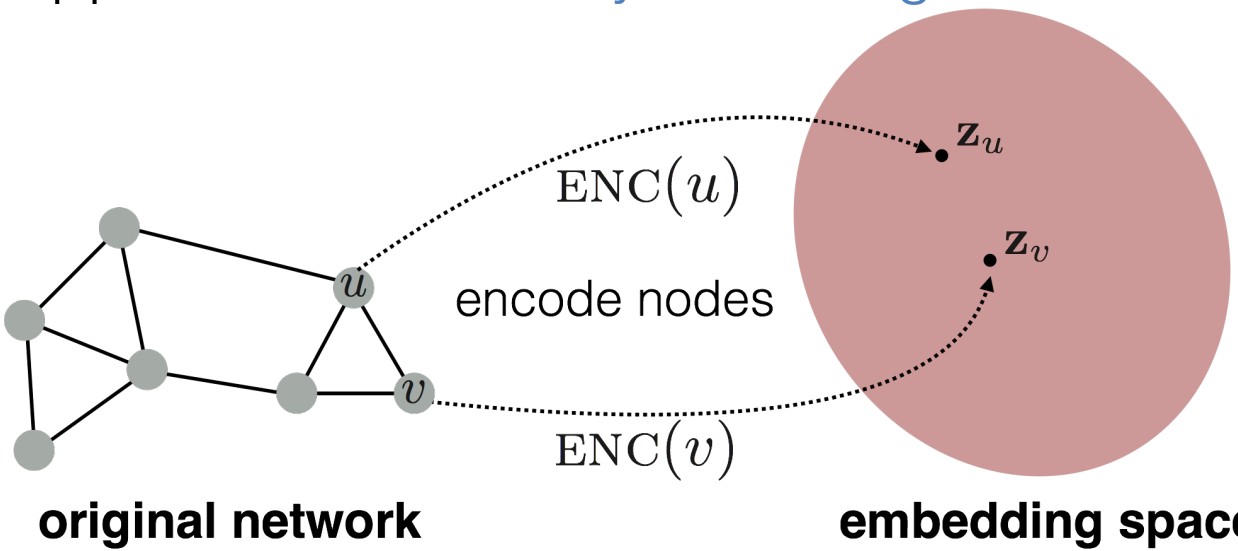
This Talk

- 1) Node embeddings ✓
  - Map nodes to low-dimensional embeddings.
- 2) Graph neural networks 
  - Deep learning architectures for graph-structured data
- 3) Applications

Part 2: Graph Neural Networks

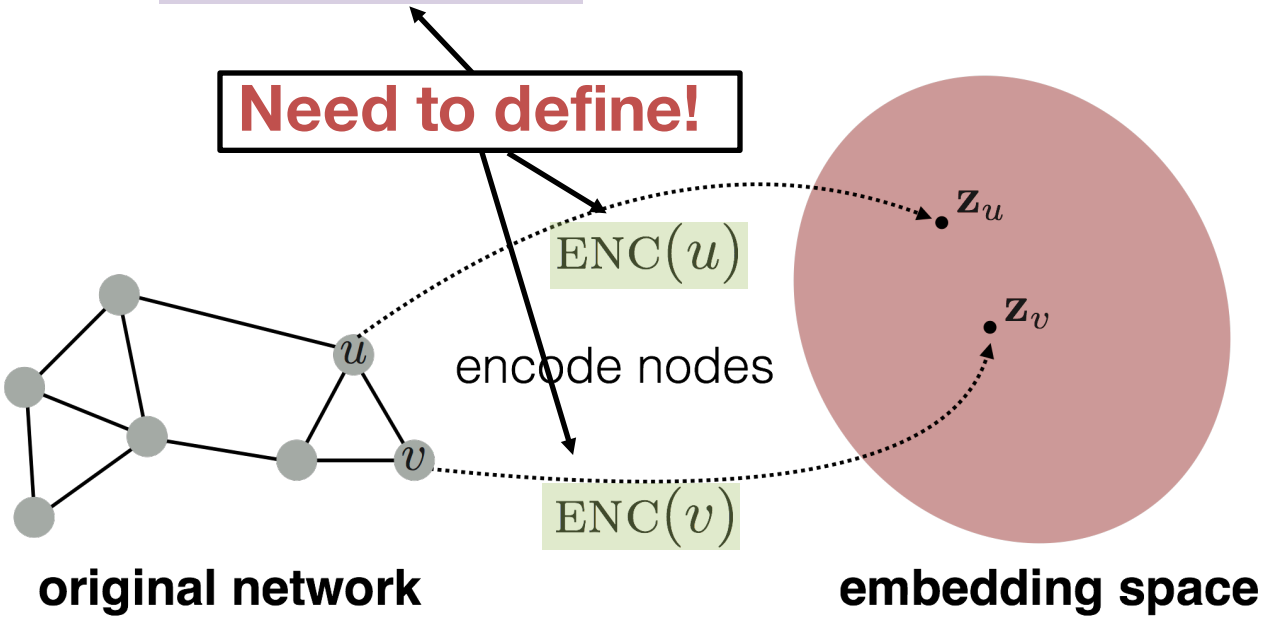
Embedding Nodes

- Goal is to encode nodes so that similarity in the embedding space (e.g., dot product) approximates similarity in the original network.



Embedding Nodes

Goal: $\text{similarity}(u, v) \approx \mathbf{z}_v^\top \mathbf{z}_u$



Two Key Components

- **Encoder** maps each node to a low-dimensional vector.

$$\text{ENC}(v) = \mathbf{z}_v$$

$\mathbf{d}$-dimensional embedding

node in the input graph

- **Similarity function** specifies how relationships in vector space map to relationships in the original network.

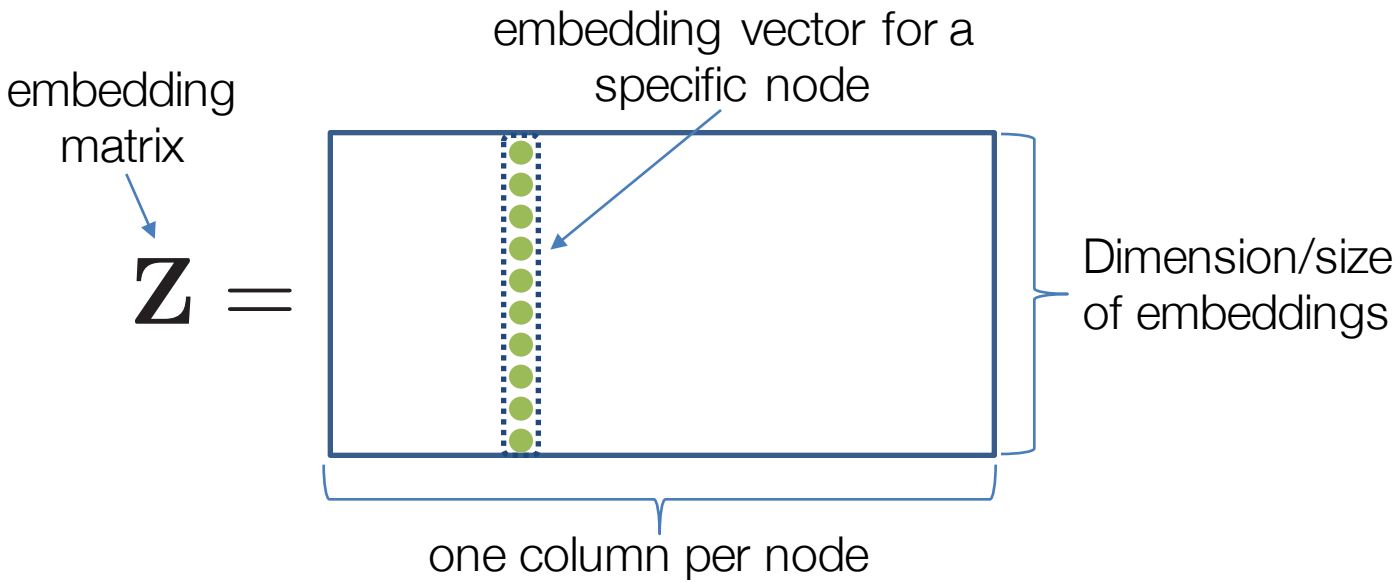
$$\text{similarity}(u, v) \approx \mathbf{z}_v^\top \mathbf{z}_u$$

Similarity of u and v in the original network

dot product between node embeddings

From "Shallow" to "Deep"

- So far we have focused on **"shallow" encoders**, i.e. embedding lookups:



From "Shallow" to "Deep"

- Limitations of shallow encoding:
  - **O(|V|) parameters are needed**: there no parameter sharing and every node has its own unique embedding vector.
  - **Inherently "transductive"**: It is impossible to generate embeddings for nodes that were not seen during training.
  - **Do not incorporate node features**: Many graphs have features that we can and should leverage.

From "Shallow" to "Deep"

- We will now discuss "deeper" methods based on **graph neural networks.**

$$\text{ENC}(v) = \text{complex function that depends on graph structure.}$$

- In general, all of these more complex encoders can be combined with the similarity functions from the previous section.

Outline for this Section

- We will now discuss "deeper" methods based on **graph neural networks.**
  1. **The Basics**
  2. **Graph Convolutional Networks (GCNs)**
  3. **GraphSAGE**
  4. **Gated Graph Neural Networks**
  5. **Subgraph Embeddings**

The Basics: Graph Neural Networks

Based on material from:

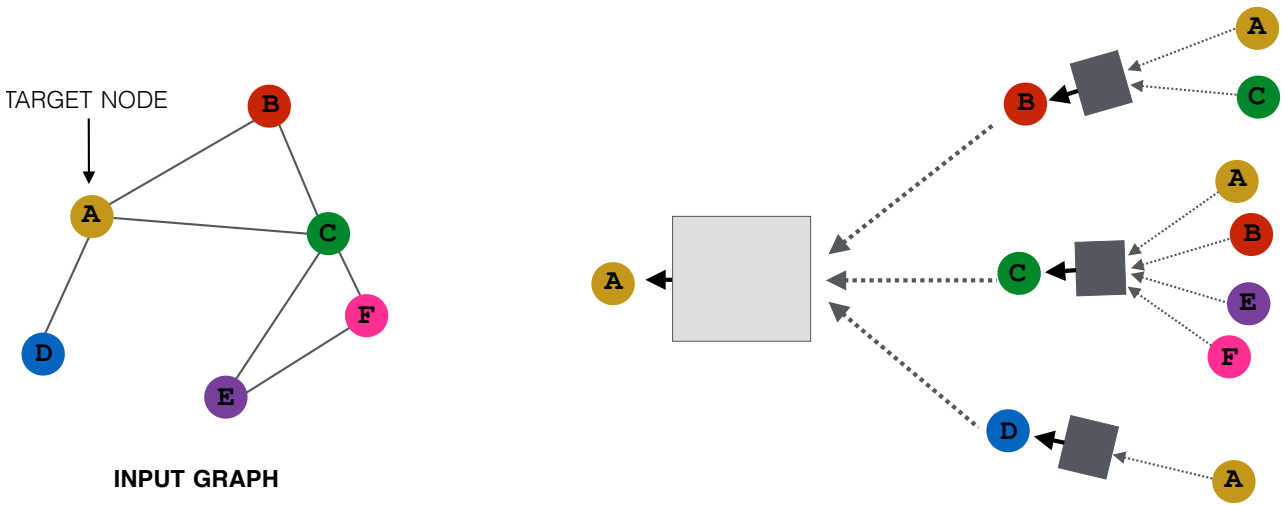
- Hamilton et al. 2017. Representation Learning on Graphs: Methods and Applications. *IEEE Data Engineering Bulletin on Graph Systems*.
- Scarselli et al. 2005. The Graph Neural Network Model. *IEEE Transactions on Neural Networks*.

Setup

- Assume we have a graph $\mathbf{G}$:
  - $\mathbf{V}$ is the vertex set.
  - $\mathbf{A}$ is the adjacency matrix (assume binary).
  - **$\mathbf{X} \in \mathbf{R}^{m \times |V|}$ is a matrix of node features.**
    - Categorical attributes, text, image data
      - E.g., profile information in a social network.
    - Node degrees, clustering coefficients, etc.
    - Indicator vectors (i.e., one-hot encoding of each node)

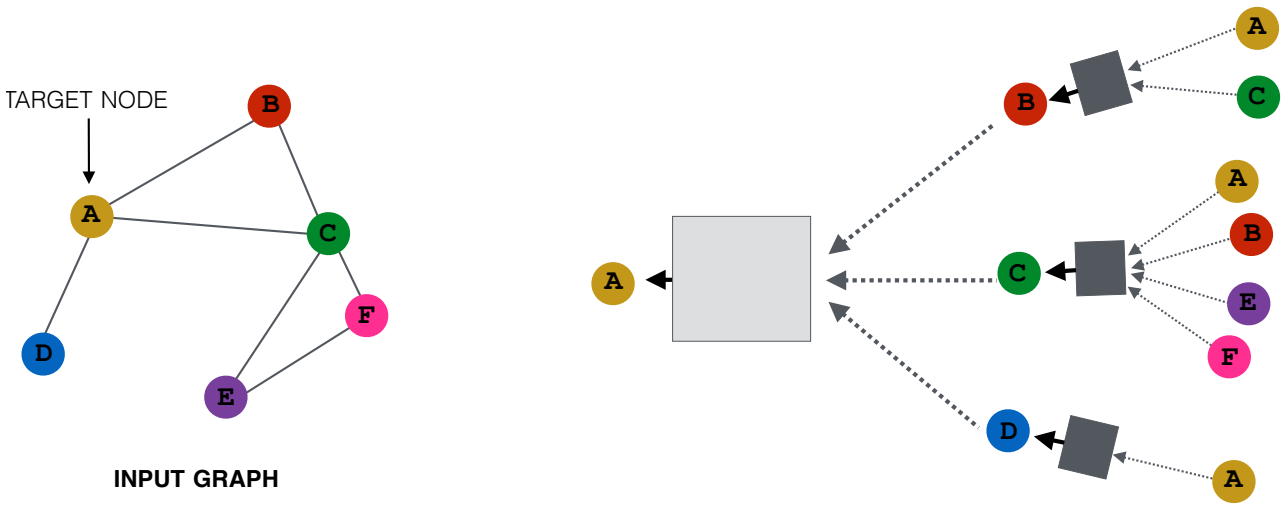
Neighborhood Aggregation

- **Key idea:** Generate node embeddings based on local neighborhoods.



Neighborhood Aggregation

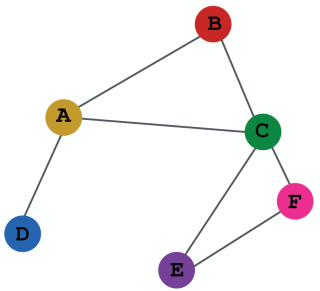
- **Intuition:** Nodes aggregate information from their neighbors using neural networks



Neighborhood Aggregation

- **Intuition:** Network neighborhood defines a computation graph

Every node defines a unique computation graph!



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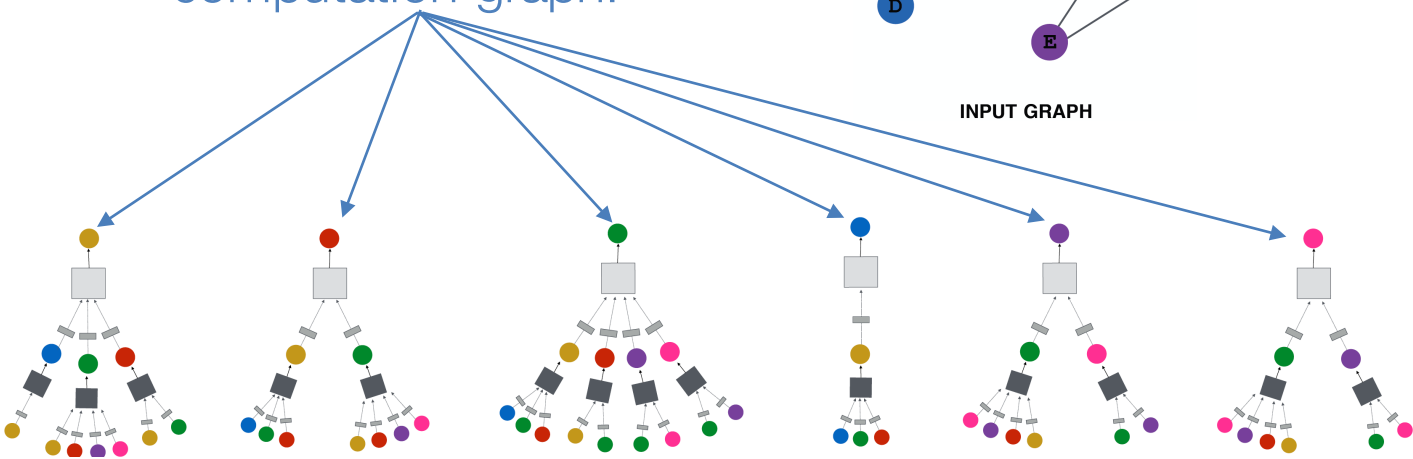
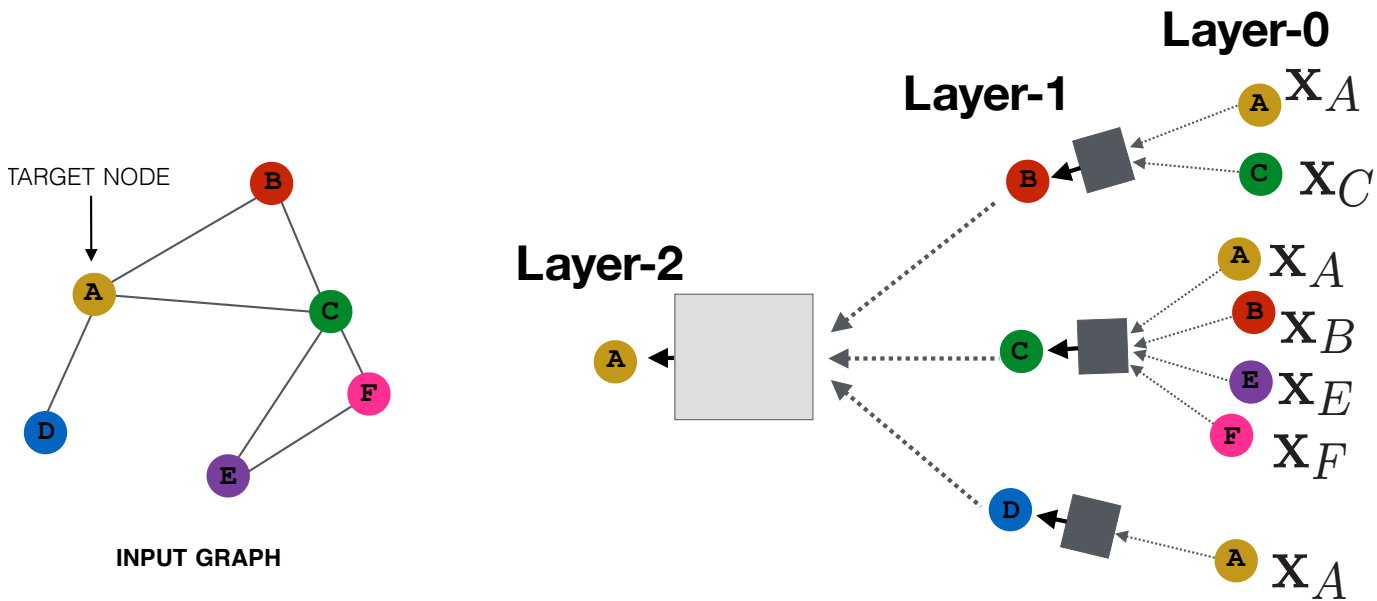


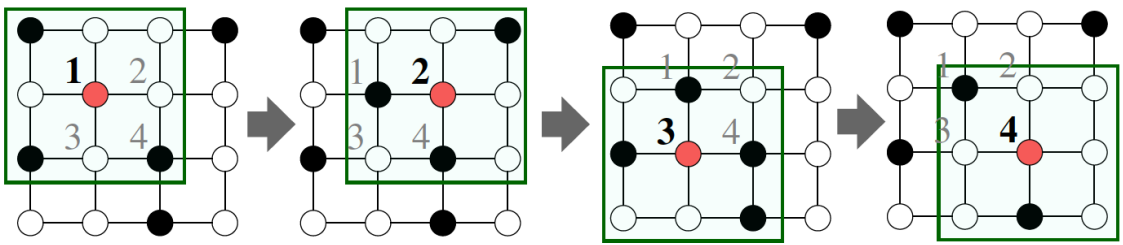
Neighborhood Aggregation

- Nodes have embeddings at each layer.
- Model can be arbitrary depth.
- "layer-0" embedding of node $\mathbf{u}$ is its input feature, i.e. $\mathbf{x}_u$.



Neighborhood "Convolutions"

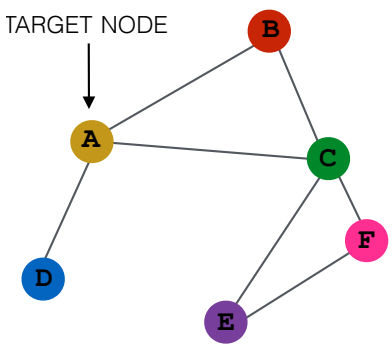
- Neighborhood aggregation can be viewed as a center-surround filter.



- Mathematically related to spectral graph convolutions (see Bronstein et al., 2017)

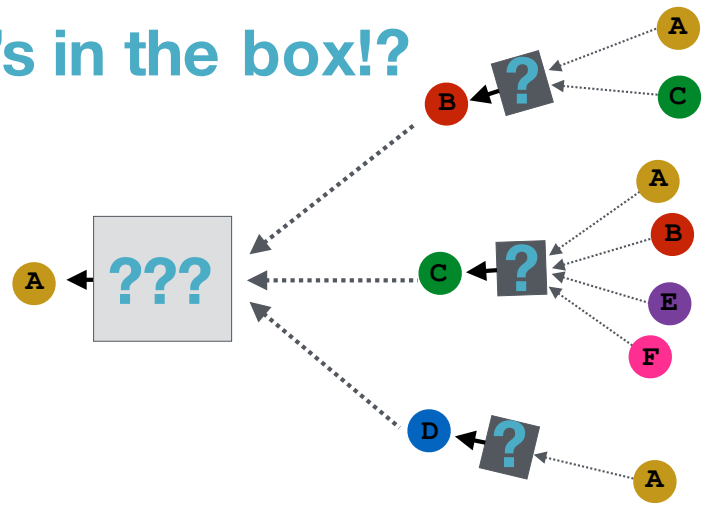
Neighborhood Aggregation

- Key distinctions are in how different approaches aggregate information across the layers.



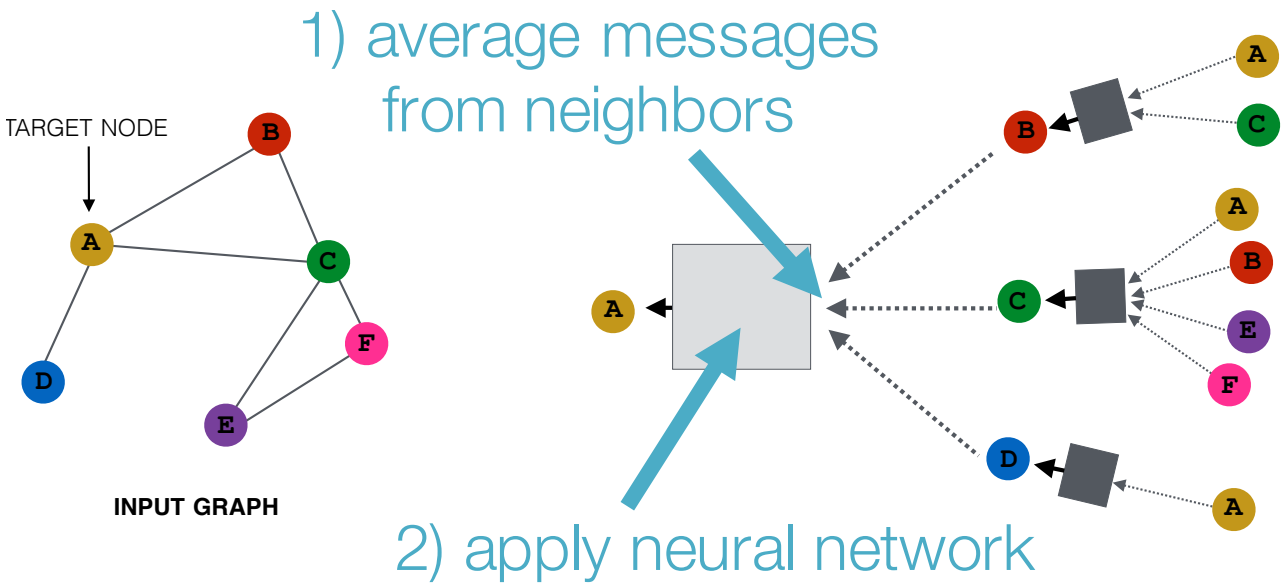
INPUT GRAPH

what's in the box!?



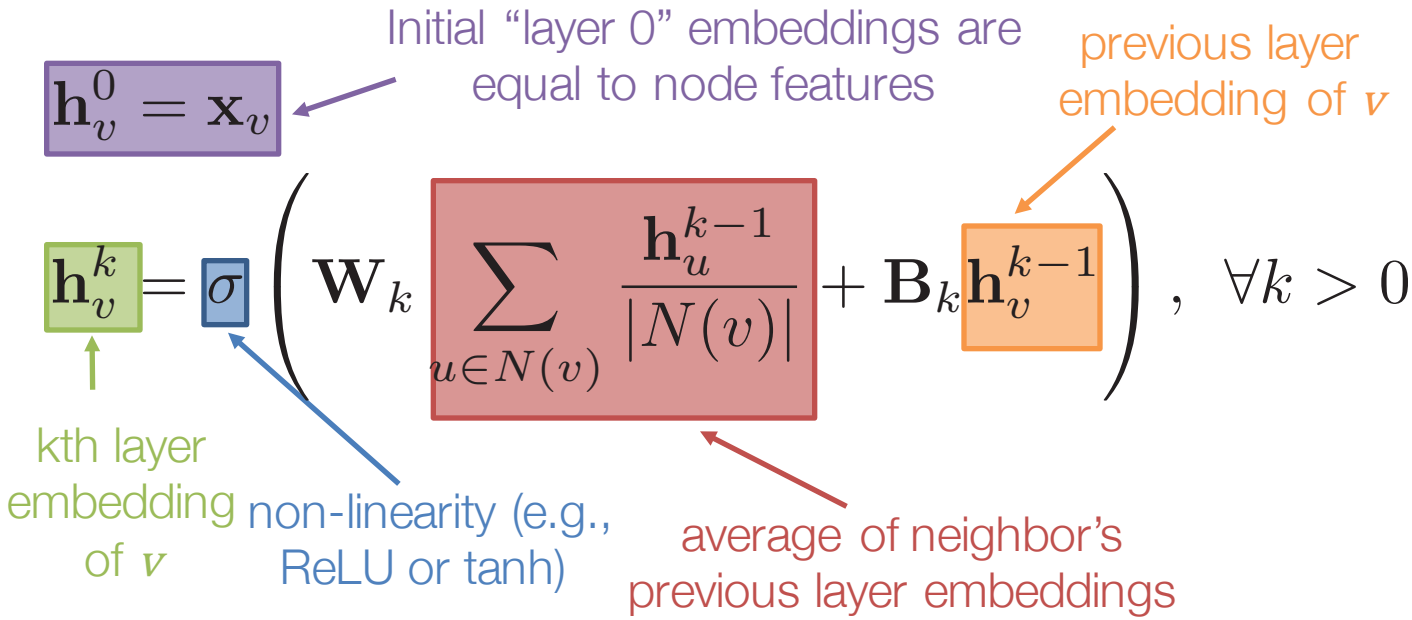
Neighborhood Aggregation

- **Basic approach:** Average neighbor information and apply a neural network.



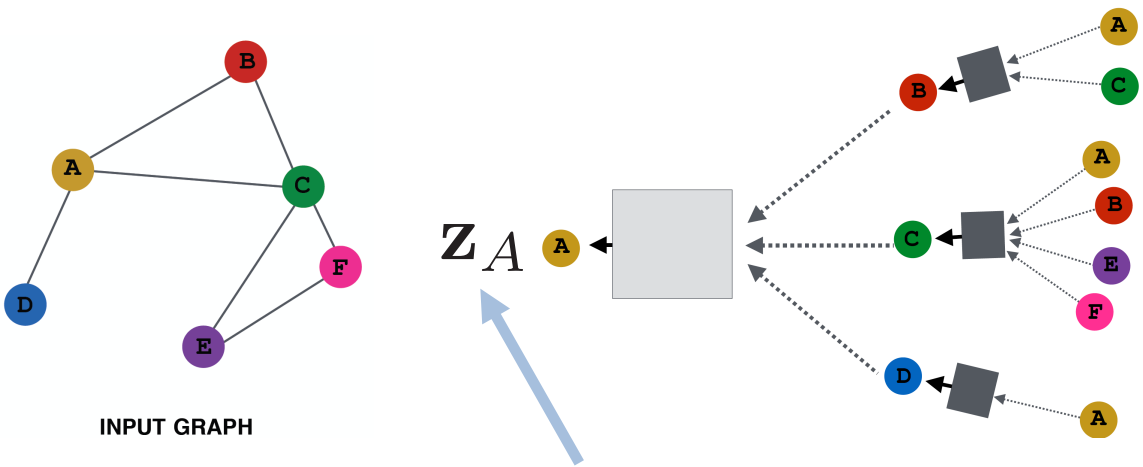
The Math

- **Basic approach:** Average neighbor messages and apply a neural network.



Training the Model

- **How do we train the model to generate "high-quality" embeddings?**



Need to define a loss function on the embeddings, $\mathcal{L}(\mathbf{z}_u)$!

Training the Model

trainable matrices
(i.e., what we learn)

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

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

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

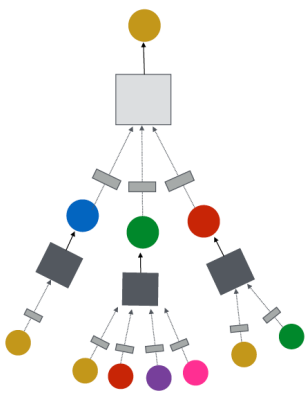
- After K-layers of neighborhood aggregation, we get output embeddings for each node.
- **We can feed these embeddings into any loss function** and run stochastic gradient descent to train the aggregation parameters.

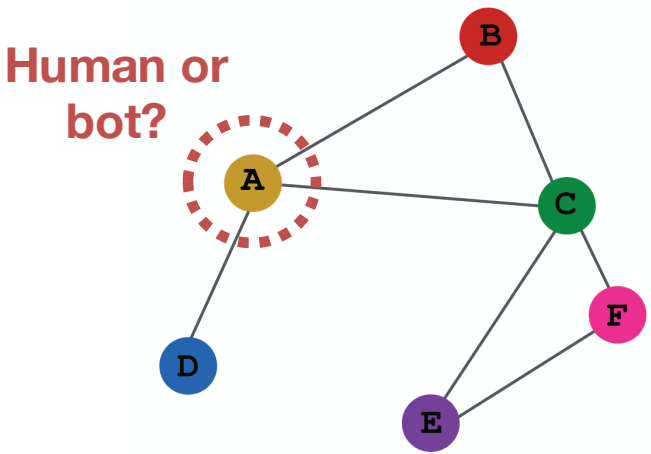
Training the Model

- Train in an **unsupervised manner** using only the graph structure.
- Unsupervised loss function can be anything from the last section, e.g., based on
  - Random walks (node2vec, DeepWalk)
  - Graph factorization
  - i.e., train the model so that "similar" nodes have similar embeddings.

Training the Model

- **Alternative**: Directly train the model for a supervised task (e.g., node classification):

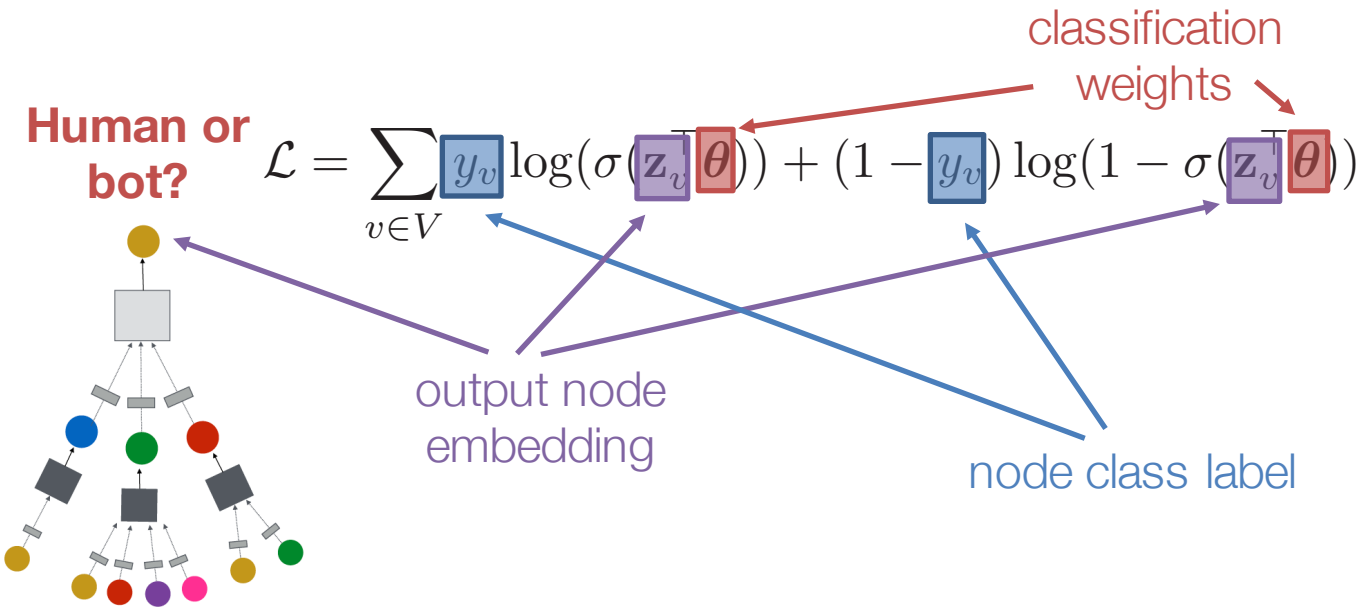




e.g., an online social network

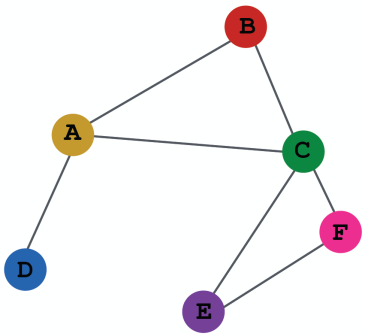
Training the Model

- **Alternative**: Directly train the model for a supervised task (e.g., node classification):



Overview of Model Design

1) Define a neighborhood aggregation function.



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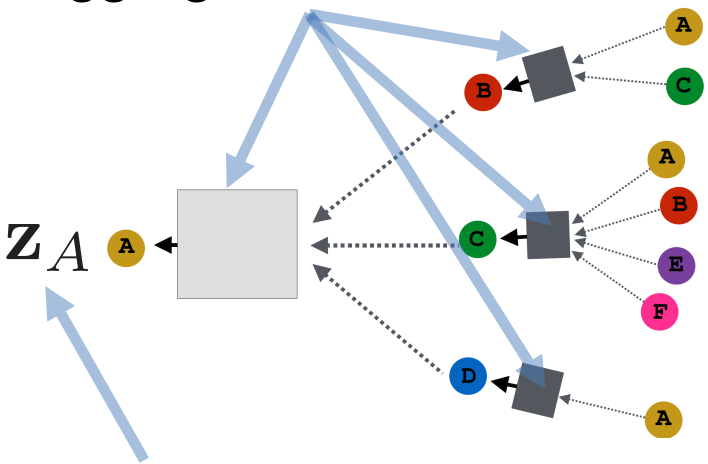
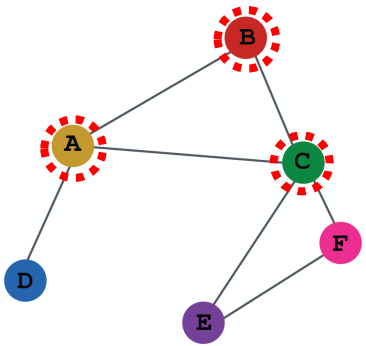


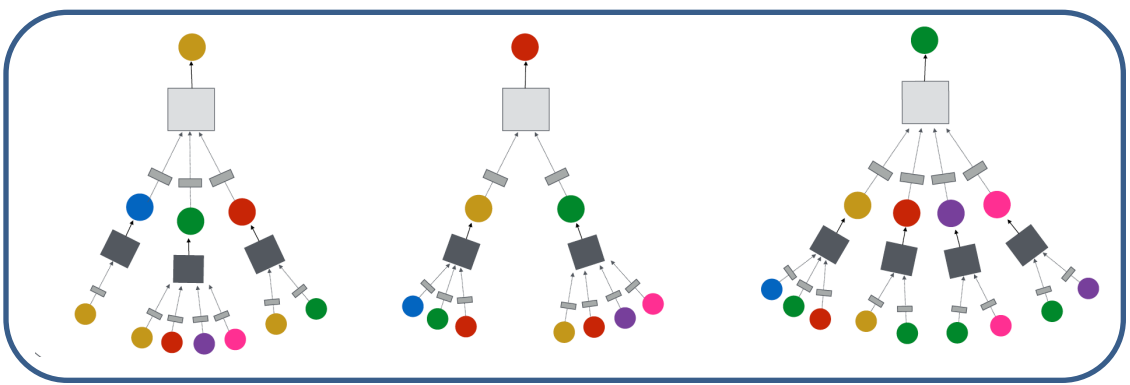
2) Define a loss function on the embeddings, $\mathcal{L}(z_u)$

Overview of Model Design

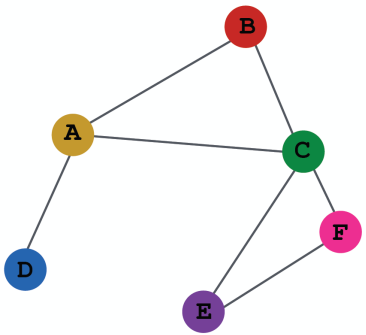


INPUT GRAPH

3) Train on a set of nodes, i.e., a batch of compute graphs



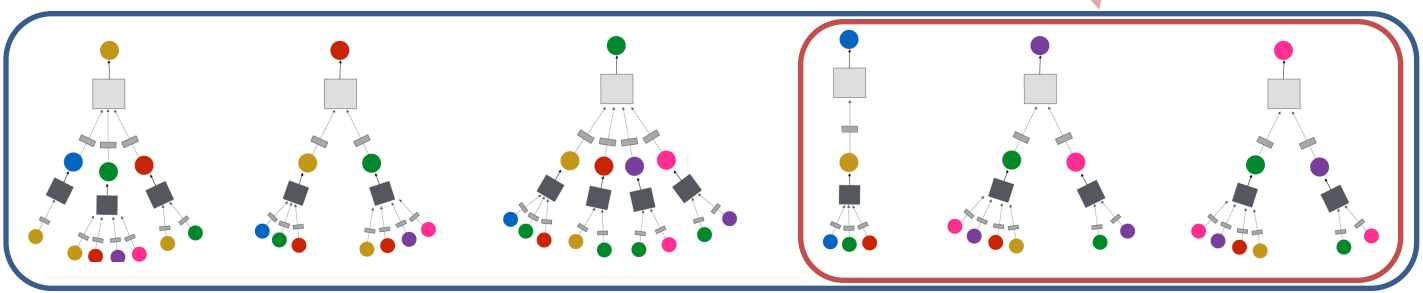
Overview of Model



INPUT GRAPH

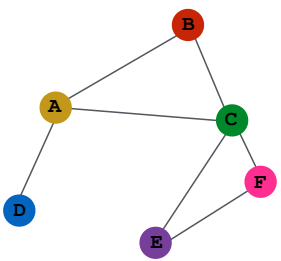
4) Generate embeddings for nodes as needed

Even for nodes we never trained on!!!!



Inductive Capability

- The same aggregation parameters are shared for all nodes.
- The number of model parameters is sublinear in $|V|$ and we can generalize to unseen nodes!



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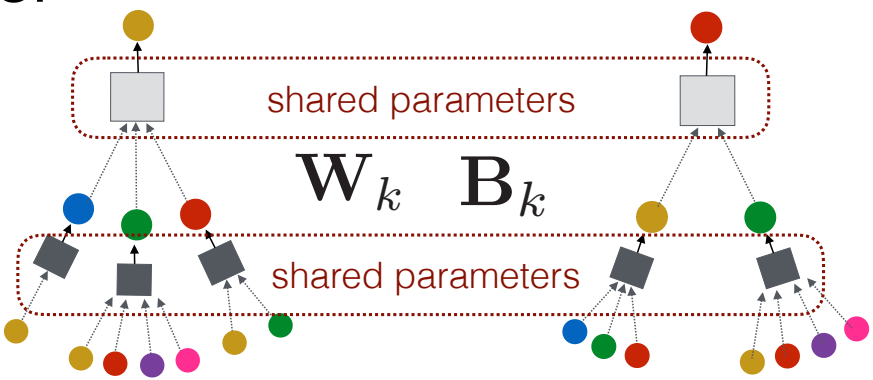
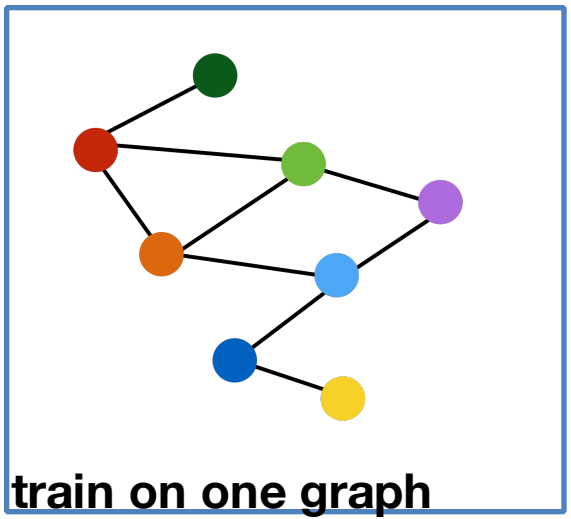
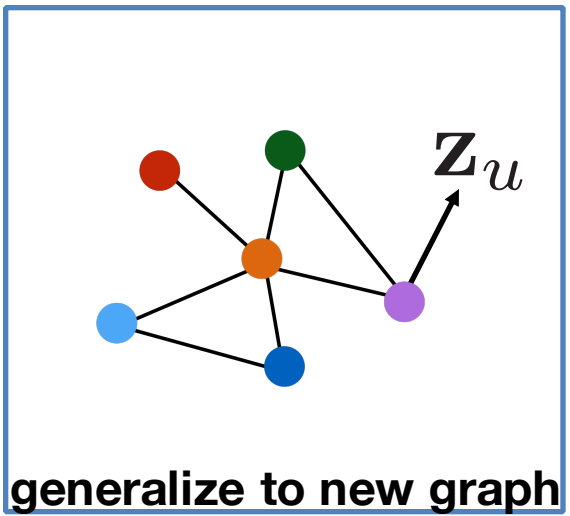


Compute graph for node A **Compute graph for node B**

Inductive Capability

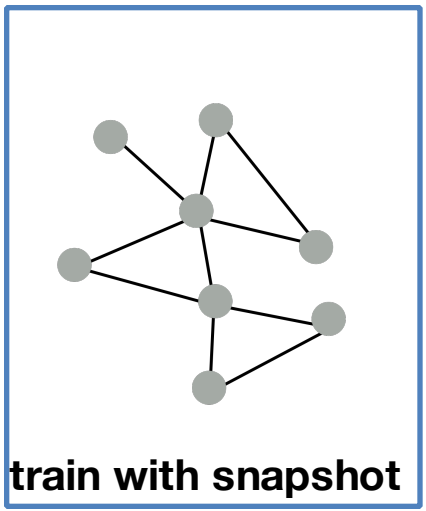


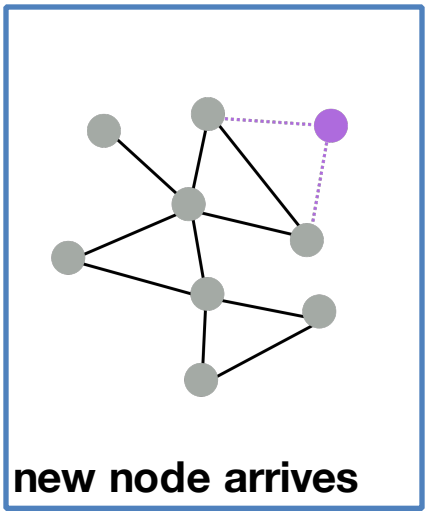


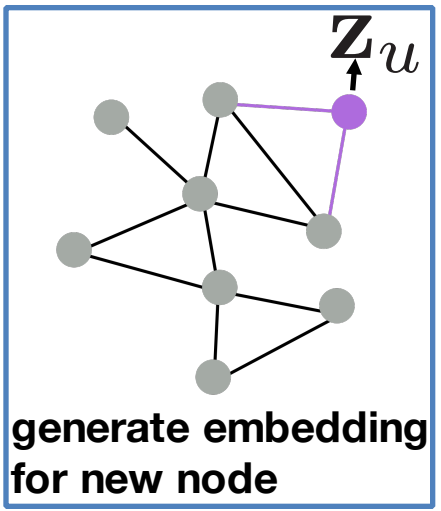
Inductive node embedding → generalize to entirely unseen graphs

e.g., train on protein interaction graph from model organism A and generate embeddings on newly collected data about organism B

Inductive Capability







Many application settings constantly encounter previously unseen nodes.

e.g., Reddit, YouTube, GoogleScholar, ….

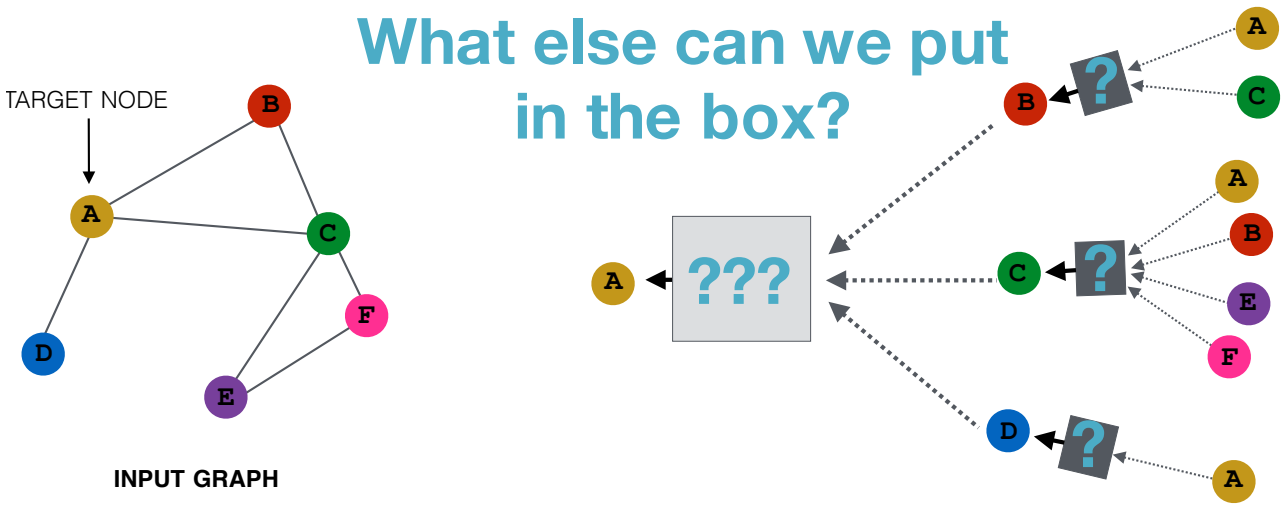
Need to generate new embeddings "on the fly"

Quick Recap

- **Recap:** Generate node embeddings by aggregating neighborhood information.
  - Allows for parameter sharing in the encoder.
  - Allows for inductive learning.
- We saw a **basic variant of this idea**… now we will cover some state of the art variants from the literature.

Neighborhood Aggregation

- Key distinctions are in how different approaches aggregate messages



Outline for this Section

1. **The Basics** ✓
2. **Graph Convolutional Networks** 
3. **GraphSAGE**
4. **Gated Graph Neural Networks**
5. **Subgraph Embeddings**

Graph Convolutional Networks

Based on material from:

- Kipf et al., 2017. Semisupervised Classification with Graph Convolutional Networks. *ICLR*.

Graph Convolutional Networks

- Kipf et al.'s **Graph Convolutional Networks (GCNs)** are a slight variation on the neighborhood aggregation idea:

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

Graph Convolutional Networks

Basic Neighborhood Aggregation

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

VS.

GCN Neighborhood Aggregation

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

same matrix for self and neighbor embeddings

per-neighbor normalization

Graph Convolutional Networks

- Empirically, they found this configuration to give the best results.
  - More parameter sharing.
  - Down-weights high degree neighbors.

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

use the same transformation matrix for self and neighbor embeddings

instead of simple average, normalization varies across neighbors

Batch Implementation

- Can be efficiently implemented using sparse batch operations:

$$\mathbf{H}^{(k+1)} = \sigma\left(\mathbf{D}^{-\frac{1}{2}}\tilde{\mathbf{A}}\mathbf{D}^{-\frac{1}{2}}\mathbf{H}^{(k)}\mathbf{W}_k\right)$$

where $\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{I}$

$$\mathbf{D}_{ii} = \sum_j \mathbf{A}_{i,j}$$

- $O(|E|)$ time complexity overall.

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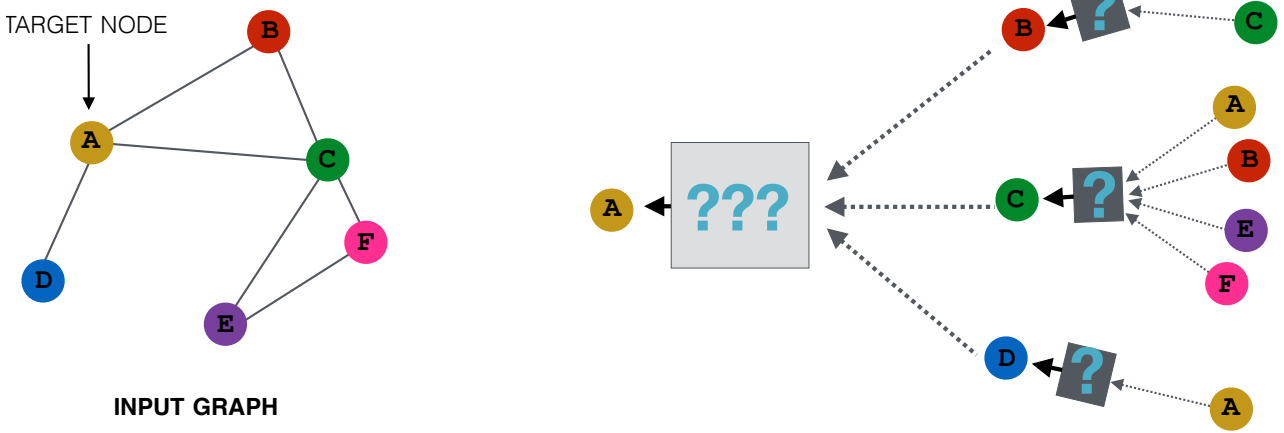
GraphSAGE

Based on material from:

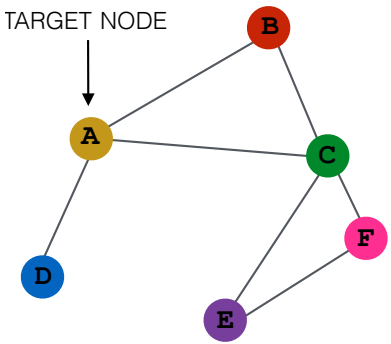
- Hamilton et al., 2017. Inductive Representation Learning on Large Graphs. *NIPS.*

GraphSAGE Idea

- So far we have aggregated the neighbor messages by taking their (weighted) average, can we do better?



GraphSAGE Idea



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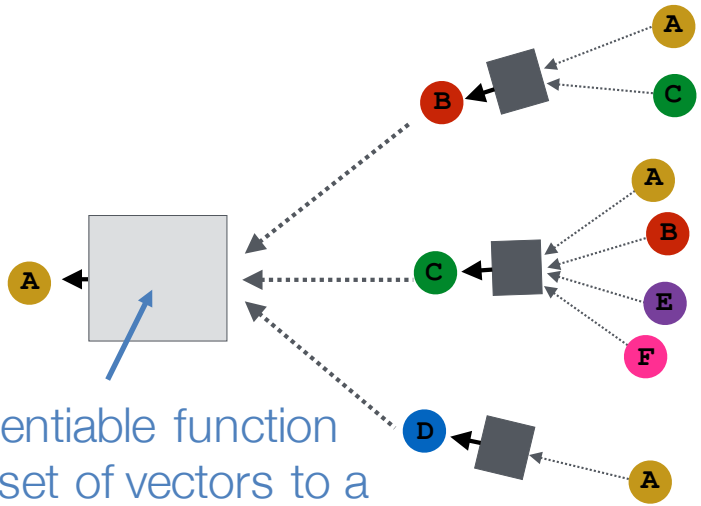

Any differentiable function that maps set of vectors to a single vector.

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

GraphSAGE Differences

- Simple neighborhood aggregation:

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

- GraphSAGE:

concatenate self embedding and neighbor embedding

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

generalized aggregation

GraphSAGE Variants

- **Mean:**

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

- **Pool**
  - Transform neighbor vectors and apply symmetric vector function.

element-wise mean/max

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

- **LSTM:**
  - Apply LSTM to random permutation of neighbors.

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

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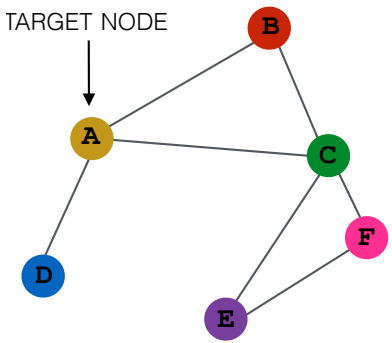
Gated Graph Neural Networks

Based on material from:

- Li et al., 2016. Gated Graph Sequence Neural Networks. *ICLR.*

Neighborhood Aggregation

- **Basic idea:** Nodes aggregate "messages" from their neighbors using neural networks



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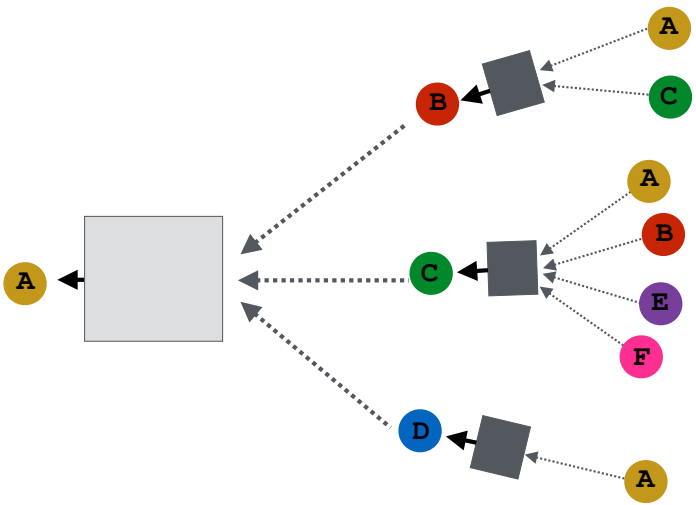
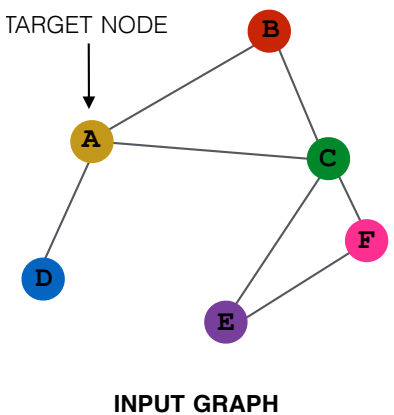


Neighborhood Aggregation

- GCNs and GraphSAGE **generally only 2-3 layers deep.**



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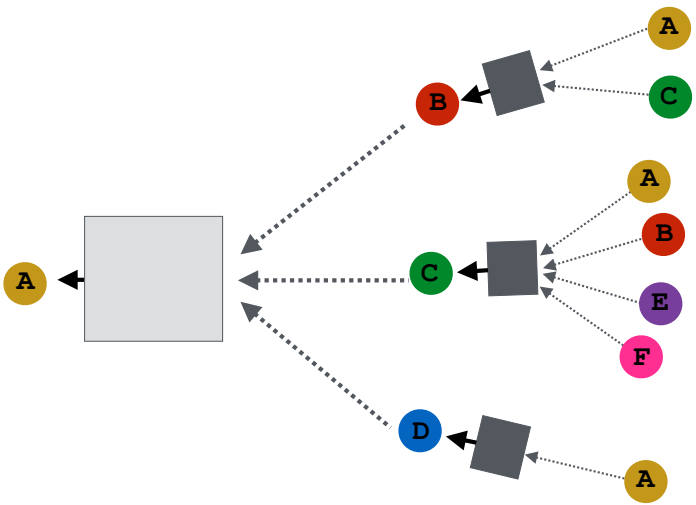
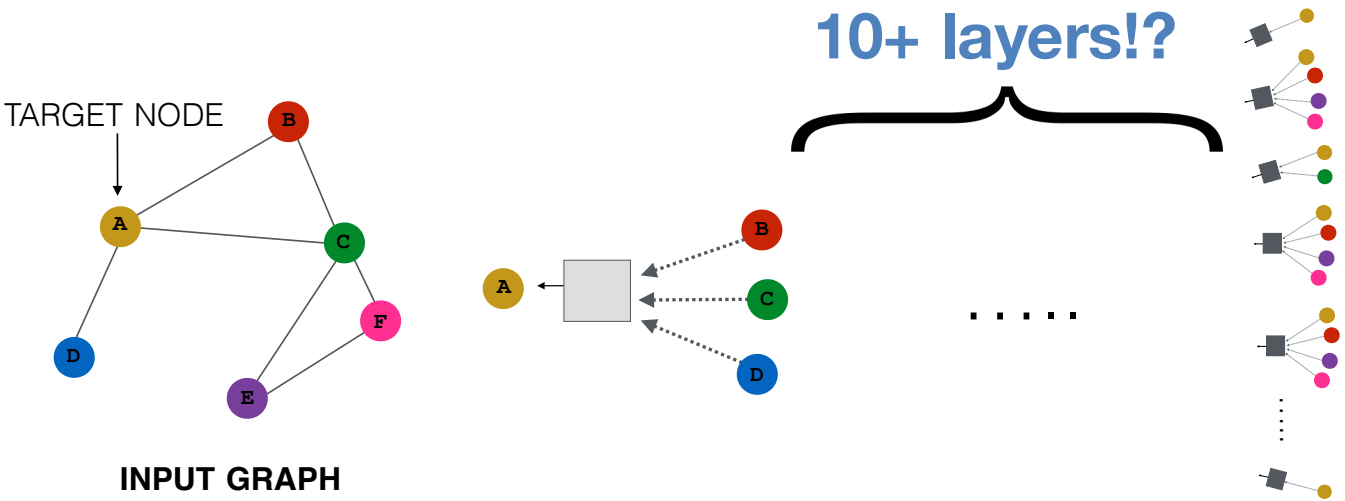


Neighborhood Aggregation

- **But what if we want to go deeper?**

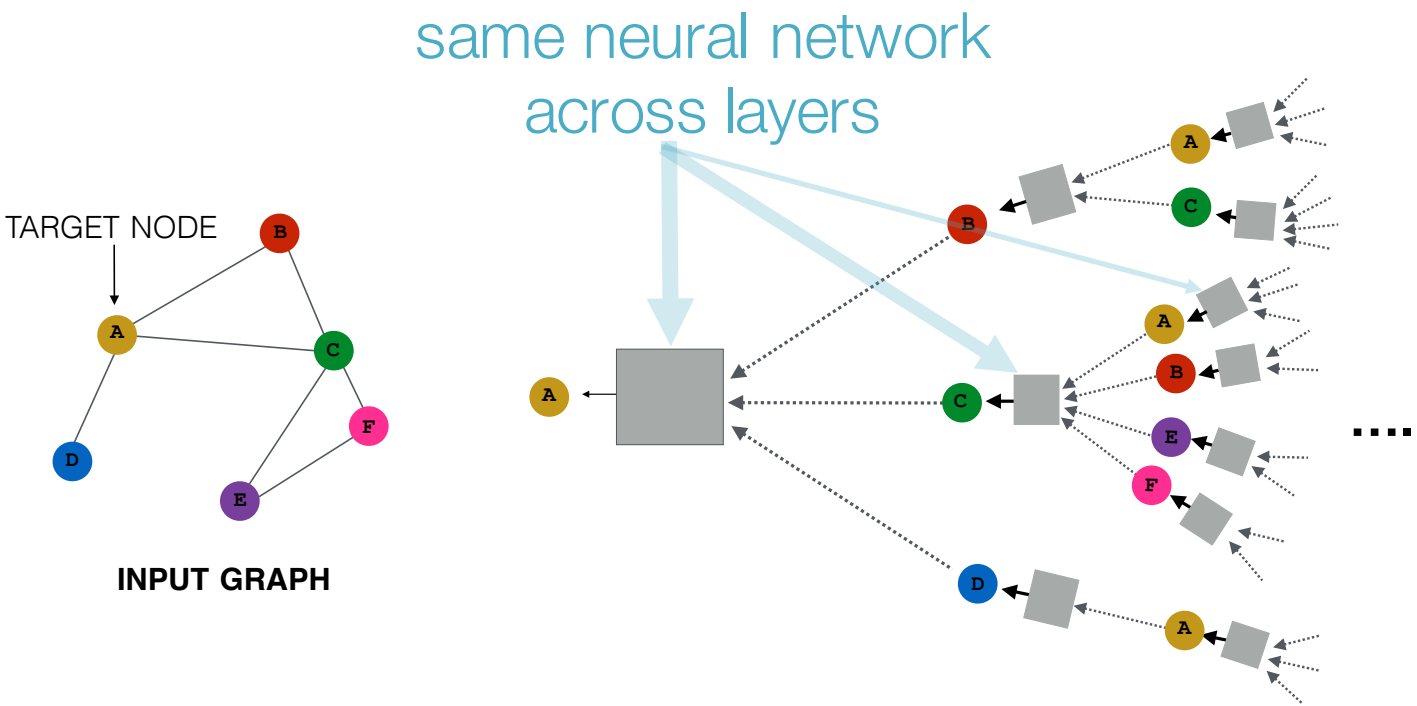


Gated Graph Neural Networks

- How can we build models with many layers of neighborhood aggregation?
- **Challenges:**
  - Overfitting from too many parameters.
  - Vanishing/exploding gradients during backpropagation.
- **Idea:** Use techniques from modern recurrent neural networks!

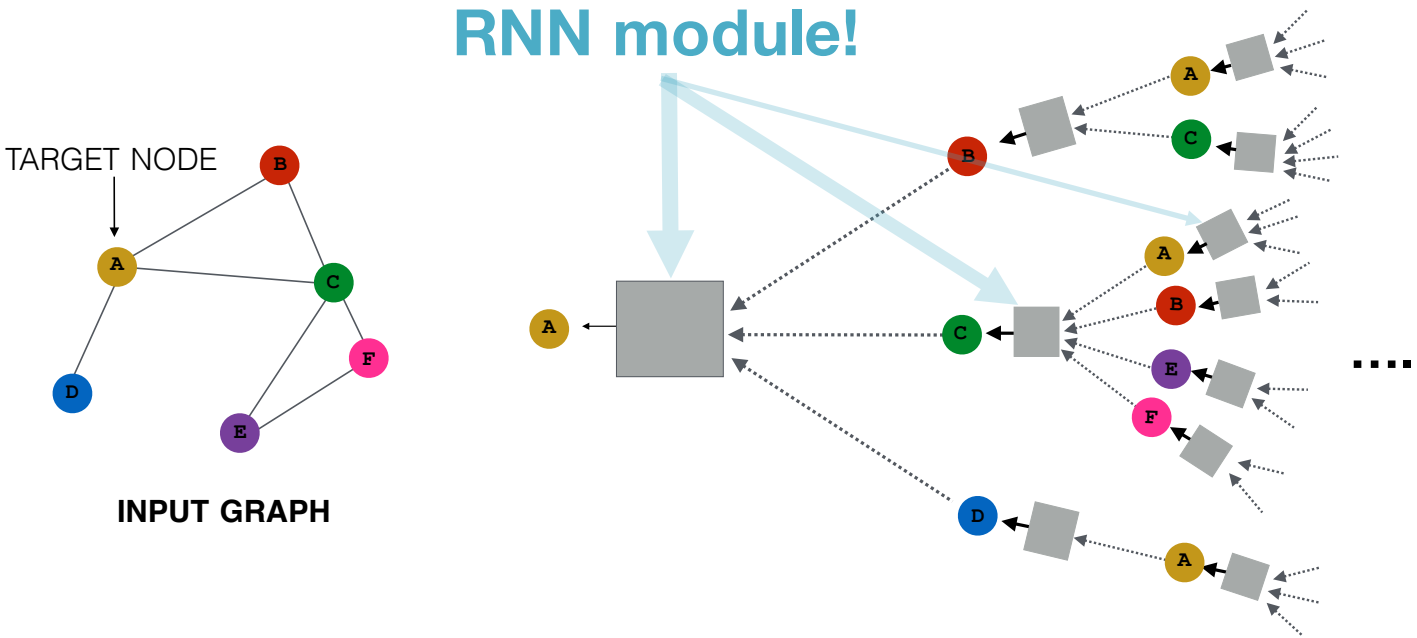
Gated Graph Neural Networks

- **Idea 1:** Parameter sharing across layers.



Gated Graph Neural Networks

- **Idea 2:** Recurrent state update.



The Math

- **Intuition:** Neighborhood aggregation with RNN state update.

1. Get "message" from neighbors at step k:

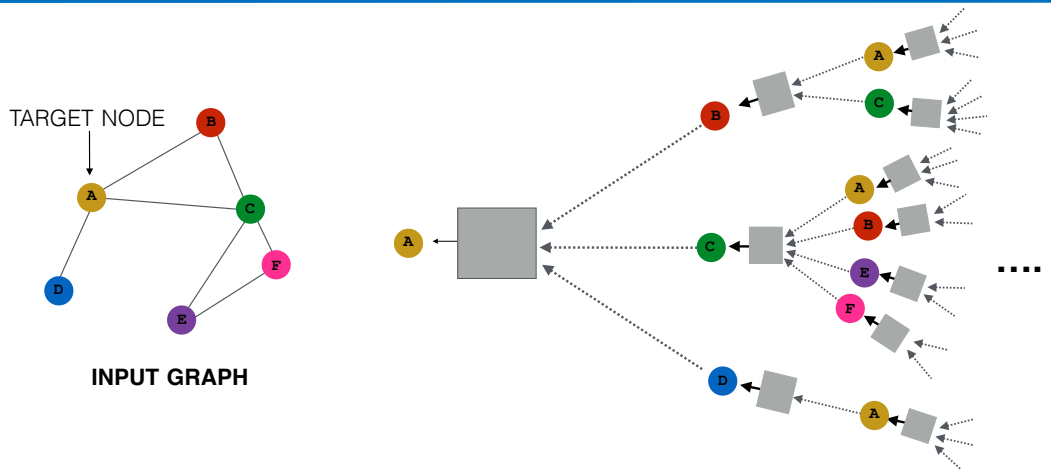
$$\mathbf{m}_v^k = \mathbf{W} \sum_{u \in N(v)} \mathbf{h}_u^{k-1}$$

aggregation function does not depend on $\mathbf{k}$

2. Update node "state" using Gated Recurrent Unit (GRU). New node state depends on the old state and the message from neighbors:

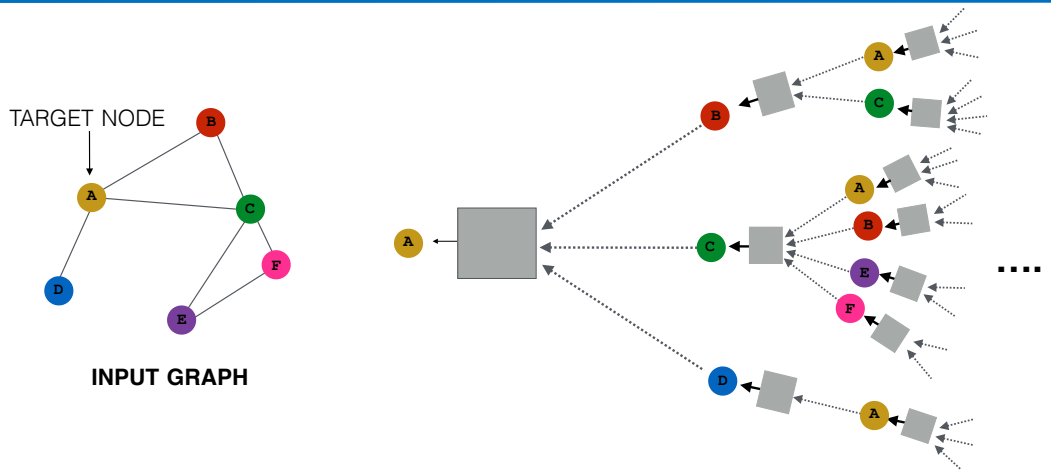
$$\mathbf{h}_v^k = \mathrm{GRU}(\mathbf{h}_v^{k-1}, \mathbf{m}_v^k)$$

Gated Graph Neural Networks



- Can handle models with >20 layers.
- Most real-world networks have small diameters (e.g., less than 7).
- Allows for complex information about global graph structure to be propagated to all nodes.

Gated Graph Neural Networks



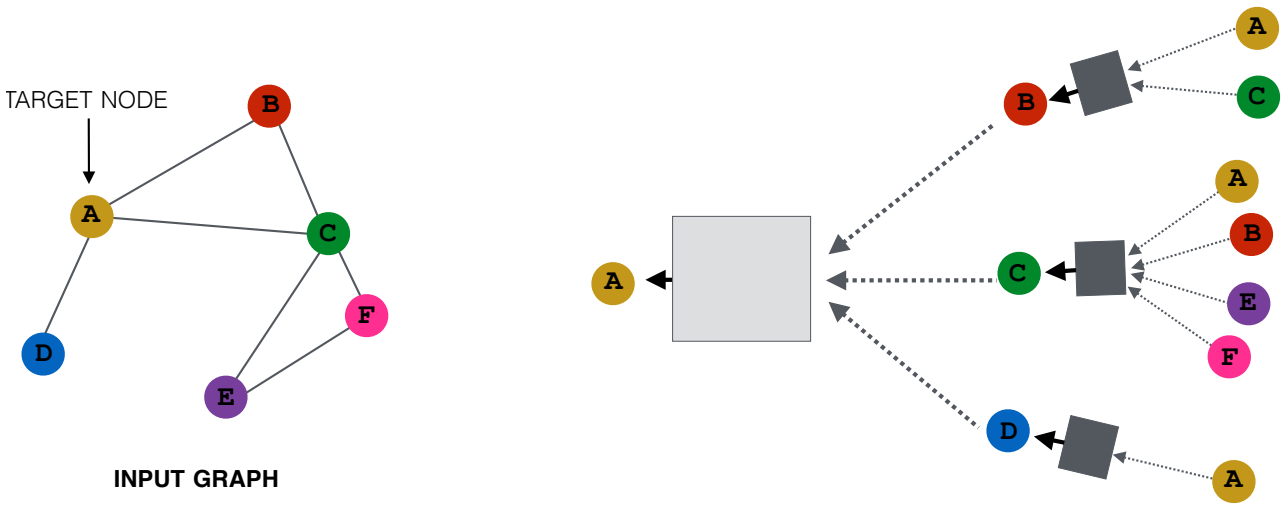
- **Useful for complex networks representing:**
  - **Logical formulas.**
  - **Programs.**

Outline for this Section

1. **The Basics** ✓
2. **Graph Convolutional Networks** ✓
3. **GraphSAGE** ✓
4. **Gated Graph Neural Networks** ✓
5. **Subgraph Embeddings**

Summary so far

- **Key idea:** Generate node embeddings based on local neighborhoods.



Summary so far

- **Graph convolutional networks**
  - Average neighborhood information and stack neural networks.
- **GraphSAGE**
  - Generalized neighborhood aggregation.
- **Gated Graph Neural Networks**
  - Neighborhood aggregation + RNNs

Recent advances in graph neural nets (not covered in detail here)

- **Attention-based neighborhood aggregation:**
  - Graph Attention Networks (Velickovic et al., 2018)
  - GeniePath (Liu et al., 2018)
- **Generalizations based on spectral convolutions:**
  - Geometric Deep Learning (Bronstein et al., 2017)
  - Mixture Model CNNs (Monti et al., 2017)
- **Speed improvements via subsampling:**
  - FastGCNs (Chen et al., 2018)
  - Stochastic GCNs (Chen et al., 2017)

Outline for this Section

1. **The Basics** ✓
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5. **Subgraph Embeddings**

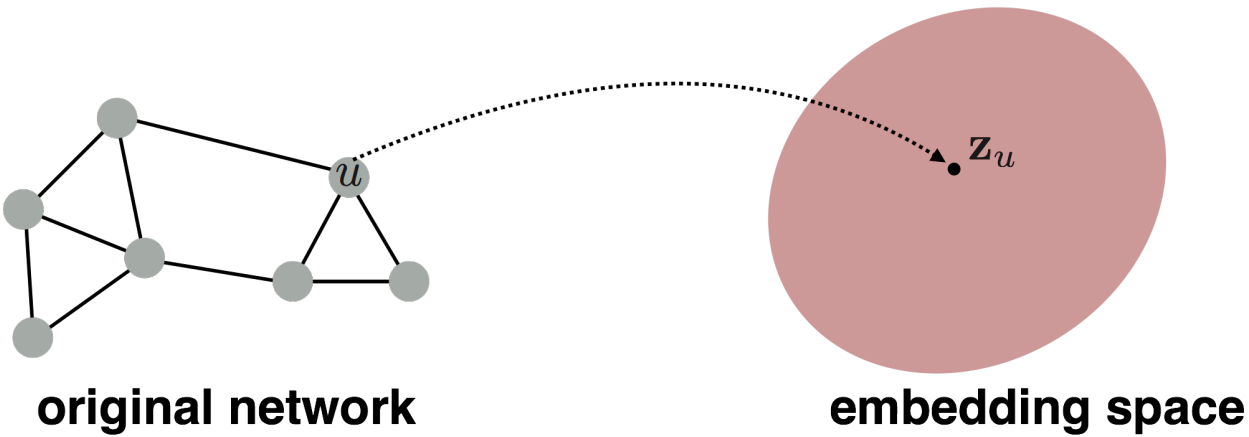
Subgraph Embeddings

Based on material from:

- Duvenaud et al. 2016. Convolutional Networks on Graphs for Learning Molecular Fingerprints. *ICML.*
- Li et al. 2016. Gated Graph Sequence Neural Networks. *ICLR.*

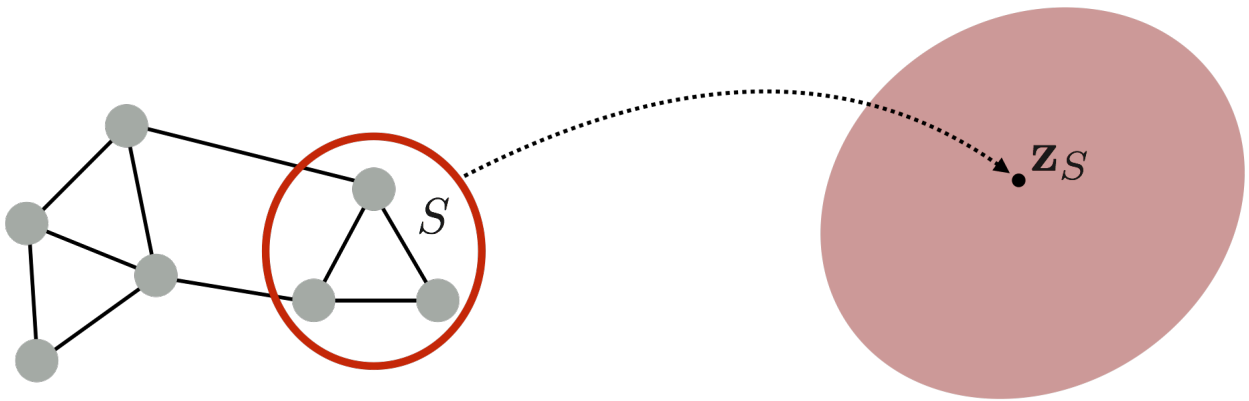
(Sub)graph Embeddings

- **So far we have focused on node-level embeddings…**



(Sub)graph Embeddings

- **But what about subgraph embeddings?**



Approach 1

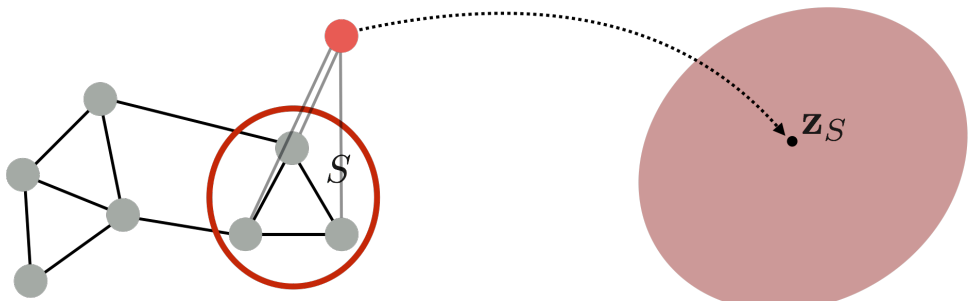
- **Simple idea:** Just sum (or average) the node embeddings in the (sub)graph

$$\mathbf{z}_S = \sum_{v \in S} \mathbf{z}_v$$

- Used by Duvenaud et al., 2016 to classify molecules based on their graph structure.

Approach 2

- **Idea:** Introduce a **"virtual node"** to represent the subgraph and run a standard graph neural network.



- Proposed by Li et al., 2016 as a general technique for subgraph embedding.

(Sub)graph Embeddings

- **Still an open research area!**
  - How to embed (sub)graphs with millions or billions of nodes?
  - How to do analogue of CNN "pooling" on networks?