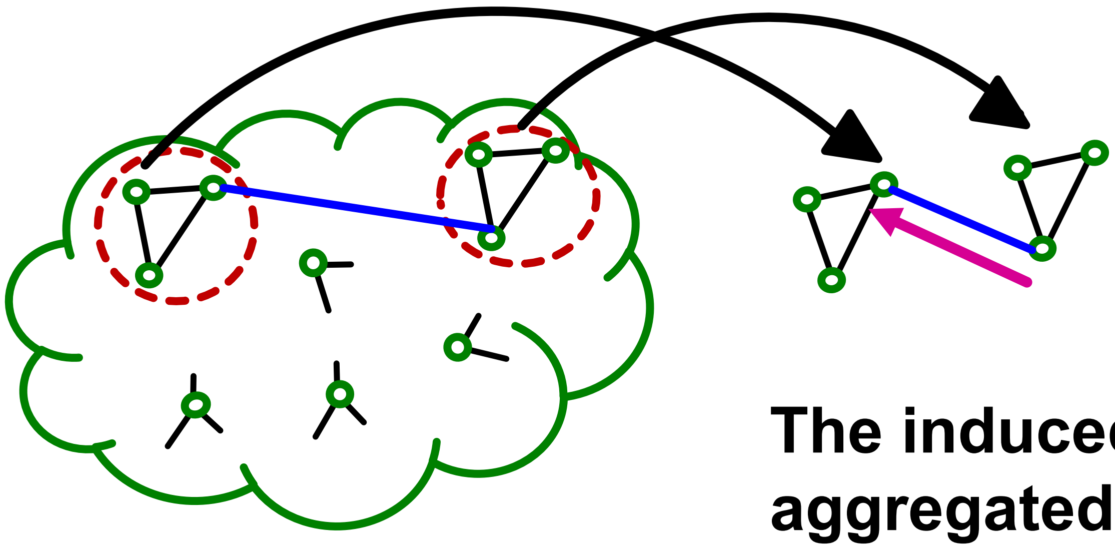
Advanced Cluster-GCN: Overview

- **Solution: Aggregate multiple node groups per mini-batch.**
- Partition the graph into **relatively-small groups of nodes.**
- **For each mini-batch:**
  - **Sample and aggregate multiple node groups.**
  - **Construct the induced subgraph of the *aggregated* node group.**
  - The rest is the same as vanilla Cluster-GCN (compute node embeddings and the loss, update parameters)

Advanced Cluster-GCN: Overview

- **Why does the solution work?**

Sampling multiple node groups
→ Makes the sampled nodes more representative of the entire nodes. Leads to less variance in gradient estimation.



The induced subgraph over aggregated node groups
→ Includes edges between groups
→ Message can flow across groups.

Advanced Cluster-GCN

Similar to vanilla Cluster-GCN, advanced Cluster-GCN also follows a 2-step approach.

1) Pre-processing step:

- Given a large graph $G = (V, E)$, partition its nodes V into C **relatively-small** groups: $V_1, \dots, V_C$.
  - $V_1, \dots, V_C$ needs to be small so that even if multiple of them are aggregated, the resulting group would not be too large.

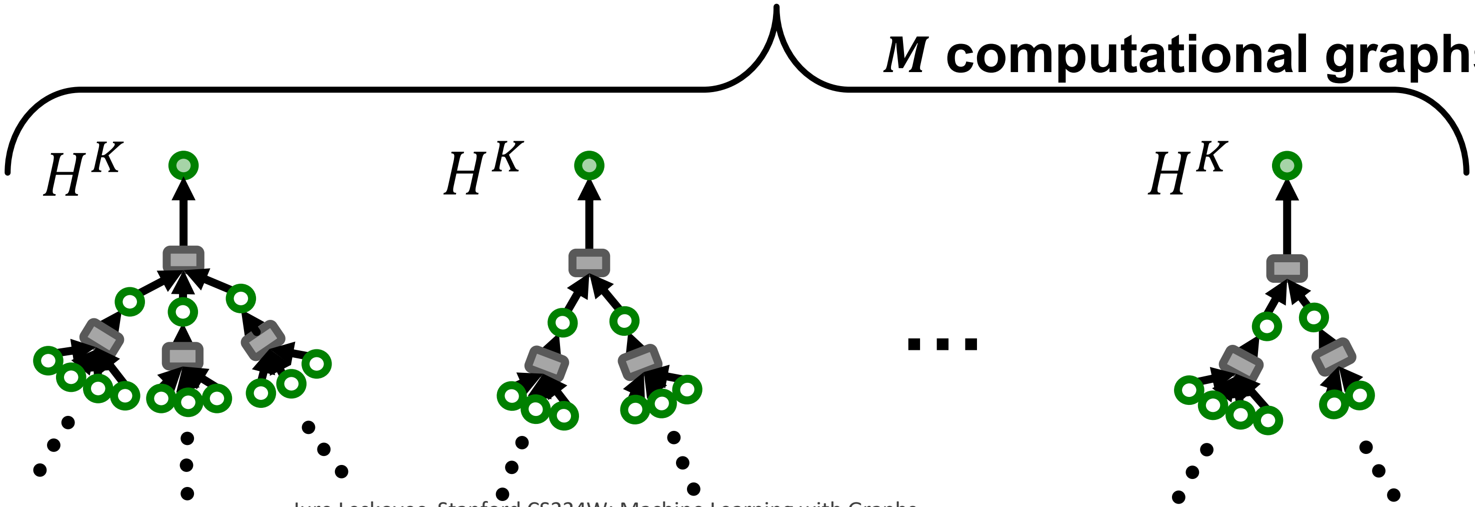
Advanced Cluster-GCN

2) Mini-batch training:

- For each mini-batch, **randomly sample a set of $\boldsymbol{q}$ node groups:** $\{V_{t_1}, \dots, V_{t_q}\} \subset \{V_1, \dots, V_C\}$.
- **Aggregate all nodes across the sampled node groups:** $V_{aggr} = V_{t_1} \cup \cdots \cup V_{t_q}$
- Extract the **induced subgraph** $\boldsymbol{G_{aggr} = (V_{aggr}, E_{aggr})}$,
  where $E_{aggr} = \{(u, v) \mid u, v \in V_{aggr}\}$
  - $\boldsymbol{E_{aggr}}$ **also includes between-group edges!**

Comparison of Time Complexity

- **Generate M ($\ll N$) node embeddings using K-layer GNN (N : #all nodes).**
- **Neighbor-sampling** (sampling H nodes per layer):
  - For each node, the size of K-layer computational graph is H^K.
  - For M nodes, the cost is $\boldsymbol{M \cdot H^K}$



Comparison of Time Complexity

- **Generate M ($\ll N$) node embeddings using K-layer GNN (N : #all nodes).**
- **Cluster-GCN:**
  - Perform message passing over a subgraph induced by the M nodes.
  - The subgraph contains $M \cdot D_{avg}$ edges, where D_{avg} is the average node degree.
  - K-layer message passing over the subgraph costs at most $\boldsymbol{K \cdot M \cdot D_{avg}}$.

Comparison of Time Complexity

- In summary, the cost to generate embeddings for M nodes using K-layer GNN is:
  - **Neighbor-sampling (sample $\boldsymbol{H}$ nodes per layer): $\boldsymbol{M \cdot H^K}$**
  - **Cluster-GCN: $\boldsymbol{K \cdot M \cdot D_{avg}}$**
- **Assume $\boldsymbol{H = D_{avg}/2}$. In other words, 50% of neighbors are sampled.**
  - **Then, Cluster-GCN (cost: $\boldsymbol{2MHK}$) is much more efficient than neighbor sampling (cost: $\boldsymbol{MH^K}$).**
  - **Linear (instead of exponential) dependency w.r.t. $\boldsymbol{K}$.**

Cluster-GCN: Summary

- Cluster-GCN first **partitions the entire nodes into a set of small node groups.**
- At each mini-batch, multiple node groups are sampled, and their nodes are aggregated.
- **GNN performs layer-wise node embeddings update over the induced subgraph**.
- Cluster-GCN is more computationally efficient than neighbor sampling, especially when #(GNN layers) is large.
- But Cluster-GCN leads to systematically biased gradient estimates (due to missing cross-community edges)

Scaling up by Simplifying GNN Architecture

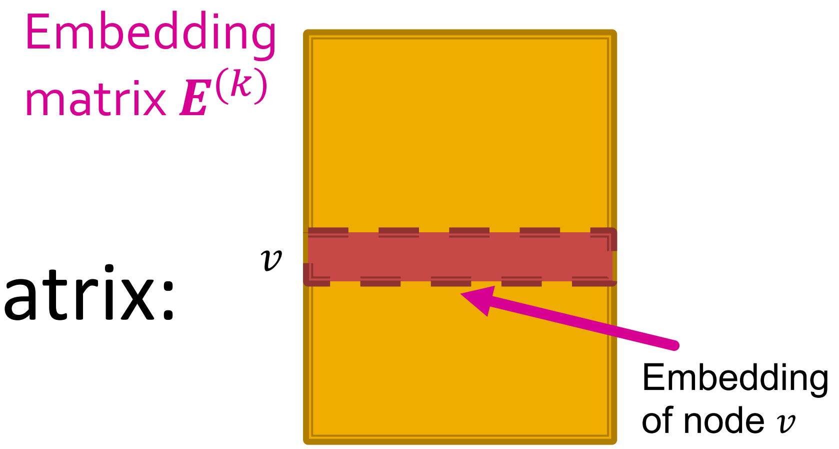
CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Roadmap of Simplifying GCN

- **We start from Graph Convolutional Network (GCN)** [Kipf & Welling ICLR 2017]**.**
- We simplify GCN ("*SimplGCN*") by **removing the non-linear activation** from the GCN [Wu et al. ICML 2019]**.**
  - SimplGCN demonstrated that the performance on benchmark is not much lower by the simplification.
  - Simplified GCN turns out to be extremely scalable by the model design.
  - **The simplification strategy is very similar to the one used by LightGCN for recommender systems.**

Quick Overview of LightGCN (1)

- Adjacency matrix: $\boldsymbol{A}$
- Degree matrix: $\boldsymbol{D}$
- Normalized adjacency matrix: $\widetilde{\boldsymbol{A}} \equiv \boldsymbol{D}^{-1/2}\boldsymbol{A}\boldsymbol{D}^{-1/2}$



- Let $\boldsymbol{E}^{(k)}$ be the embedding matrix at k-th layer.
- Let $\boldsymbol{E}$ be the input embedding matrix.
  - We backprop into $\boldsymbol{E}$.
- GCN's aggregation in the matrix form
  - $\boldsymbol{E}^{(k+1)} = \mathrm{ReLU}\left(\widetilde{\boldsymbol{A}}\boldsymbol{E}^{(k)}\boldsymbol{W}^{(k)}\right)$

Quick Overview of LightGCN (2)

- Removing ReLU non-linearity gives us
  - $\boldsymbol{E}^{(K)} = \boxed{\widetilde{\boldsymbol{A}}^{K}\ \boldsymbol{E}}\,\boldsymbol{W}$, where $\boldsymbol{W} \equiv \boldsymbol{W}^{(0)} \cdots \boldsymbol{W}^{(K-1)}$

    Diffusing node embeddings along the graph

- Efficient algorithm to obtain $\widetilde{\boldsymbol{A}}^{K}\ \boldsymbol{E}$
  - Start from input embedding matrix $\boldsymbol{E}$.
  - Apply $\boldsymbol{E} \leftarrow \widetilde{\boldsymbol{A}}\ \boldsymbol{E}$ for K times.
- Weight matrix $\boldsymbol{W}$ can be ignored for now.
  - $\boldsymbol{W}$ acts as a linear classifier over the diffused node embeddings $\widetilde{\boldsymbol{A}}^{K}\ \boldsymbol{E}$.

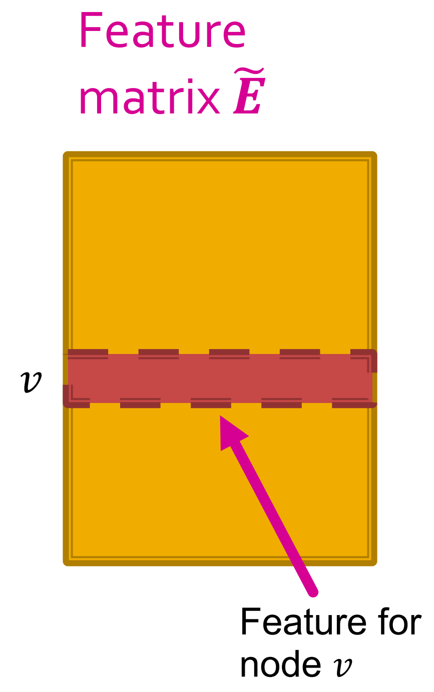
Differences to LightGCN

- SimplGCN adds **self-loops** to adjacency matrix $\boldsymbol{A}$:
  - $\boldsymbol{A} \leftarrow \boldsymbol{A} + \boldsymbol{I}$
    - Follows the original GCN by Kipf & Welling.

- SimplGCN assumes input node embeddings $\boldsymbol{E}$ to be **given as features**:
  - Input embedding matrix $\boldsymbol{E}$ is **fixed** rather than learned.
  - **Important consequence**: $\widetilde{\boldsymbol{A}}^{K}\ \boldsymbol{E}$ needs to be calculated **only once**.
    - Can be treated as a **pre-processing step**.

Simplified GCN: "SimplGCN"

- Let $\widetilde{\boldsymbol{E}} = \widetilde{\boldsymbol{A}}^K\ \boldsymbol{E}$ be pre-processed feature matrix.
  - Each row stores the pre-processed feature for each node.
  - $\widetilde{\boldsymbol{E}}$ can be used as input to any scalable ML models (e.g., linear model, MLP).
- SimplGCN empirically shows learning a linear model over $\widetilde{\boldsymbol{E}}$ often gives performance comparable to GCN!



Comparison with Other Methods

- Compared to neighbor sampling and cluster-GCN, **SimplGCN is much more efficient**.
  - **SimplGCN computes $\widetilde{\boldsymbol{E}}$ only once at the beginning.**
    - **The pre-processing (sparse matrix vector product, ($\boldsymbol{E} \leftarrow \widetilde{\boldsymbol{A}}\,\boldsymbol{E}$) can be performed efficiently on CPU.**
  - Once $\widetilde{\boldsymbol{E}}$ is obtained, getting an embedding for node v only takes **constant time!**
    - Just look up a row for node v in $\widetilde{\boldsymbol{E}}$.
    - No need to build a computational graph or sample a subgraph.
- But the model is **less** expressive (next).

Potential Issue of Simplified GCN

- Compared to the original GNN models, **SimplGCN's expressive power is limited due to the lack of non-linearity in generating node embeddings.**

Performance of Simplified GCN

- Surprisingly, in semi-supervised node classification benchmark, **SimplGCN works comparably to the original GNNs despite being less expressive.**

- **Why?**

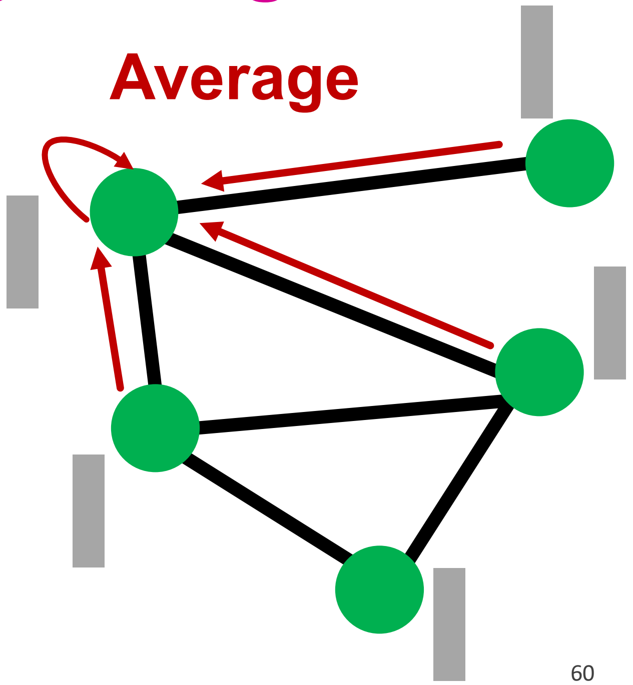
Graph Homophily

- Many node classification tasks exhibit homophily structure, i.e., **nodes connected by edges tend to share the same target labels.**
- **Examples**:
  - Paper category classification in paper-citation network
    - Two papers tend to share the same category if one cites another.
  - Movie recommendation for users in social networks
    - Two users tend to like the same movie if they are friends in a social network.

When does Simplified GCN Work?

- Recall the preprocessing step of the simplified GCN: **Do $E \leftarrow \widetilde{A}\, E$ for K times.**
    - E **is node feature matrix** $E = X$
- Pre-processed features are obtained **by iteratively averaging their neighboring node features.**

- **As a result, nodes connected by edges tend to have similar pre-processed features.**



When does Simplified GCN Work?

- **Premise**: Model uses the pre-processed node features to make prediction.
- Nodes connected by edges tend to get similar pre-processed features.

→ **Nodes connected by edges tend to be predicted the same labels by the model**

- **Simplified SGC's prediction aligns well with the graph homophily in many node classification benchmark datasets.**

Simplified GCN: Summary

- **Simplified GCN removes non-linearity in GCN and reduces to the simple pre-processing of node features.**
- Once the pre-processed features are obtained, scalable mini-batch SGD can be directly applied to optimize the parameters.
- **Simplified GCN works surprisingly well in node classification benchmark.**
  - The feature pre-processing aligns well with graph homophily in real-world prediction tasks.