Scaling Up Graph Neural Networks to Large Graphs

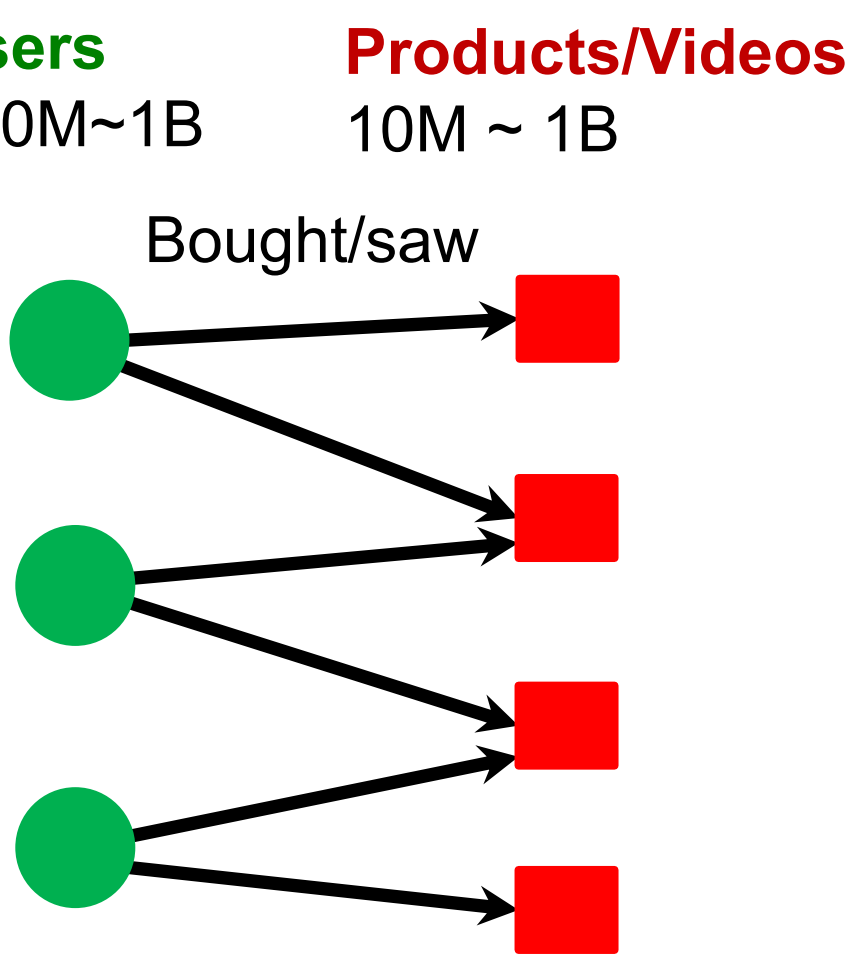
CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

http://cs224w.stanford.edu

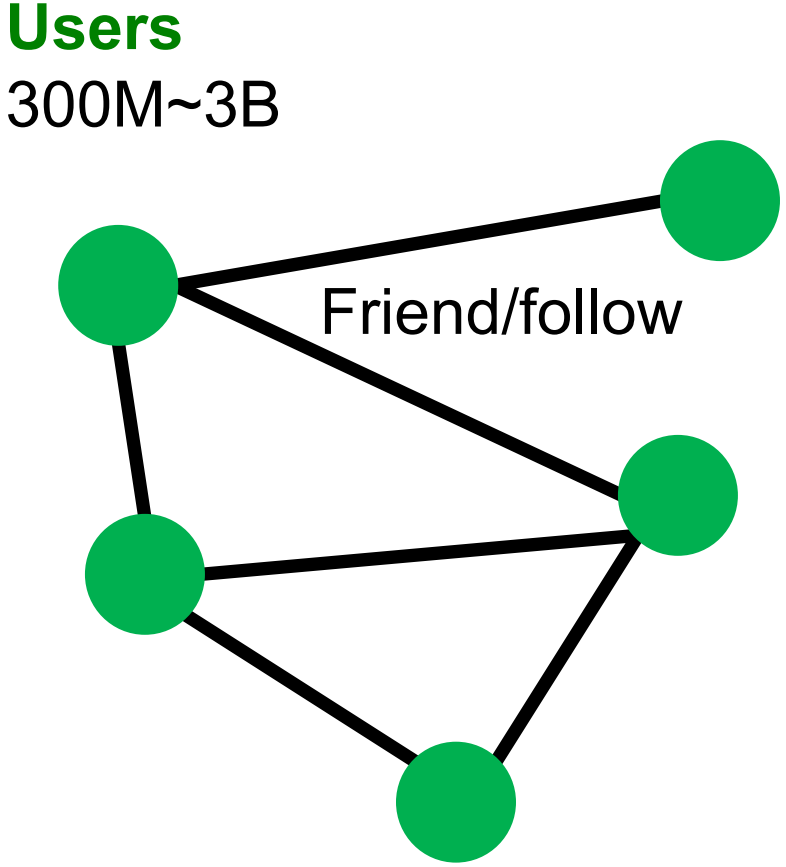
Graphs in Modern Applications

- **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)



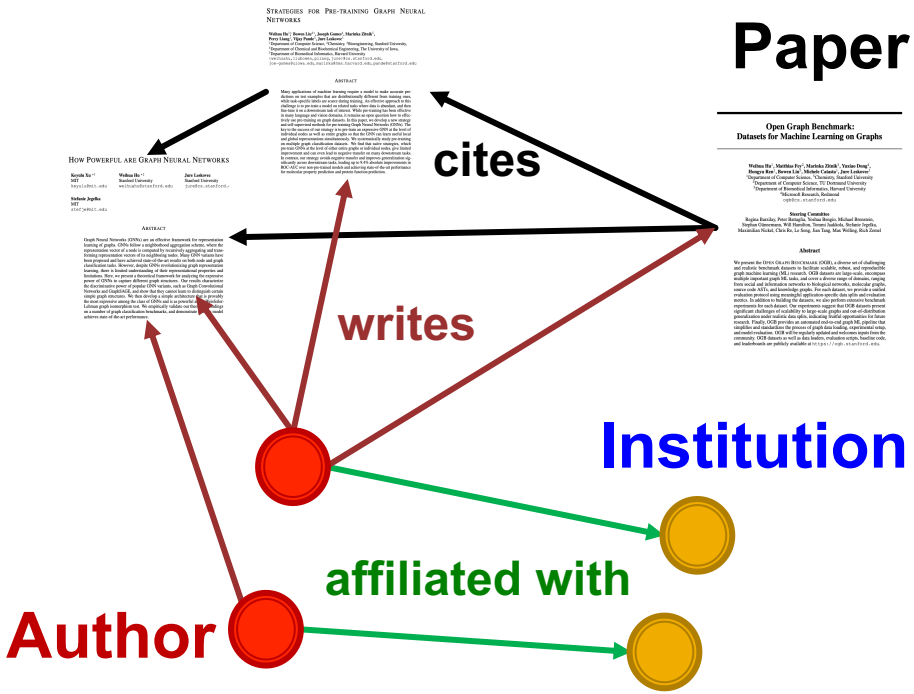
Graphs in Modern Applications

- **Academic graph:**
  - Microsoft Academic Graph

Papers 120M

Authors 120M

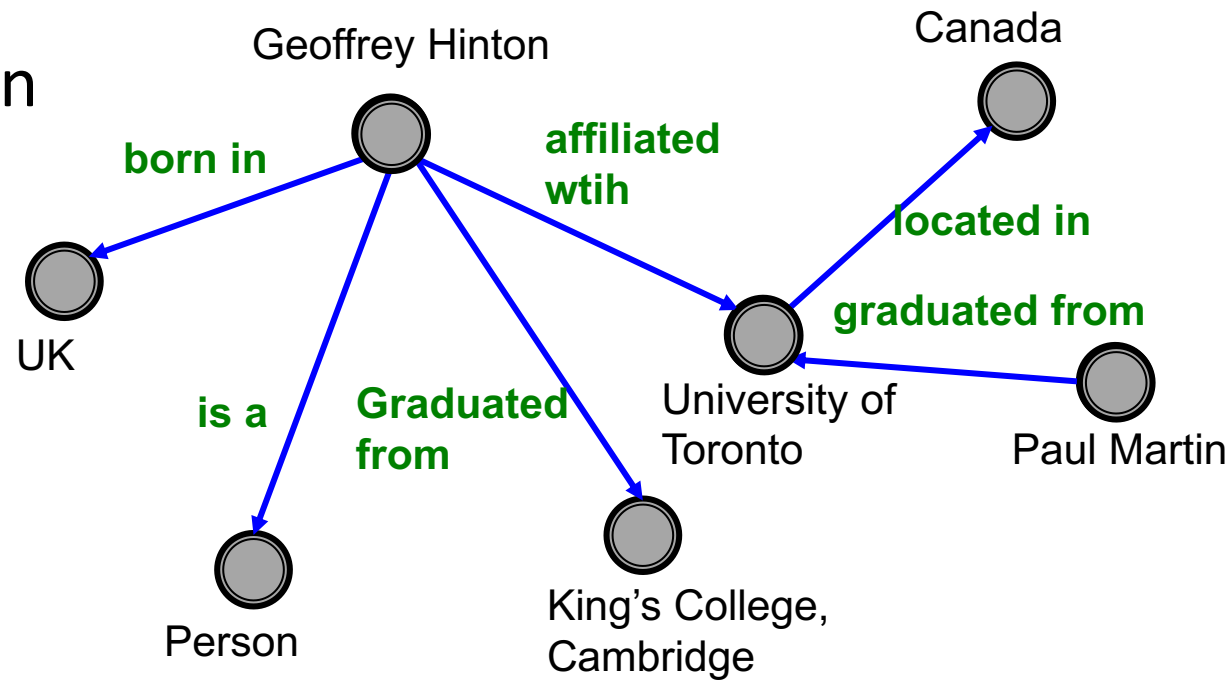
- **ML tasks:**
  - Paper categorization (node classification)
  - Author collaboration recommendation
  - Paper citation recommendation (link prediction)



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

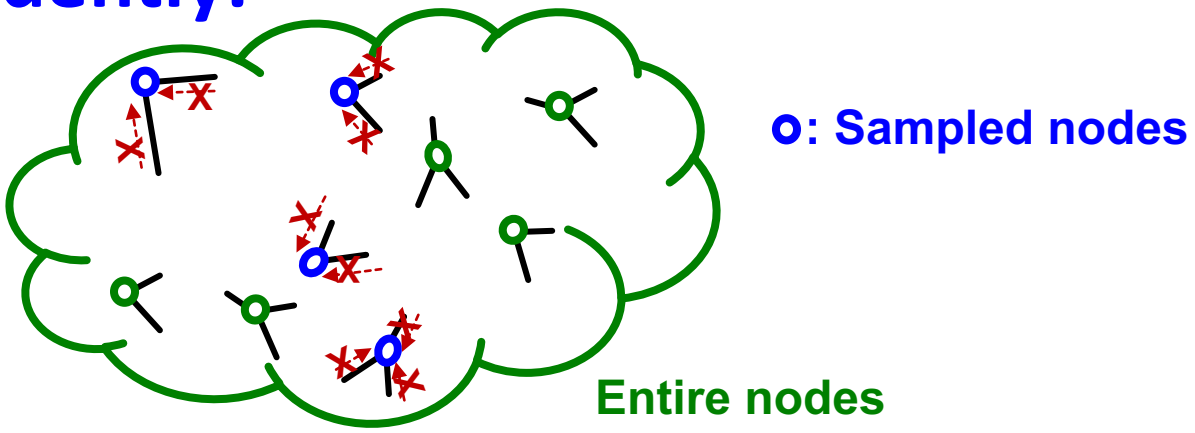
$$\ell(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=0}^{N-1} \ell_i(\boldsymbol{\theta})$$

  - $\boldsymbol{\theta}$: model parameters, $\ell_i(\boldsymbol{\theta})$: loss for i-th data point.
- We perform **Stochastic Gradient Descent (SGD)**.
  - Randomly sample M $(<< N)$ data (**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 use the standard SGD for GNN?

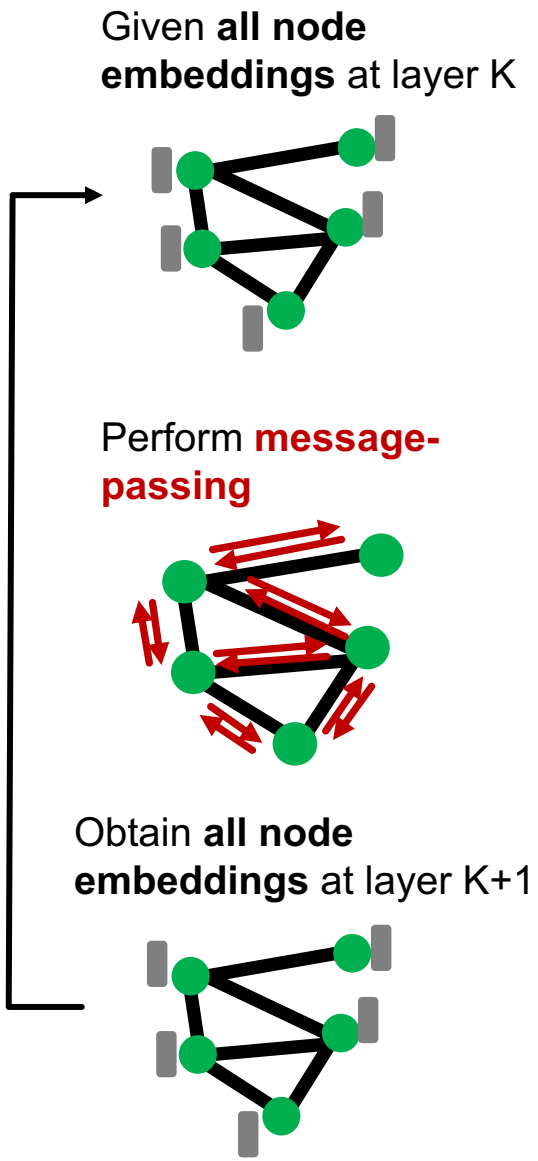
- **In mini-batch, we sample M ($<<N$) nodes independently:**



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

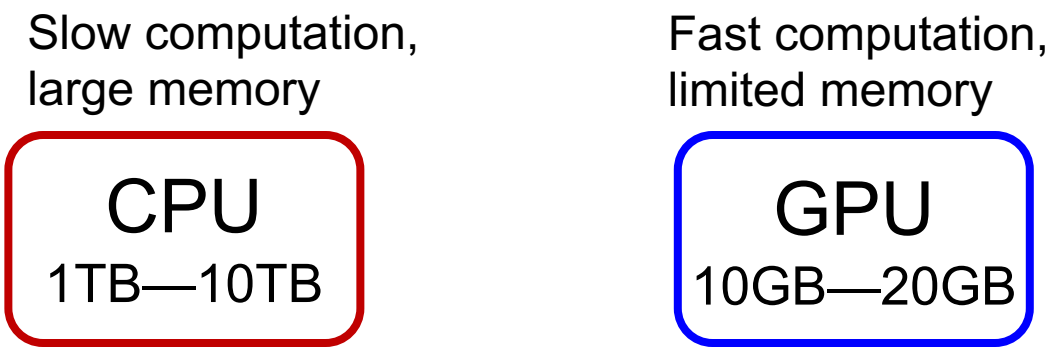
Why is it Hard?

- **Naïve full-batch implementation**: Generate embeddings of all the nodes **at the same time.**
  - Load **the entire graph and features**
  - **At each GNN layer:**
    - **Compute embeddings of all nodes using all the node embeddings from the previous layer.**
  - Compute the loss
  - Perform gradient descent



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 (only 10GB--20GB).
  - **The entire graph and the features cannot be loaded on GPU.**



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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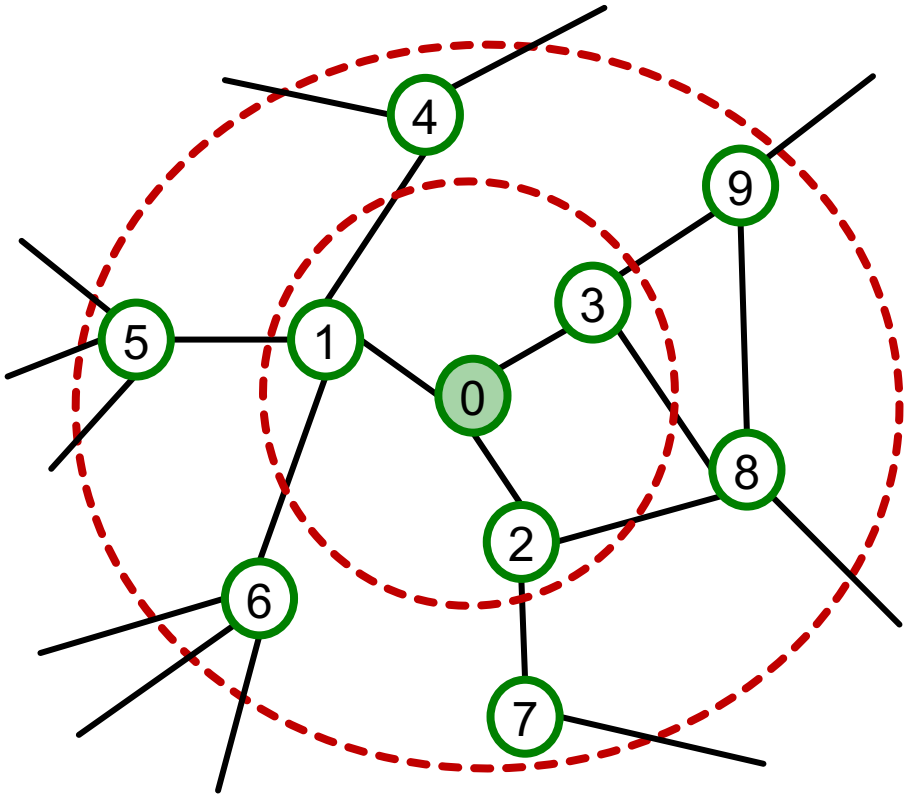
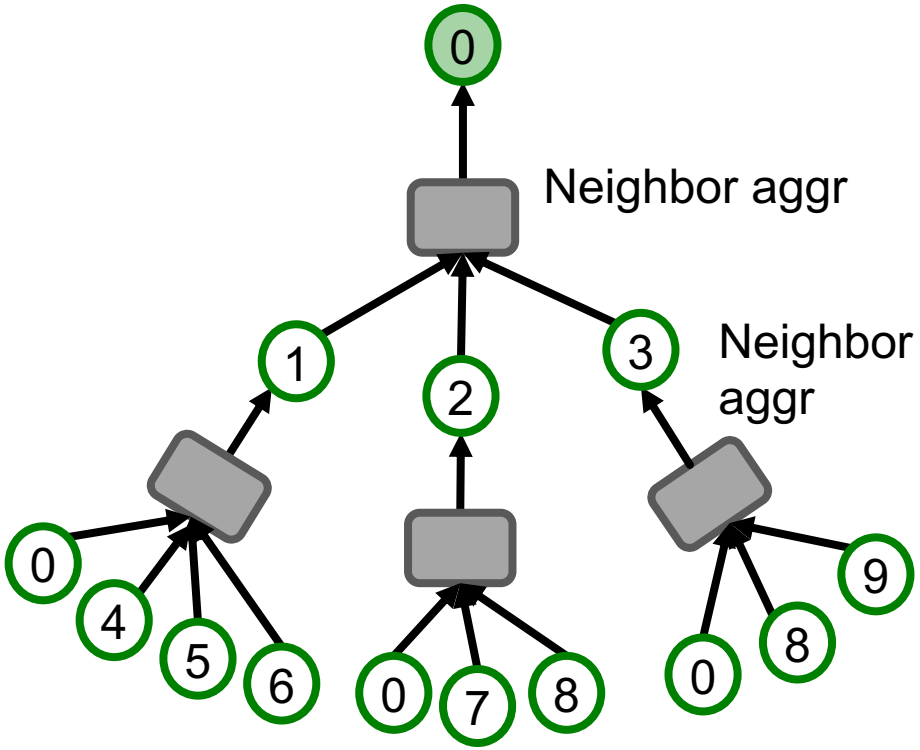
Recall: Computational Graph

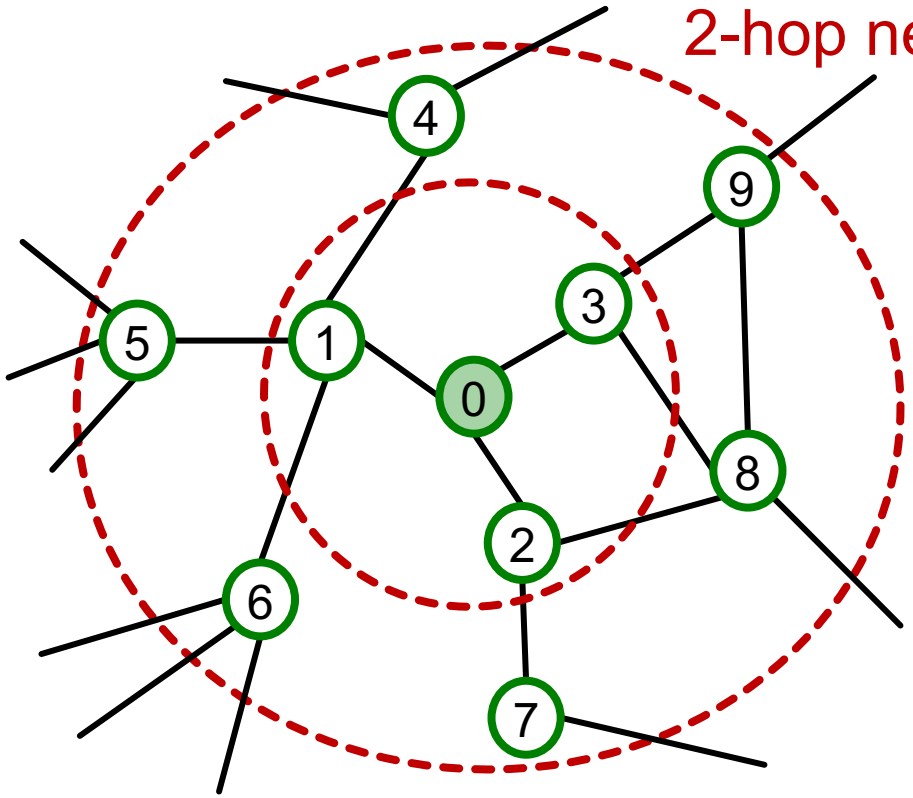
- **Recall**: GNNs generate node embeddings via neighbor aggregation.
  - Represented as a computational graph (right).

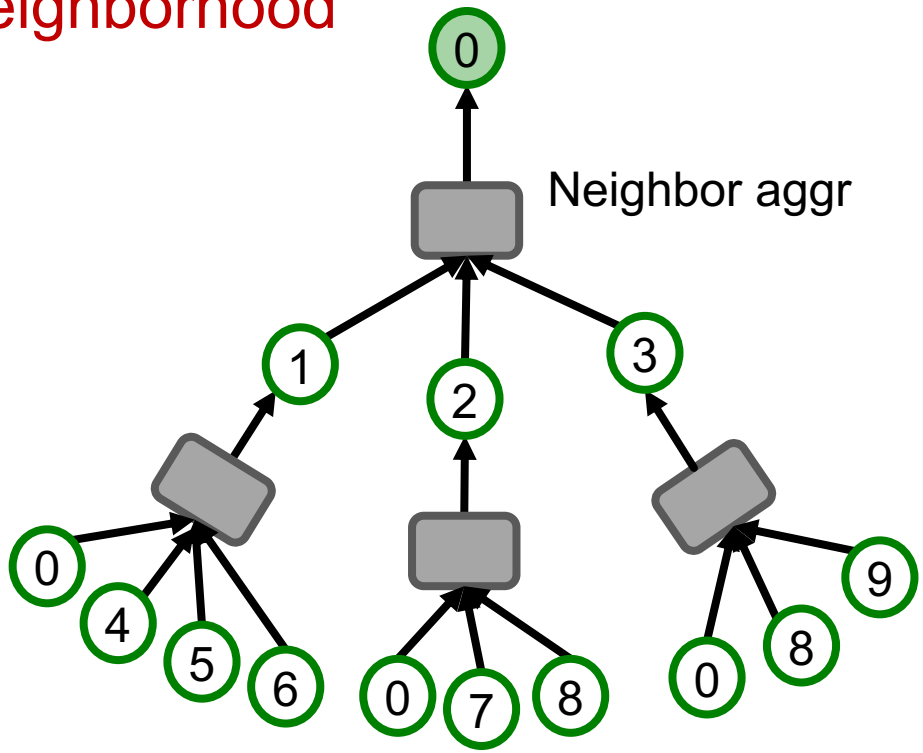




Recall: Computational Graph

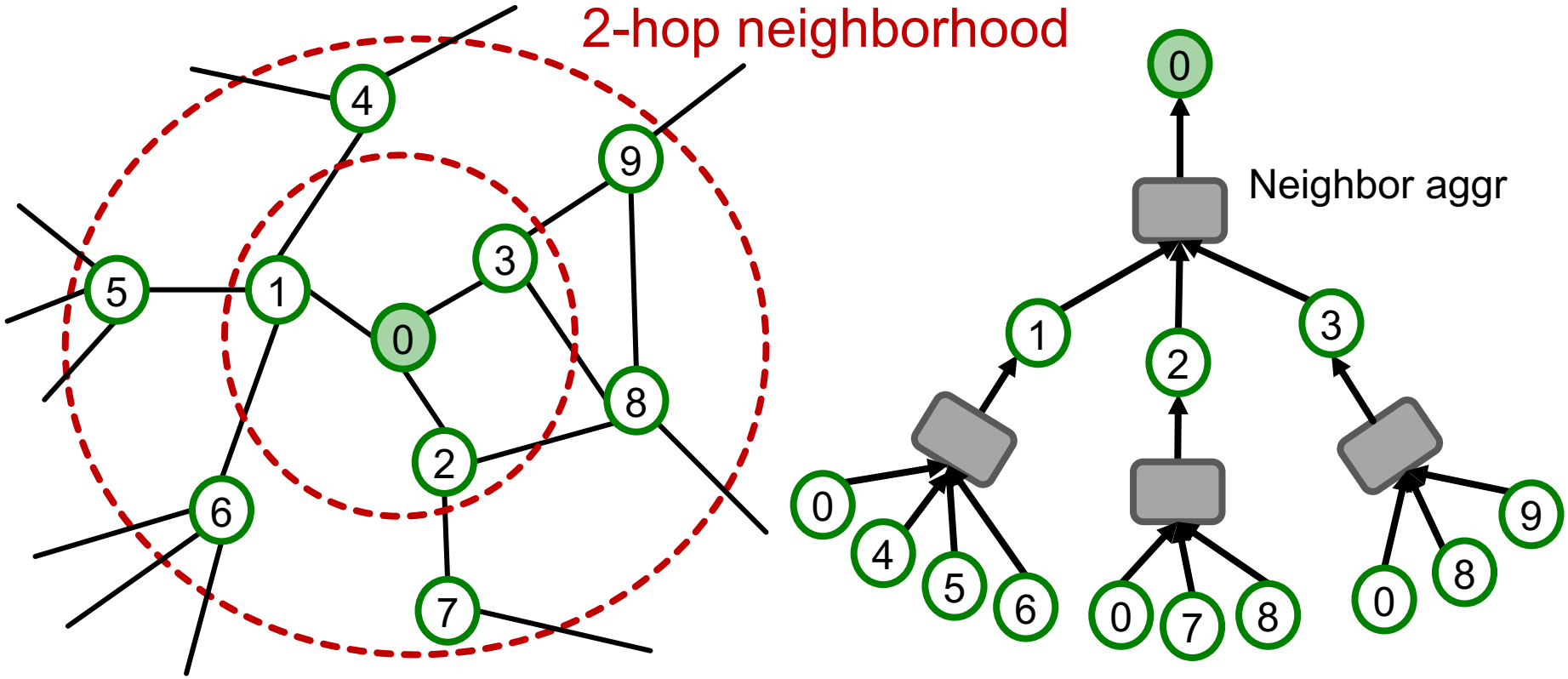
- **Observation:** A 2-layer GNN generates embedding of node "0" using 2-hop neighborhood structure and features.





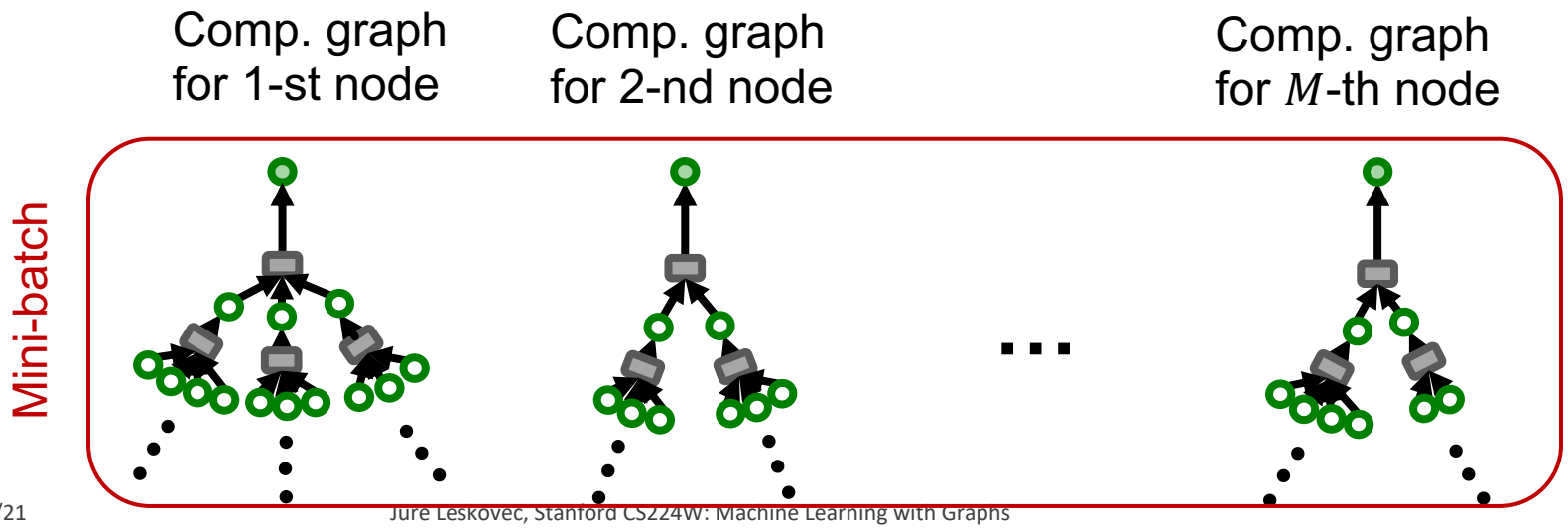
Recall: Computational Graph

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



Computing Node Embeddings

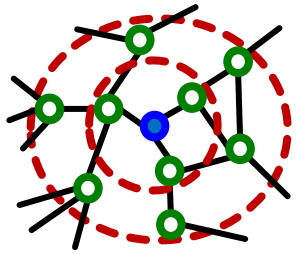
- **Key insight**: To compute embedding of a single node, all we need is **the K-hop neighborhood** (which defines the computation graph).
- Given a set of M different nodes in a **mini-batch**, we can generate their embeddings using M computational graphs. **Can be computed on GPU!**



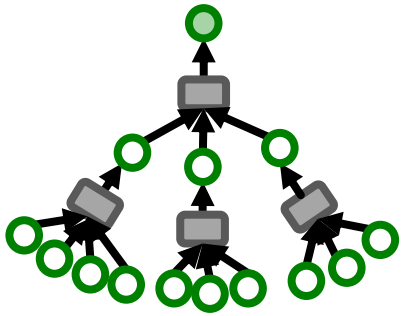
Stochastic Training of GNNs

- **We can now consider the following SGD strategy for training K-layer GNNs:**
  - Randomly sample M ($<< N$) nodes.
  - For each sampled 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

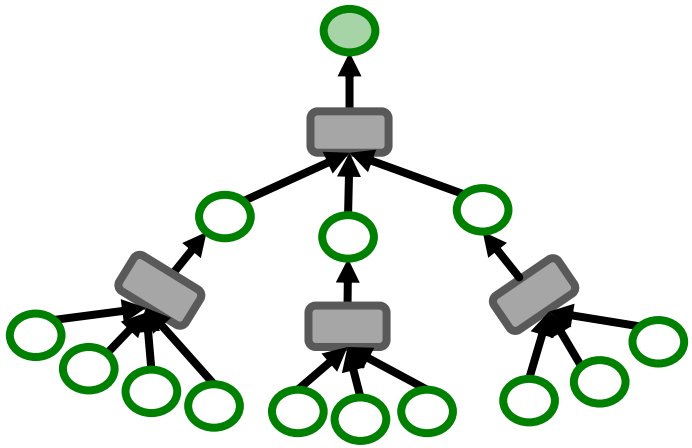


Computational graph



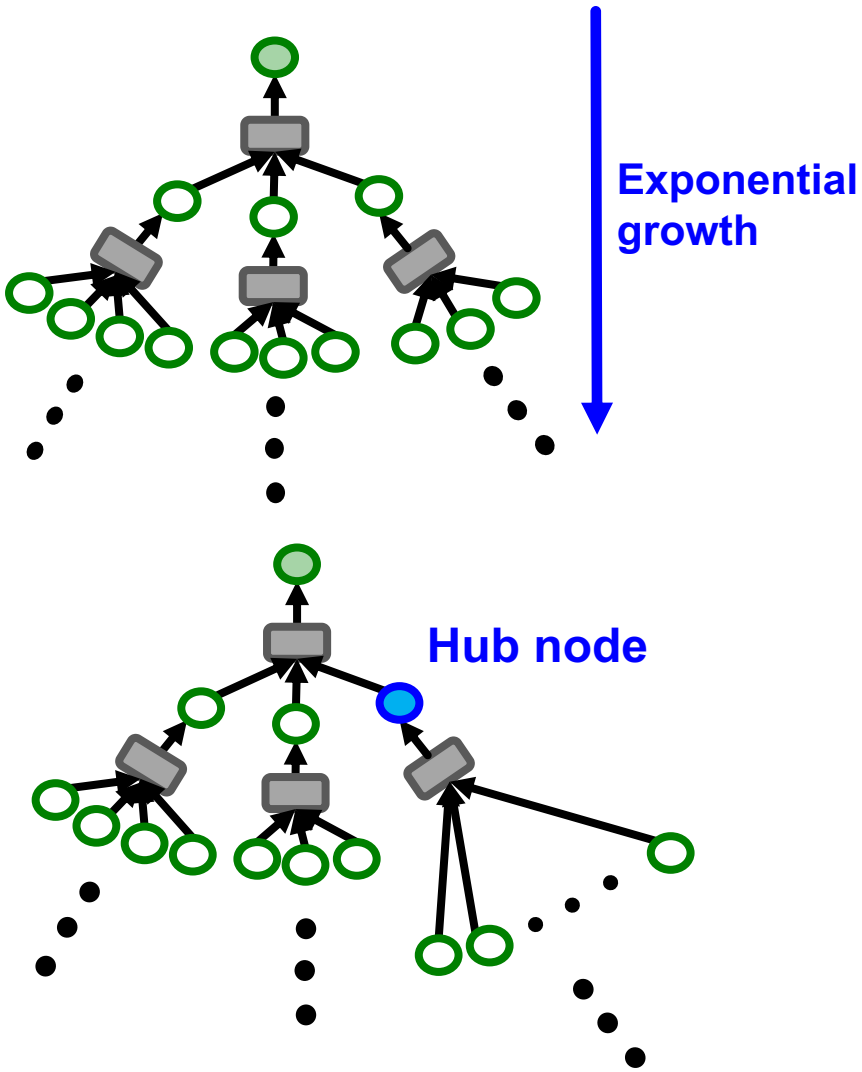
Issue with Stochastic Training

- **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.
- **Computationally expensive.**



Issue with Stochastic Training

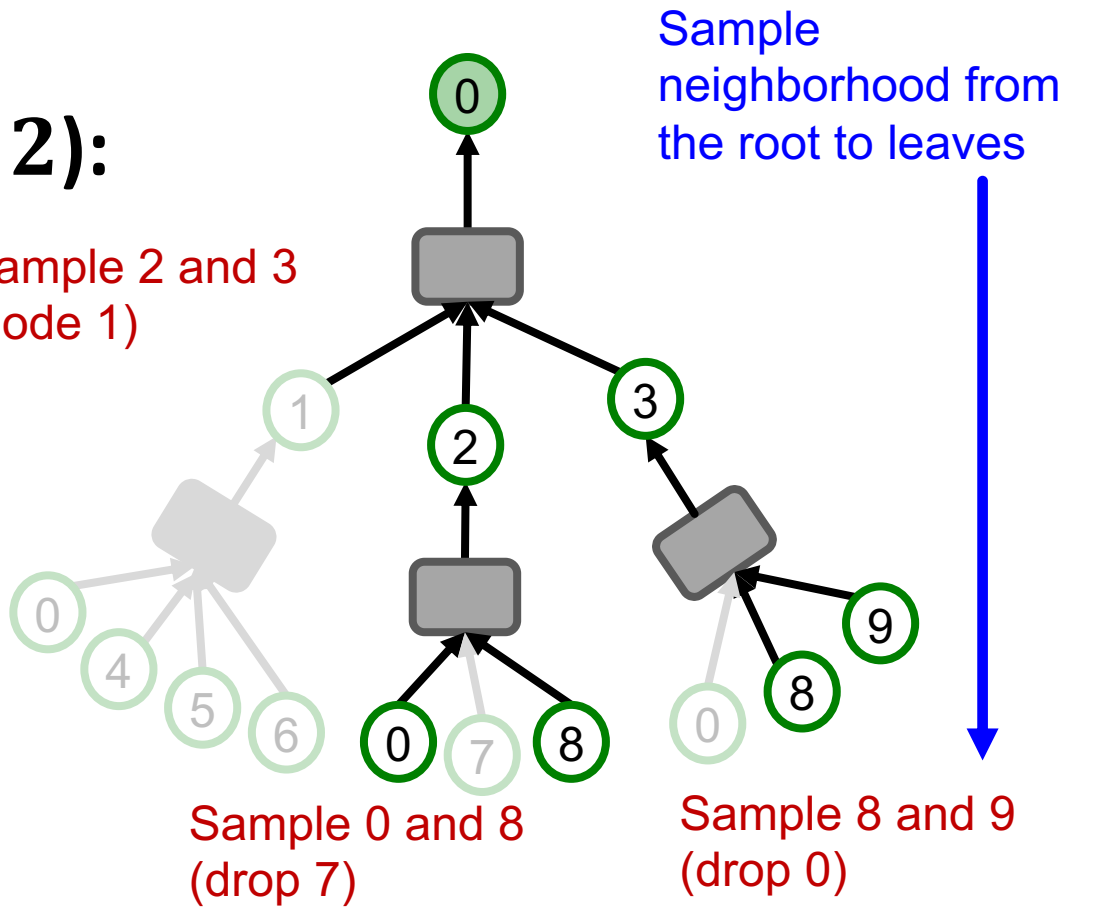
- **More details:**
  - Computation graph becomes **exponentially large** with respect to the layer size K.
  - Computation graph explodes when it hits a **hub node** (high-degree node).
- **Next:** Make the comp. graph more compact!



Neighbor Sampling

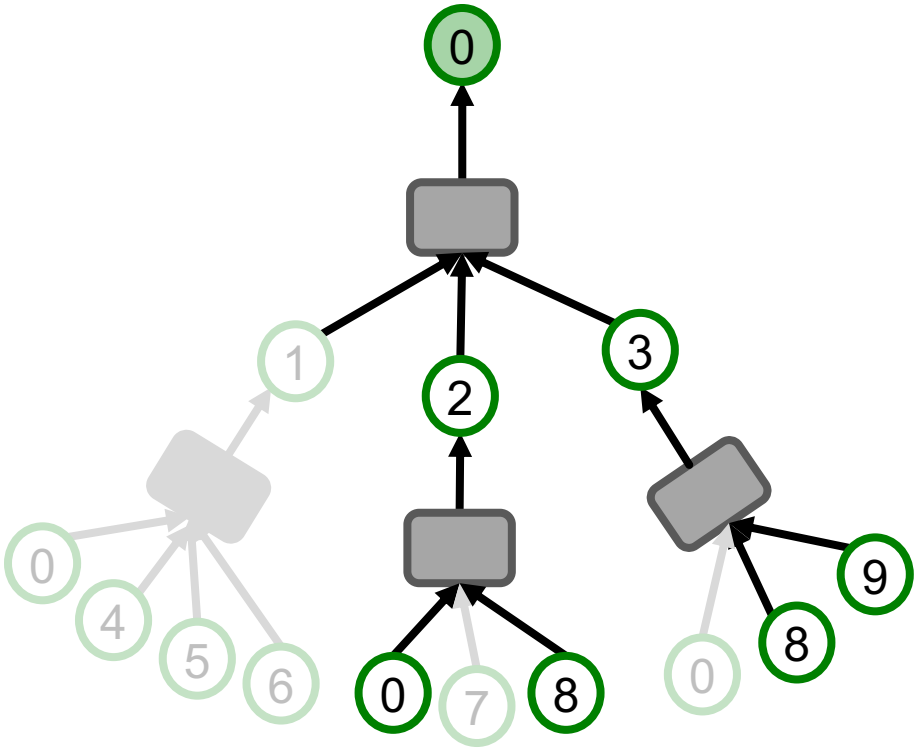
Key idea: **Construct the computational graph** by (randomly) sampling at most H neighbors at each hop.

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



Neighbor Sampling

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



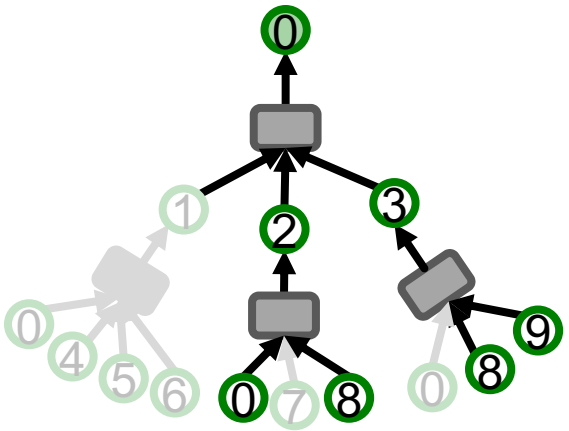
Neighbor Sampling Algorithm

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



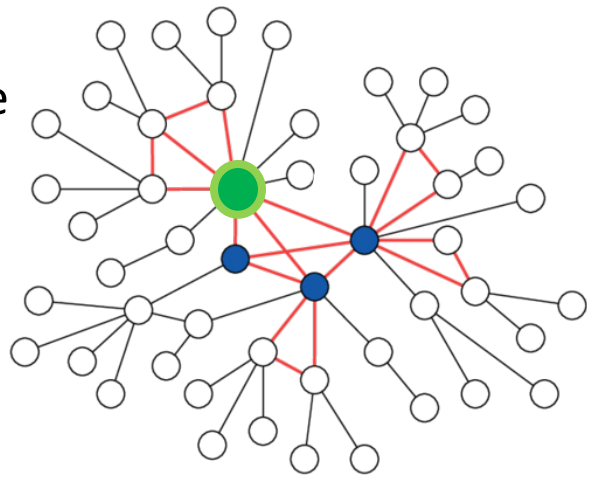
- K-layer GNN will at most involve $\prod_{k=1}^{K} H_k$ leaf nodes in comp. graph.

Remarks on Neighbor Sampling (1)

- **Remark 1: Trade-off in sampling number H**
  - Smaller H leads to more efficient neighbor aggregation, but results in more unstable 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.**
  - Increasing 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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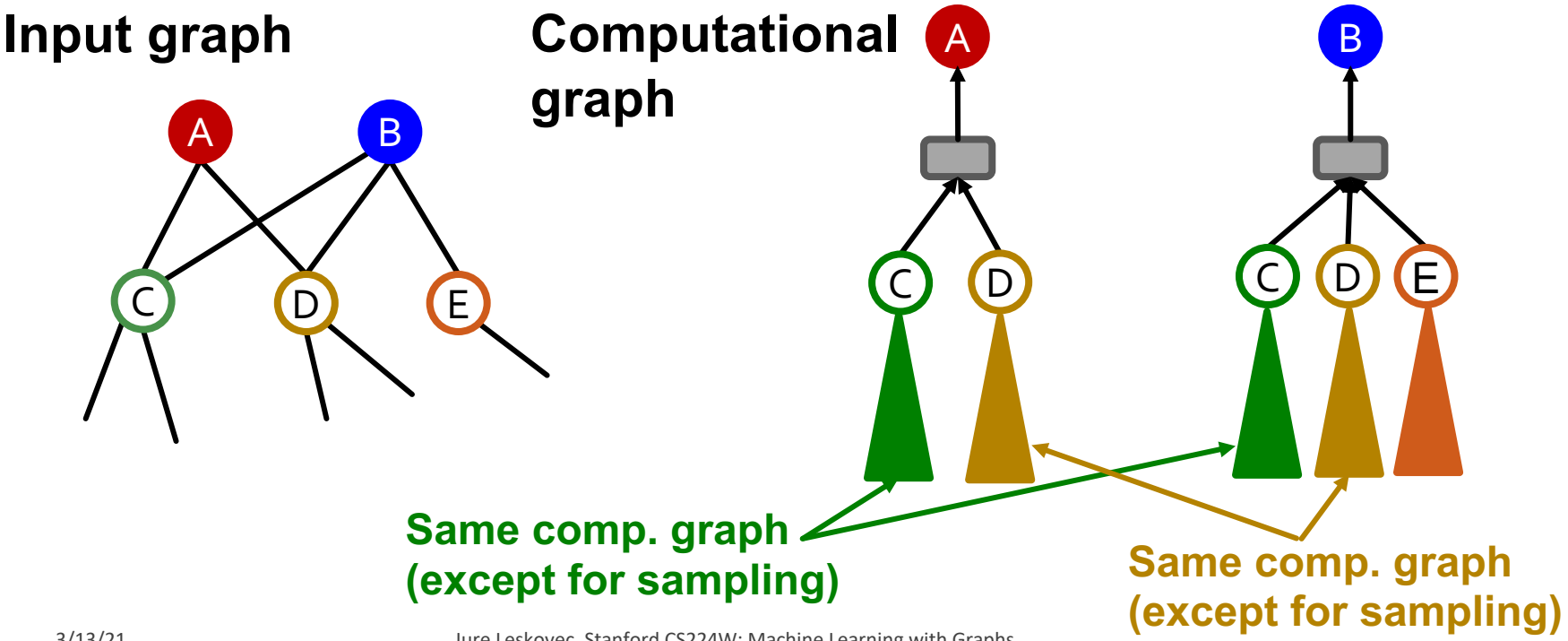
Issues with Neighbor Sampling

- **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.



Recall: Full Batch GNN

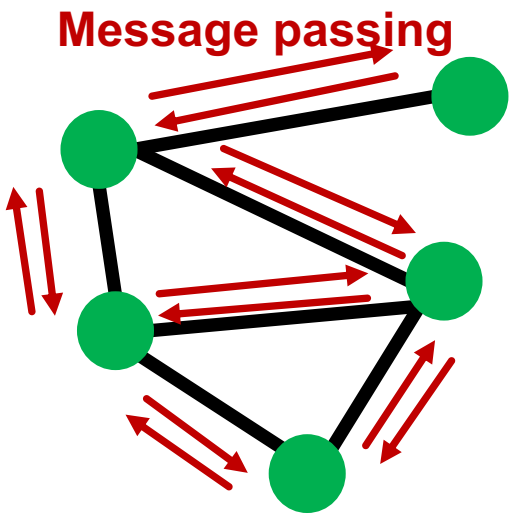
- In full-batch GNN implementation, **all the node embeddings are updated together using embeddings of the previous layer.**

Update for all $v \in V$

Message

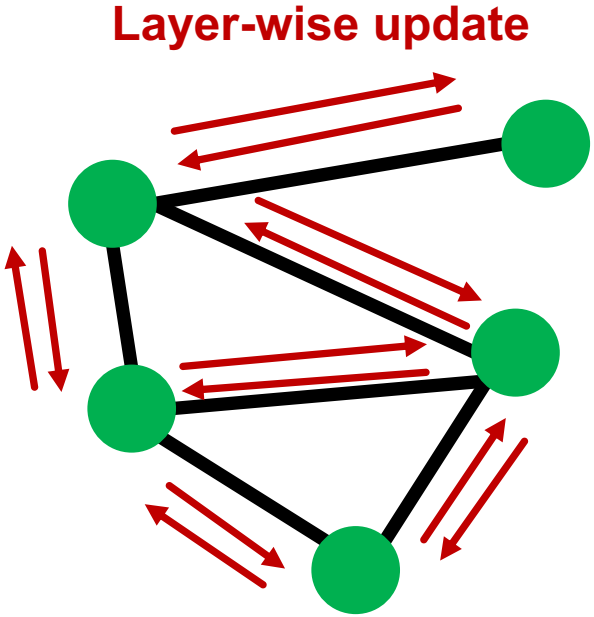
$$h_v^{(\ell)} = COMBINE\left(h_v^{(\ell-1)}, AGGR\left(\left\{\boldsymbol{h_u^{(\ell-1)}}\right\}_{u \in N(v)}\right)\right)$$

- 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

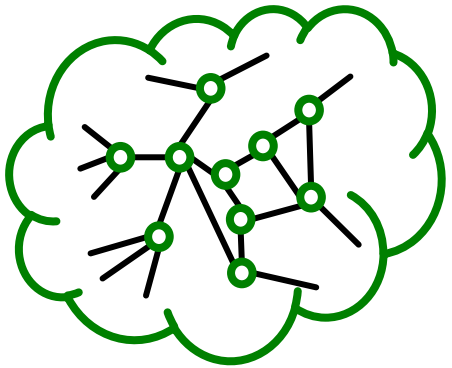
- **The layer-wise node embedding update allows the re-use of embeddings from the previous layer.**
- **This significantly reduces the computational redundancy of neighbor sampling.**
  - Of course, the **layer-wise** update is **not feasible** for a large graph due to **limited GPU memory**.



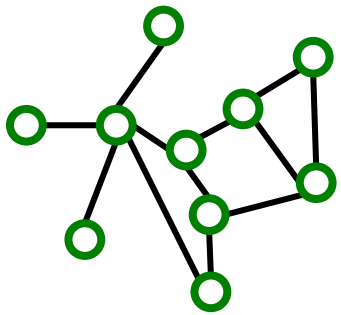
Subgraph Sampling

- **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.

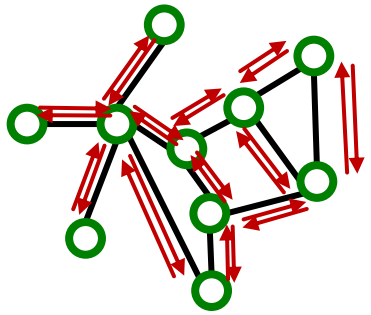
Large graph



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



Layer-wise node embeddings update on the GPU



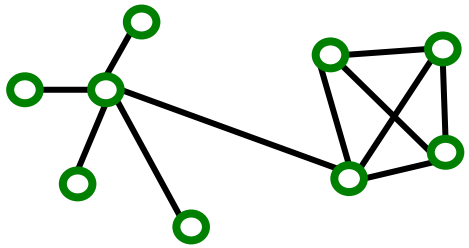
Subgraph Sampling

- **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.

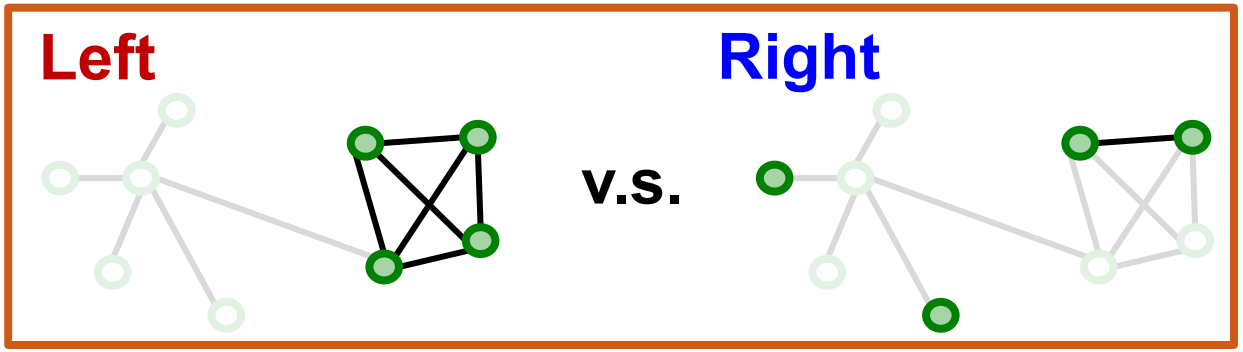
Subgraph Sampling: Case Study

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

Original graph



Subgraphs (both 4-node induced subgraph)



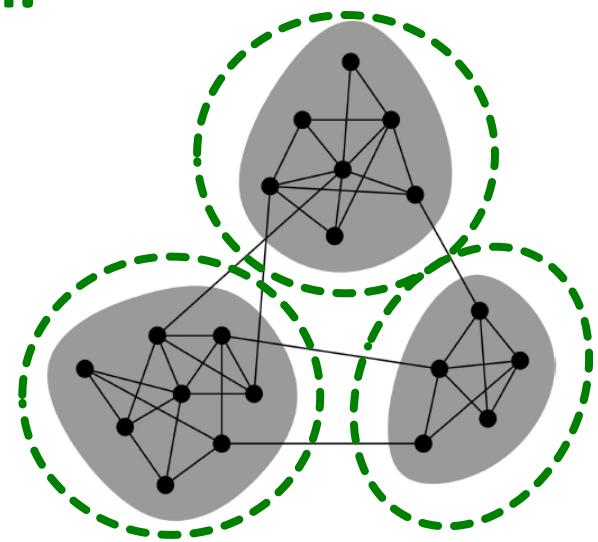
- **Left subgraph** retains the essential community structure among the 4 nodes → **Good**
- **Right subgraph** drops many connectivity patterns, even leading to isolated nodes → **Bad**

Exploiting Community Structure

Real-world graph exhibits community structure

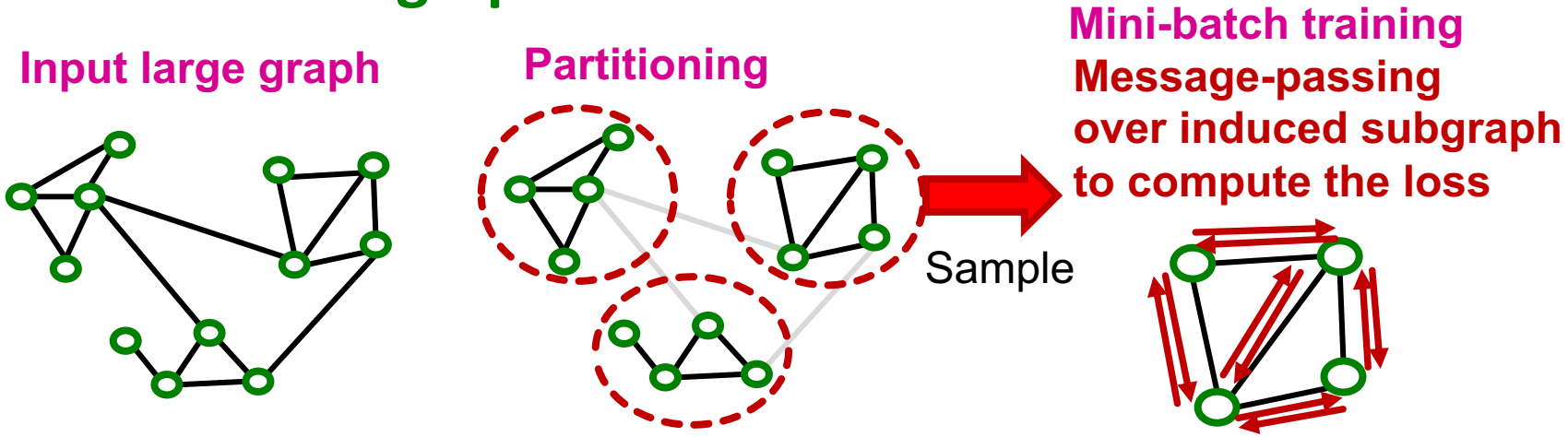
- A large graph can be decomposed into many small communities.

- **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

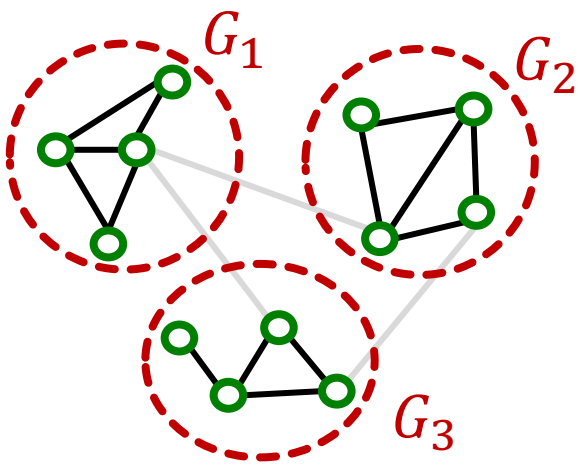
- **We first introduce "vanilla" Cluster-GCN.**
- **Cluster-GCN** consists of two steps:
  - **Pre-processing**: Given a large graph, partition it into groups of nodes (i.e., subgraphs).
  - **Mini-batch training**: Sample one node group at a time. Apply GNN's message passing over the **induced subgraph**.



Cluster-GCN: Pre-processing

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

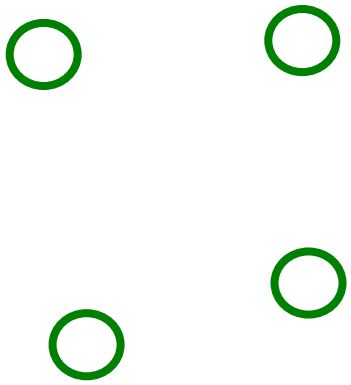
Notice: Between-group edges are *not* included in $G_1, \ldots, G_C$.



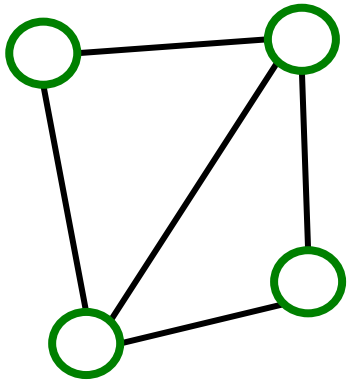
Cluster-GCN: Mini-batch Training

- 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



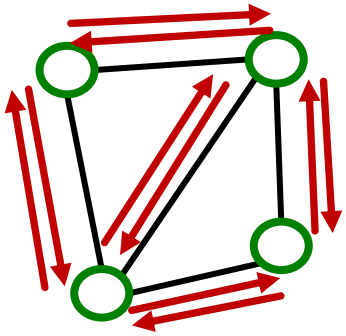
Induced subgraph G_c



Cluster-GCN: Mini-batch Training

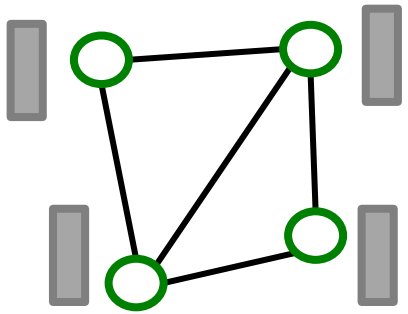
- Apply GNN's **layer-wise node update** over $\boldsymbol{G_c}$ to obtain embedding $\boldsymbol{h_v}$ for each node $v \in V_c$.
- Compute the loss for each node $v \in V_c$ and take average: $\ell_{sub}(\boldsymbol{\theta}) = (1/|V_c|) \cdot \sum_{v \in V_c} \ell_v(\boldsymbol{\theta})$
- Update params: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

Induced subgraph G_c



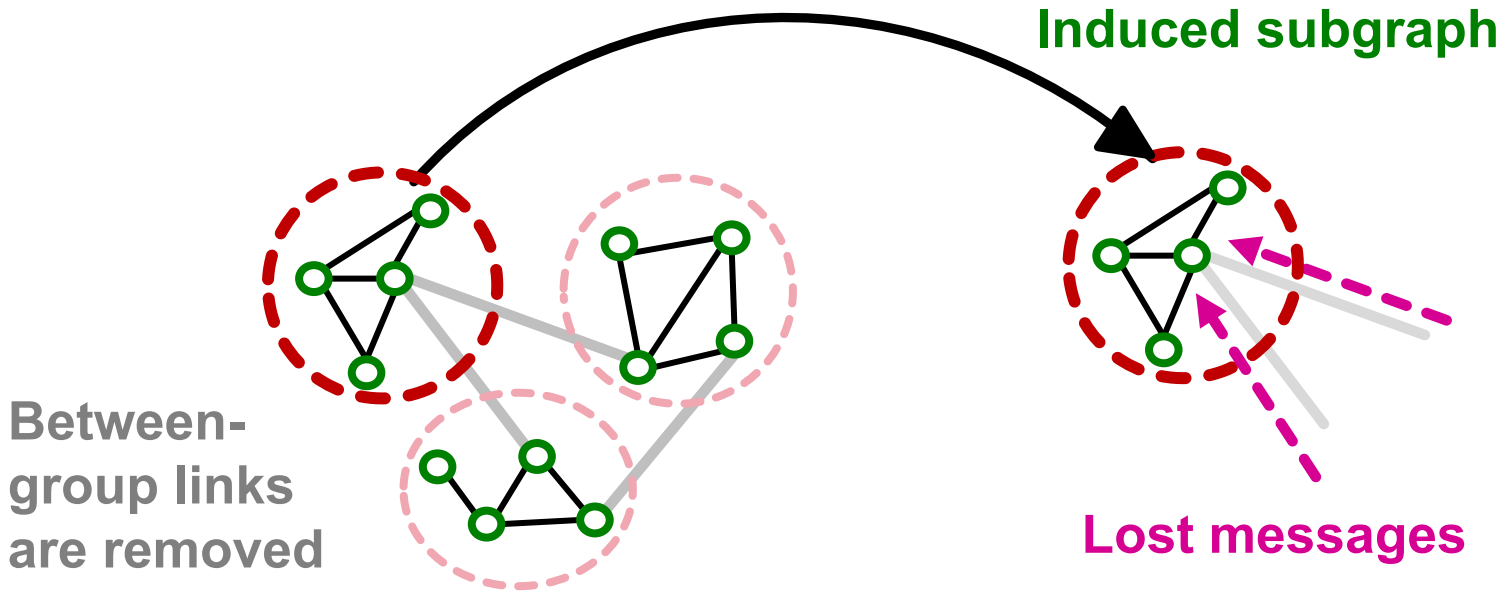
Layer-wise node embedding update

Embedding



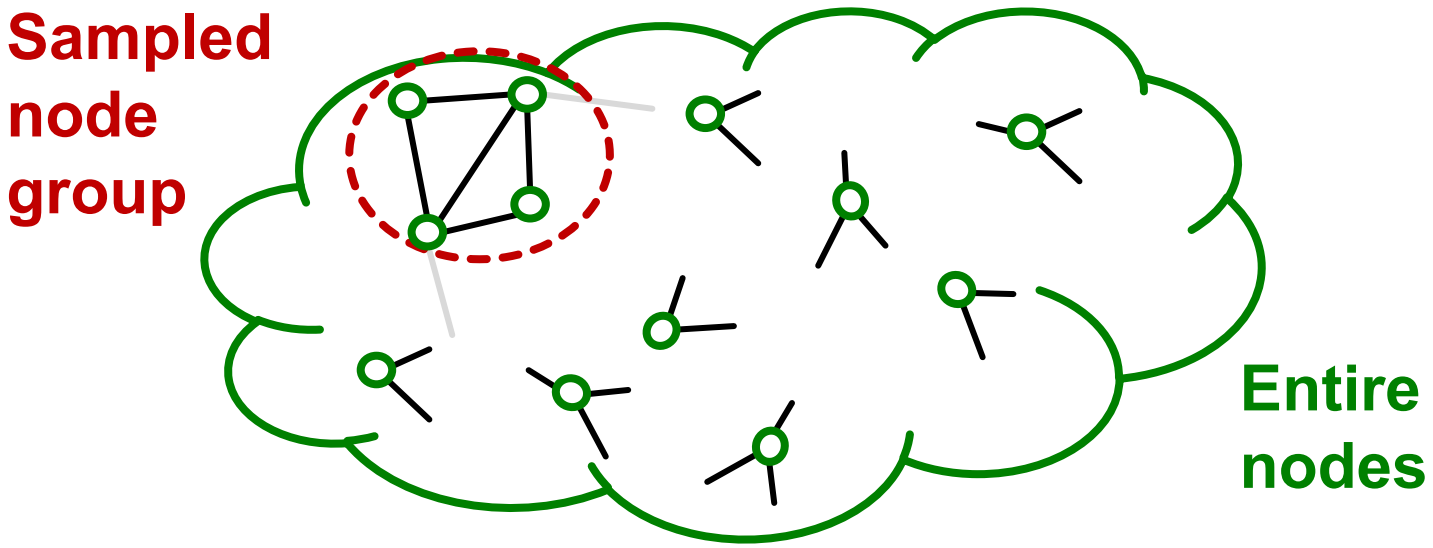
Issues with Cluster-GCN (1)

- **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, $\frac{1}{|V_c|}\sum_{v \in V_c} \nabla \ell_v(\boldsymbol{\theta})$, 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

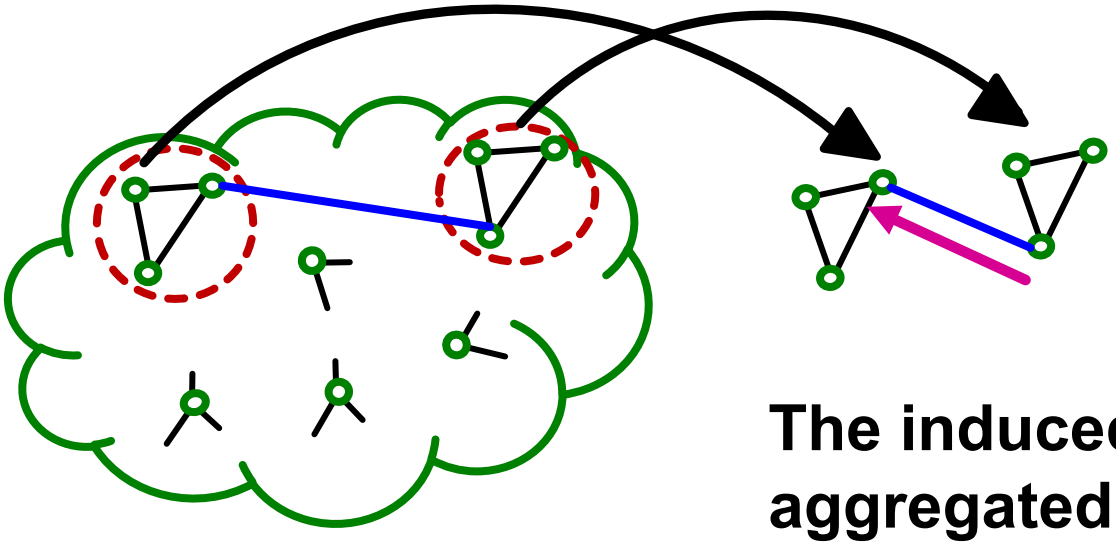
- **Solution: Aggregate multiple node groups per mini-batch.**
- Partition the graph into **relatively-small groups of nodes.**
- **For each mini-batch:**
  - **Sample and aggregate multiple node groups.**
  - **Construct the induced subgraph of the *aggregated* node group.**
  - The rest is the same 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 between-group edges

→ Message can flow across groups.

Advanced Cluster-GCN

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

Pre-processing step:

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

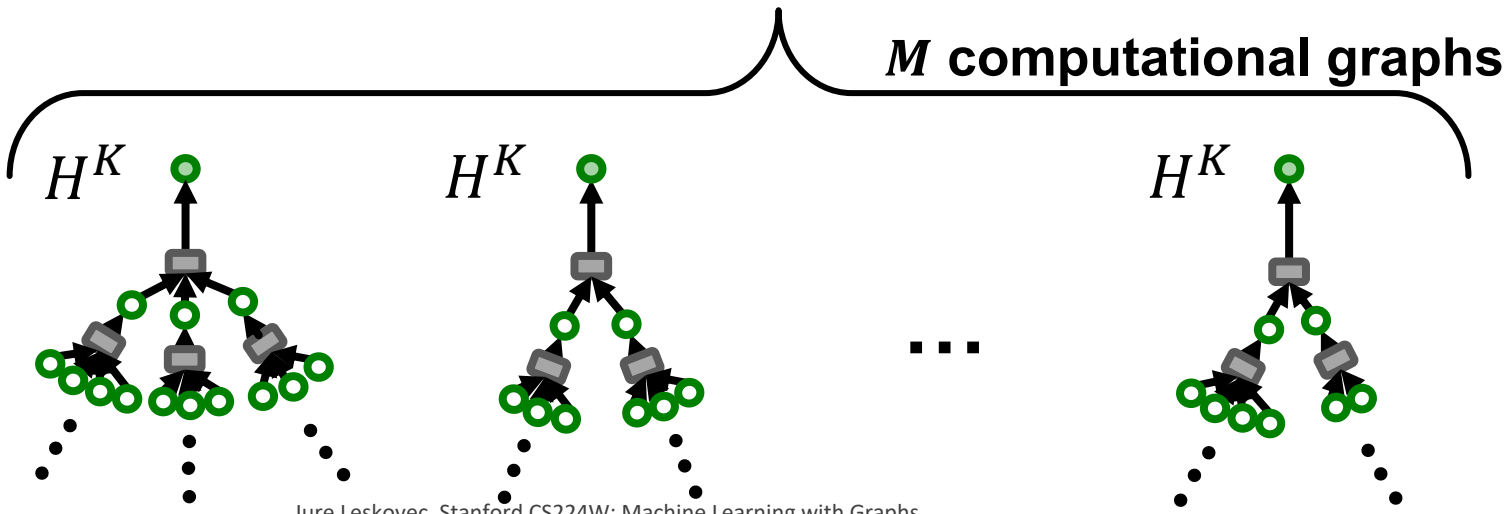
Advanced Cluster-GCN

Mini-batch training:

- For each mini-batch, **randomly sample a set of 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** $G_{aggr} = (V_{aggr}, E_{aggr})$, where $E_{aggr} = \{(u, v) \mid u, v \in V_{aggr}\}$
  - E_{aggr} **also includes between-group edges!**

Comparison of Time Complexity

- **Generate M $(<< N)$ 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 $(<< N)$ 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 H nodes per layer): $M \cdot H^K$**
  - **Cluster-GCN: $K \cdot M \cdot D_{avg}$**
- **Assume $H = D_{avg}/2$. In other words, 50% of neighbors are sampled.**
  - **Then, Cluster-GCN (cost: $2MHK$) is much more efficient than neighbor sampling (cost: MH^K).**
  - **Linear (instead of exponential) dependency w.r.t. 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 GNNs

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

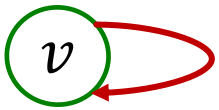
http://cs224w.stanford.edu

Roadmap of Simplifying GCN

- **We start from Graph Convolutional Network** (GCN) [Kipf & Welling ICLR 2017].
- We simplify GCN by **removing the non-linear activation** from the GCN [Wu et al. ICML 2019].
  - *Wu et al.* 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.

Recall: GCN (mean-pool)

- **Given**: Graph $G = (V, E)$ with input node features X_v for $v \in V$, where $\boldsymbol{E}$ **includes the self-loop**:
  - $(\boldsymbol{v}, \boldsymbol{v}) \in \boldsymbol{E}$ **for all** $\boldsymbol{v} \in \boldsymbol{V}$.



- Set input node embeddings: $h_v^{(0)} = X_v$ for $v \in V$.
- For $k \in \{0, \ldots, K-1\}$:
  - For all $v \in V$, aggregate neighboring information as

$$h_v^{(k+1)} = \mathrm{ReLU}\left(\boldsymbol{W_k} \frac{1}{|N(v)|} \sum_{u \in N(v)} h_u^{(k)}\right)$$

Trainable weight matrices (i.e., what we learn)

Mean-pooling

- **Final node embedding**: $z_v = h_v^{(K)}$

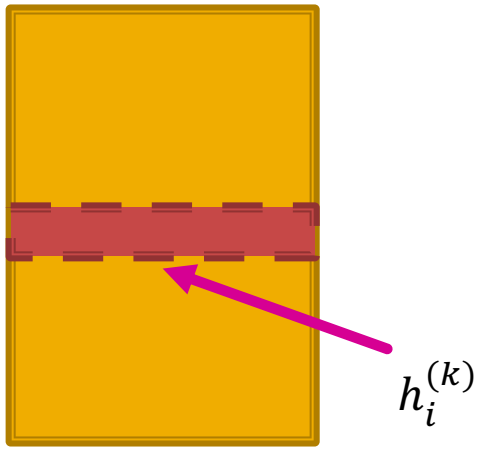
Recall: Matrix Formulation of GCN

GCN aggregations can be formulated as matrix vector product:

- Let $\boldsymbol{H}^{(k)} = [h_1^{(1)} \ldots h_{|V|}^{(k)}]^{\mathrm{T}}$
- Let $\boldsymbol{A}$ be the adjacency matrix (w/ self-loop)
- Then: $\sum_{u \in N(v)} h_u^{(k)} = A_{v,:}\boldsymbol{H}^{(k)}$
- Let $\boldsymbol{D}$ be diagonal matrix where $D_{v,v} = \mathrm{Deg}(v) = |N(v)|$
  - The inverse of D: D^{-1} is also diagonal: $D_{v,v}^{-1} = 1/|N(v)|$
- **Therefore,**

$$\frac{1}{|N(v)|}\sum_{u \in N(v)} h_u^{(k)} \Rightarrow \boldsymbol{D}^{-1}\boldsymbol{A}\boldsymbol{H}^{(k)}$$

Matrix of hidden embeddings $\boldsymbol{H}^{(k)}$



Recall: Matrix Formulation of GCN

- **GCN's neighbor aggregation:**

$$h_v^{(k+1)} = \mathrm{ReLU}\left(\boldsymbol{W_k} \frac{1}{|N(v)|} \sum_{u \in N(v)} h_u^{(k)}\right)$$

- **In matrix form**:

$$\boldsymbol{H}^{(k+1)} = \mathrm{ReLU}\left(\tilde{\boldsymbol{A}} \boldsymbol{H}^{(k)} \boldsymbol{W}_k^{\mathrm{T}}\right)$$

where $\tilde{\boldsymbol{A}} = \boldsymbol{D}^{-1}\boldsymbol{A}$.

- **Note:** The original GCN uses re-normalized version: $\tilde{\boldsymbol{A}} = \boldsymbol{D}^{-1/2}\boldsymbol{A}\boldsymbol{D}^{-1/2}$.
  - Empirically, this version of $\tilde{\boldsymbol{A}}$ often gives better performance than $\boldsymbol{D}^{-1}\boldsymbol{A}$.

Simplifying GCN

- **Simplify GCN by removing ReLU non-linearity:**

$$\boldsymbol{H}^{(k+1)} = \widetilde{\boldsymbol{A}}\boldsymbol{H}^{(k)}\boldsymbol{W}_{\boldsymbol{k}}^{\mathrm{T}}$$

- The final node embedding matrix is given as

$$\boldsymbol{H}^{(K)} = \widetilde{\boldsymbol{A}}\,\boldsymbol{H}^{(K-1)}\,\boldsymbol{W}_{\boldsymbol{K-1}}^{\mathrm{T}}$$

$$= \widetilde{\boldsymbol{A}}\left(\widetilde{\boldsymbol{A}}\boldsymbol{H}^{(K-2)}\boldsymbol{W}_{\boldsymbol{K-2}}^{T}\right)\boldsymbol{W}_{\boldsymbol{K-1}}^{\mathrm{T}}$$

$$\cdots = \widetilde{\boldsymbol{A}}\left(\widetilde{\boldsymbol{A}}\left(\cdots\left(\widetilde{\boldsymbol{A}}\,\boldsymbol{H}^{(0)}\,\boldsymbol{W}_{\boldsymbol{0}}^{\mathrm{T}}\right)\cdots\right)\boldsymbol{W}_{\boldsymbol{K-2}}^{\mathrm{T}}\right)\boldsymbol{W}_{\boldsymbol{K-1}}^{\mathrm{T}}$$

$$= \widetilde{\boldsymbol{A}}^{K}\,\boldsymbol{X}\left(\boldsymbol{W}_{\boldsymbol{0}}^{\mathrm{T}}\cdots\boldsymbol{W}_{\boldsymbol{K-1}}^{\mathrm{T}}\right)$$

Composition of linear transformation is still linear!

$$= \widetilde{\boldsymbol{A}}^{K}\,\boldsymbol{X}\,\boldsymbol{W}^{\mathrm{T}} \quad \text{where } \boldsymbol{W} \equiv \boldsymbol{W}_{\boldsymbol{K-1}}\cdots\boldsymbol{W}_{\boldsymbol{0}}$$

Simplifying GCN (1)

- Removing ReLU significantly simplifies GCN!

$$\boldsymbol{H}^{(K)} = \widetilde{\boldsymbol{A}}^{K}\,\boldsymbol{X}\,\boldsymbol{W}^{\mathrm{T}}$$

- Notice $\widetilde{\boldsymbol{A}}^{K}\,\boldsymbol{X}$ does not contain any learnable parameters; hence, it **can be pre-computed.**
  - Efficiently computable as a sequence of sparse-matrix vector products:
  - Do $\boldsymbol{X} \leftarrow \widetilde{\boldsymbol{A}}\,\boldsymbol{X}$ for K times.

Simplifying GCN (2)

- Let $\tilde{\boldsymbol{X}} = \tilde{\boldsymbol{A}}^K \boldsymbol{X}$ be pre-computed matrix.
- Simplified GCN's final embedding is

$$\boldsymbol{H}^{(K)} = \tilde{\boldsymbol{X}} \boldsymbol{W}^{\mathrm{T}}$$

- It's just a **linear transformation of pre-computed matrix!**
- Back to the node embedding form:

$$h_v^{(K)} = \boldsymbol{W} \boxed{\tilde{\boldsymbol{X}}_v}$$

Pre-computed feature vector for node v

- Embedding of node v only depends on its own (pre-processed) feature!

Simplifying GCN (3)

- Once $\tilde{\boldsymbol{X}}$ is pre-computed, embeddings of M nodes can be generated in time linear in M:
  - Given M nodes $\{v_1, v_2, \ldots, v_M\}$, their embeddings are
    - $h_{v_1}^{(K)} = \boldsymbol{W}\tilde{\boldsymbol{X}}_{v_1}$,
    - $h_{v_2}^{(K)} = \boldsymbol{W}\tilde{\boldsymbol{X}}_{v_2}$,
    - ...
    - $h_{v_M}^{(K)} = \boldsymbol{W}\tilde{\boldsymbol{X}}_{v_M}$.

Simplified GCN: Summary

In summary, simplified GCN consists of **two steps**:

- **Pre-processing step**:
  - Pre-compute $\widetilde{\boldsymbol{X}} = \widetilde{\boldsymbol{A}}^K \boldsymbol{X}$. Can be done on CPU.
- **Mini-batch training step**:
  - For each mini-batch, randomly-sample M nodes $\{v_1, v_2, \ldots, v_M\}$.
  - Compute their embeddings by
    - $h_{v_1}^{(K)} = \boldsymbol{W}\widetilde{\boldsymbol{X}}_{v_1}, h_{v_2}^{(K)} = \boldsymbol{W}\widetilde{\boldsymbol{X}}_{v_2}, \ldots, h_{v_M}^{(K)} = \boldsymbol{W}\widetilde{\boldsymbol{X}}_{v_M}$
  - Use the embeddings to make prediction and compute the loss averaged over the M data points.
  - Perform SGD parameter update.

Comparison with Other Methods

- **Compared to neighbor sampling:**
  - Simplified GCN generates node embeddings much more efficiently (no need to construct the giant computational graph for each node).
- **Compared to Cluster-GCN:**
  - Mini-batch nodes of simplified GCN can be sampled completely randomly from the entire nodes (no need to sample from multiple groups as Cluster-GCN does)
  - Leads to lower SGD variance during training.
- But the model is much **less** expressive (next).

Potential Issue of Simplified GCN

- Compared to the original GNN models, **simplified GCN'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, **simplified GCN works comparably to the original GNNs despite being less expressive.**

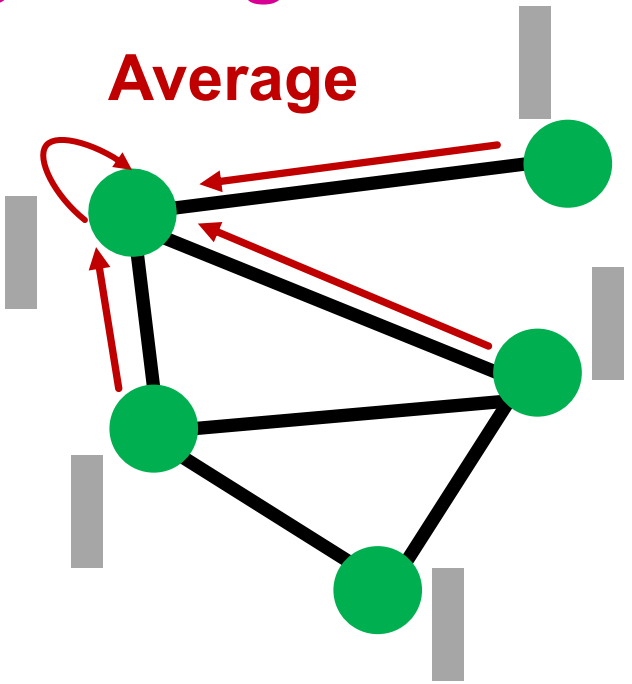
- **Why?**

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 $X \leftarrow \tilde{A}\,X$ for K times.**
- 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.