Message Passing Mechanism & Graph Neural Networks

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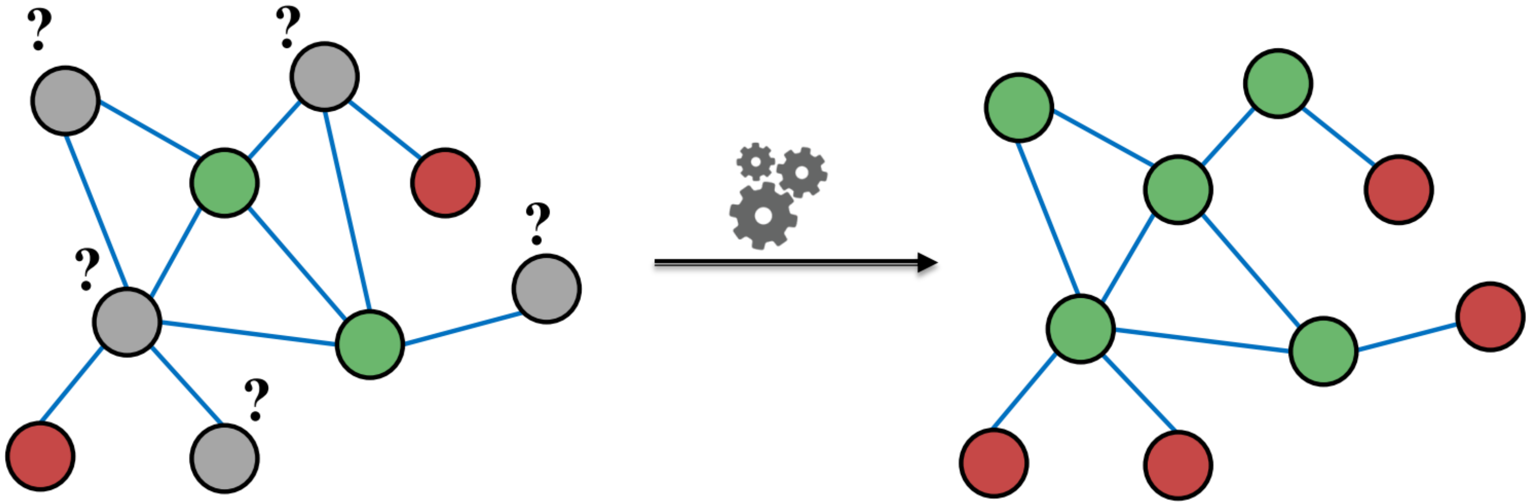
- Relational Classification and Node Classification
- From “Shallow” to “Deep” Representation Learning
- Message Passing Mechanism.
- Graph Convolutional Network.
- Libraries for deep learning on graphs

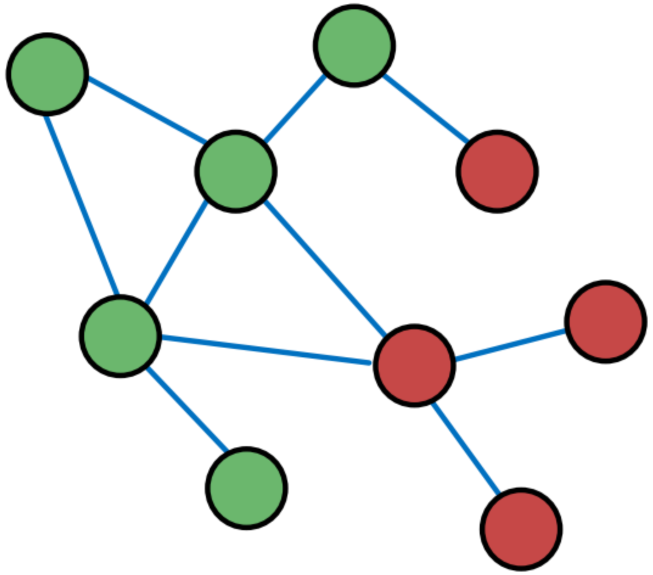
Main Question

- Given a network with labels on some nodes, how do we assign labels to all other nodes in the network?
- Node embedding (shallow encoding) is a method to solve this
- Message passing is an alternative framework



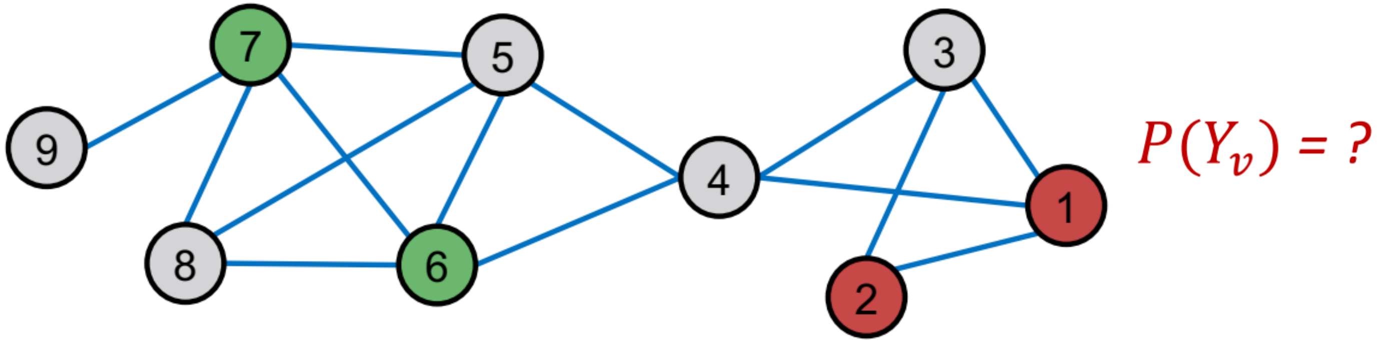
Message Passing Intuition

- **Intuition**: Correlations (dependency) exist in network
  - Similar nodes are connected.
  - Homophily: individual character → social connections.
  - Influence: social connections → individual character.
- **Key concept**: collective classification, assign labels to all nodes in a network together.
- We will look at 2 **techniques**:
  - Relational classification.
  - Iterative classification.



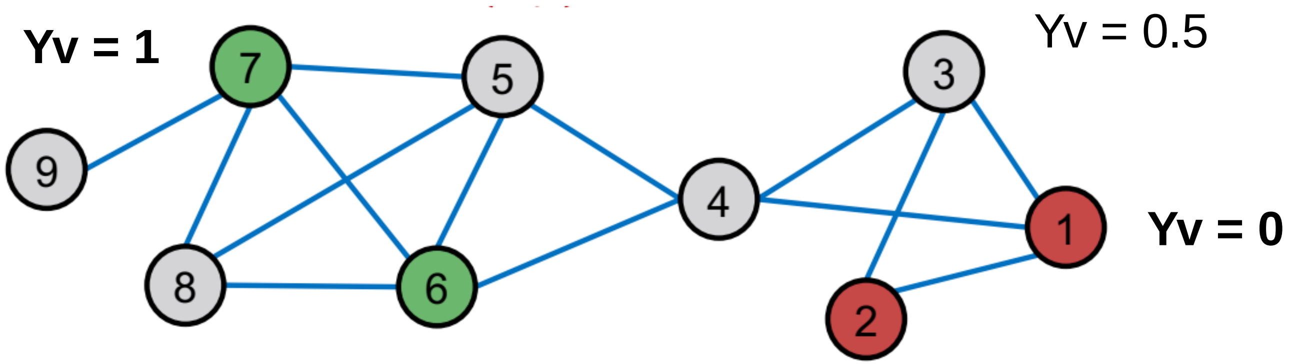
Classification with Network Data

- How do we leverage node correlations in networks to help prediction?
- Motivation 1: Similar nodes are typically close together or directly connected in the network.
- Motivation 2: Classification label of node v in network may depend on:
  - features of v.
  - labels of the nodes in v ‘s neighbourhood.
  - features of the nodes in v ‘s neighbourhood.
- Many applications are under the same setting



Relational Classification

- Idea: Propagate node labels across the network
  - Class probability Yv of node v is a weighted average of class probabilities of its neighbors.
- Labeled nodes: initialize Yv with ground-truth label Yv*.
- Unlabeled nodes: initialize Yv = 0.5.
- Update all nodes in a random order until convergence or until maximum number of iterations.

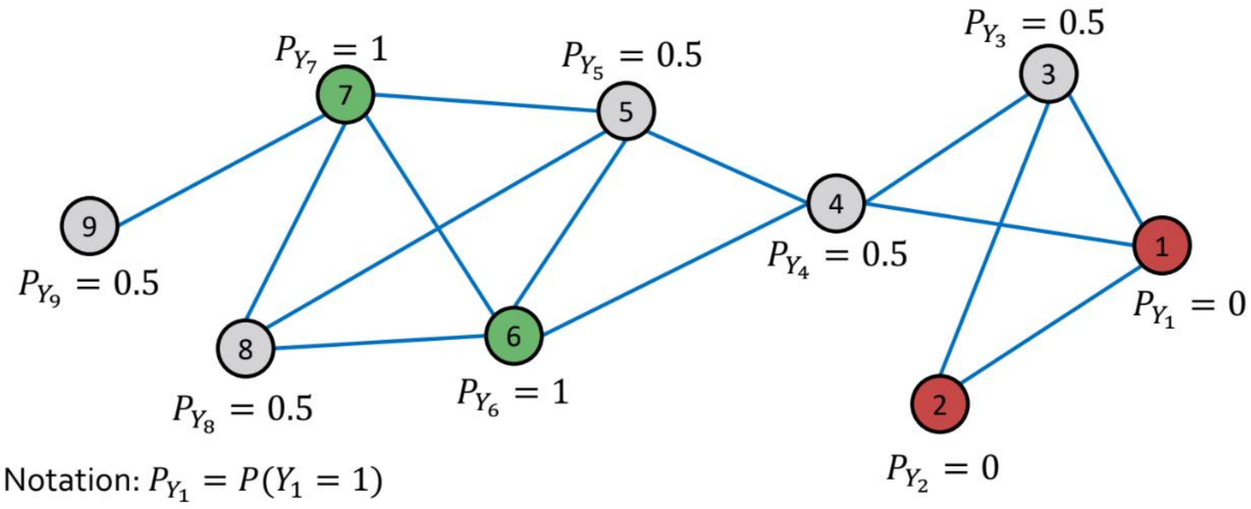


Update for Relational Classifier

- Update for each node v and label c (0 or 1)

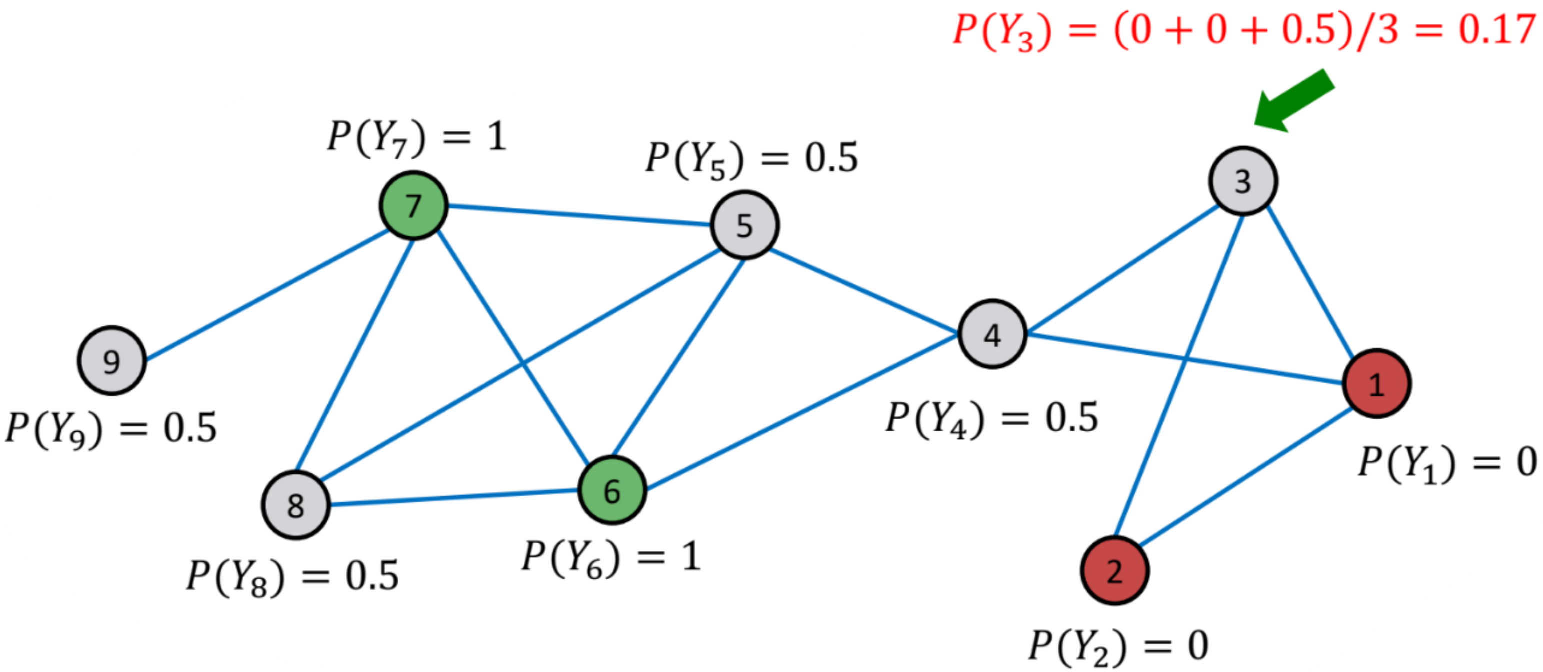
$$P(Y_v = c) = \frac{1}{\sum_{(v,u)\in E} A_{v,u}} \sum_{(v,u)\in E} A_{v,u}\, P(Y_u = c)$$

- If edges have weight/strength, $A_{v,u}$ can represent the edge weight
- For example:



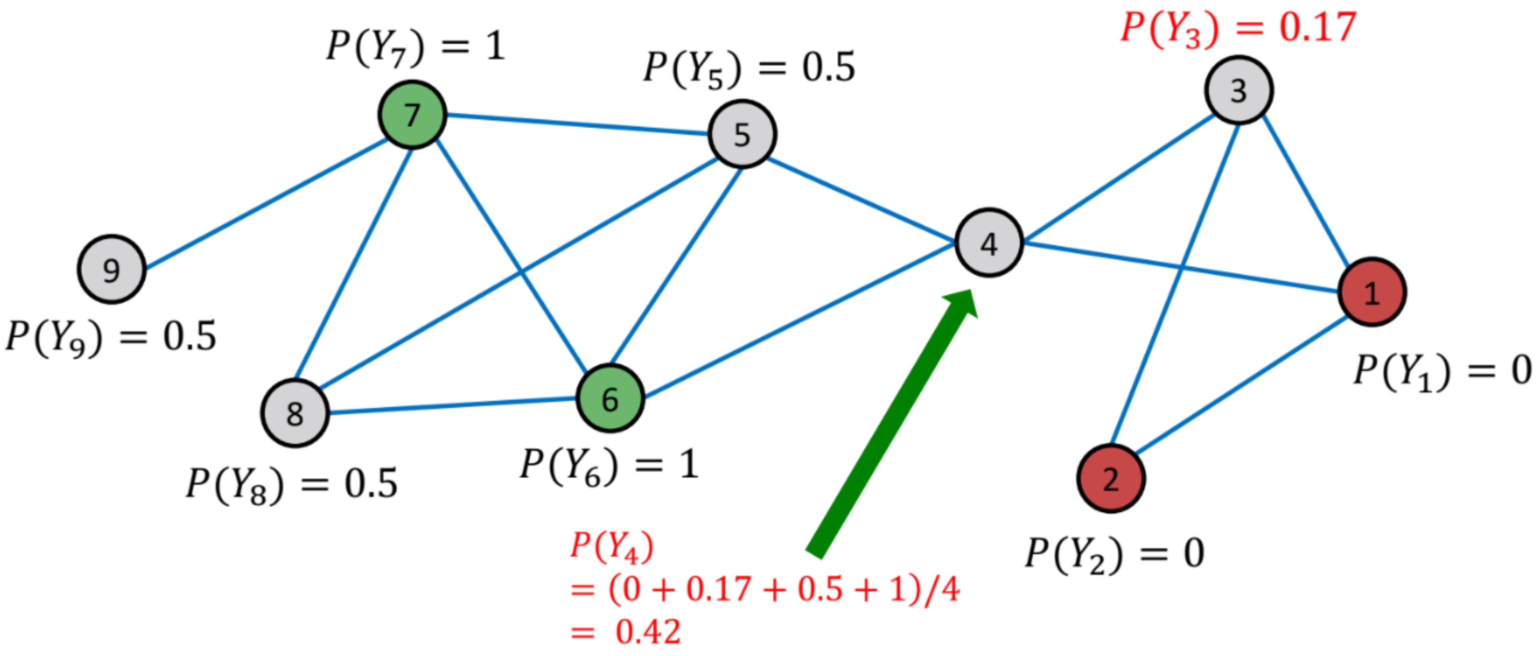
Example: 1st Iteration, Update Node 3

- Update for the 1st iteration:
  - For node 3, N(3) = {1, 2, 4}



Example: 1st Iteration, Update Node 4

- Update for the 1st iteration:
  - For node 3, N(3) = {1, 2, 4}

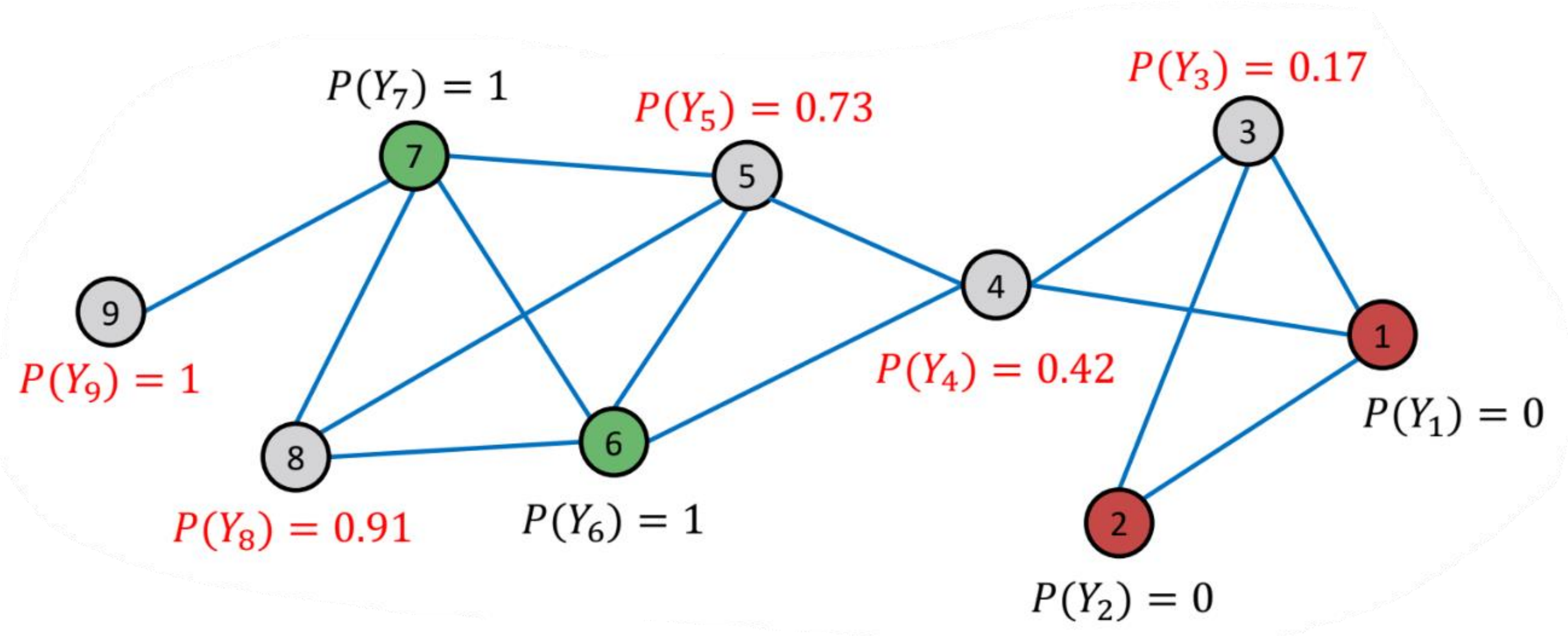


$P(Y_4)$
$= (0 + 0.17 + 0.5 + 1)/4$
$= 0.42$

After Node 3 is updated

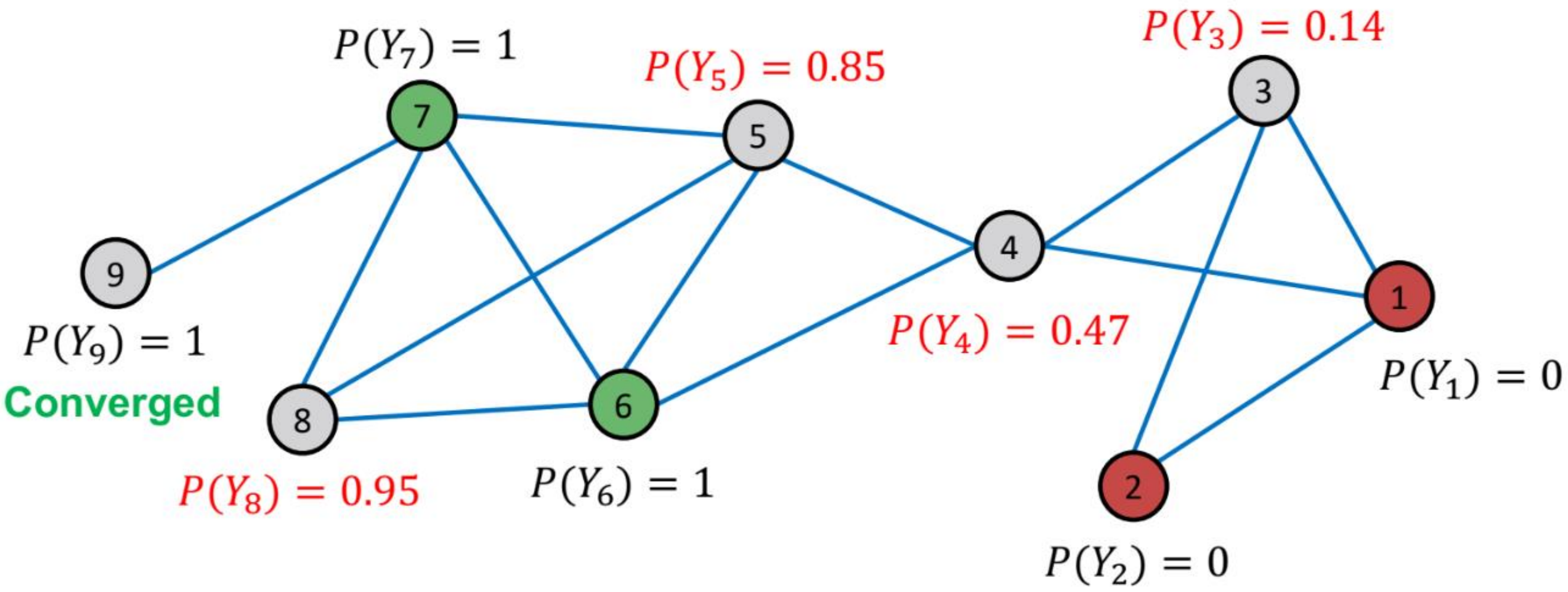
Example: After 1st Iteration

- Then after update for node 5, 8, 9
    - 1 iteration



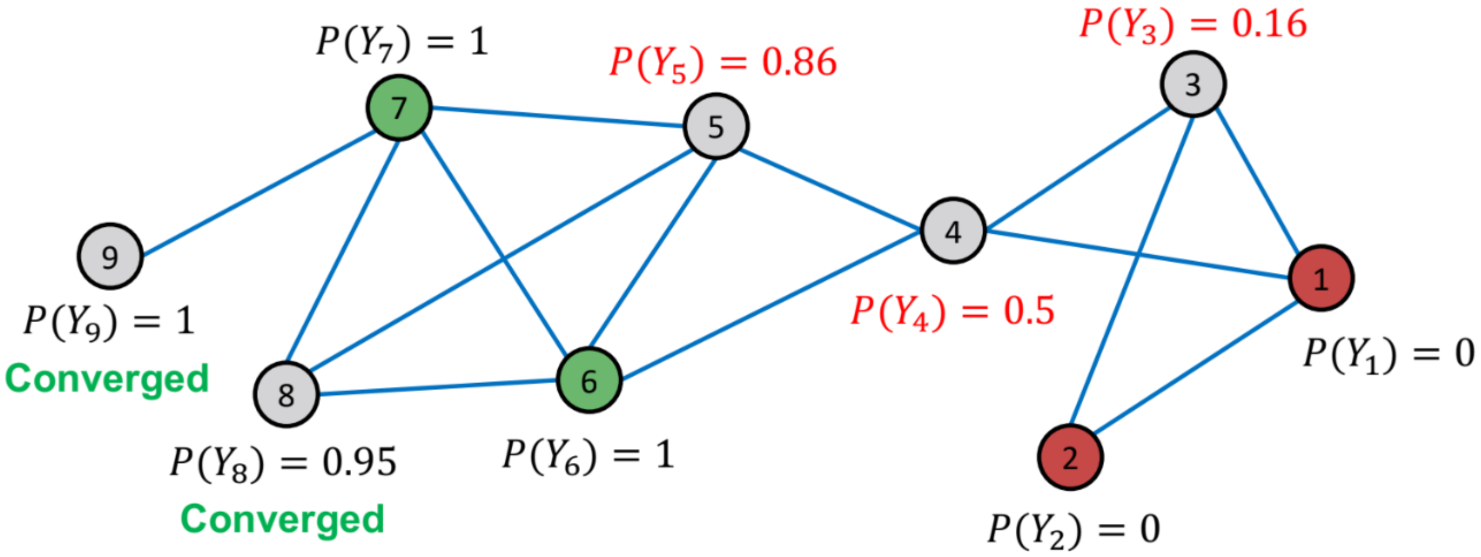
Example: After 2nd Iteration

- Update nodes with another random order
  - After 2nd iteration:



Example: After 3rd Iteration

- Update nodes with another random order
  - After 3rd iteration:

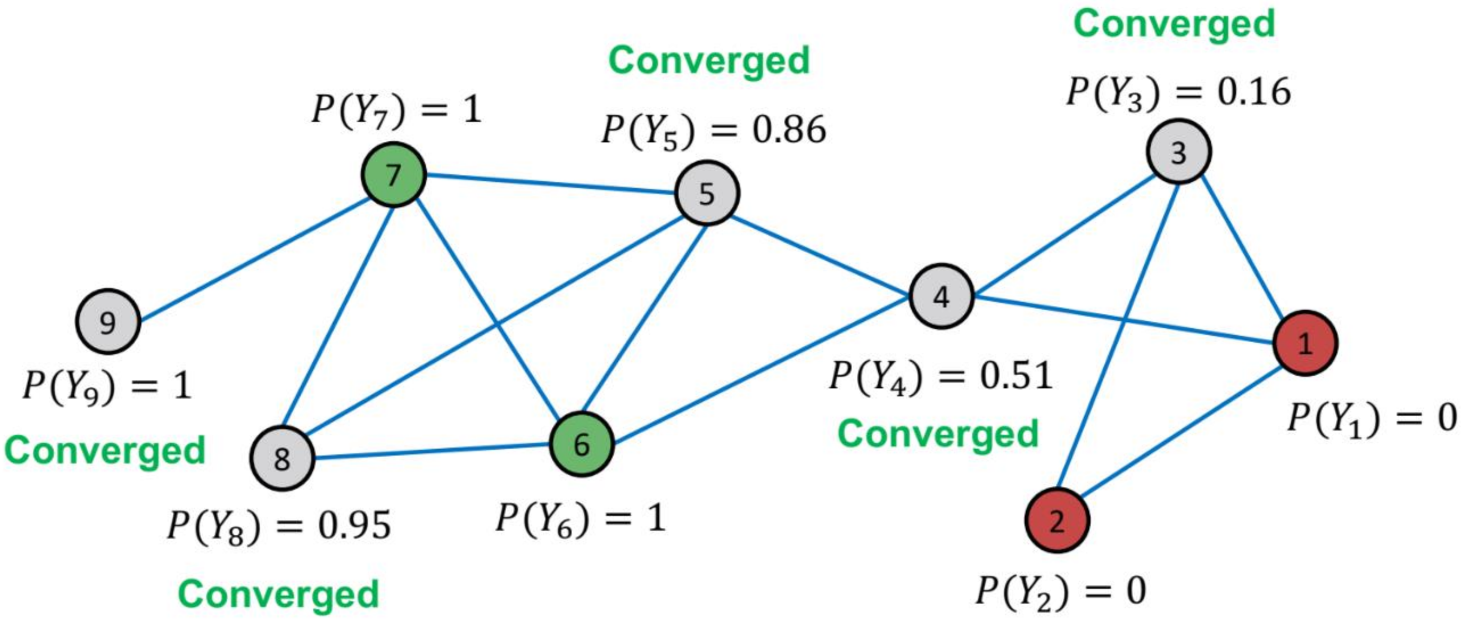


Example: Convergence

- After 4th iteration, it converged, we therefore predict:
  - Nodes 4, 5, 8, 9 belong to Class 1 $(P_{Y_v} > 0.5)$
  - Node 3 belong to Class 0 $(P_{Y_v} < 0.5)$
- **Challenges:**

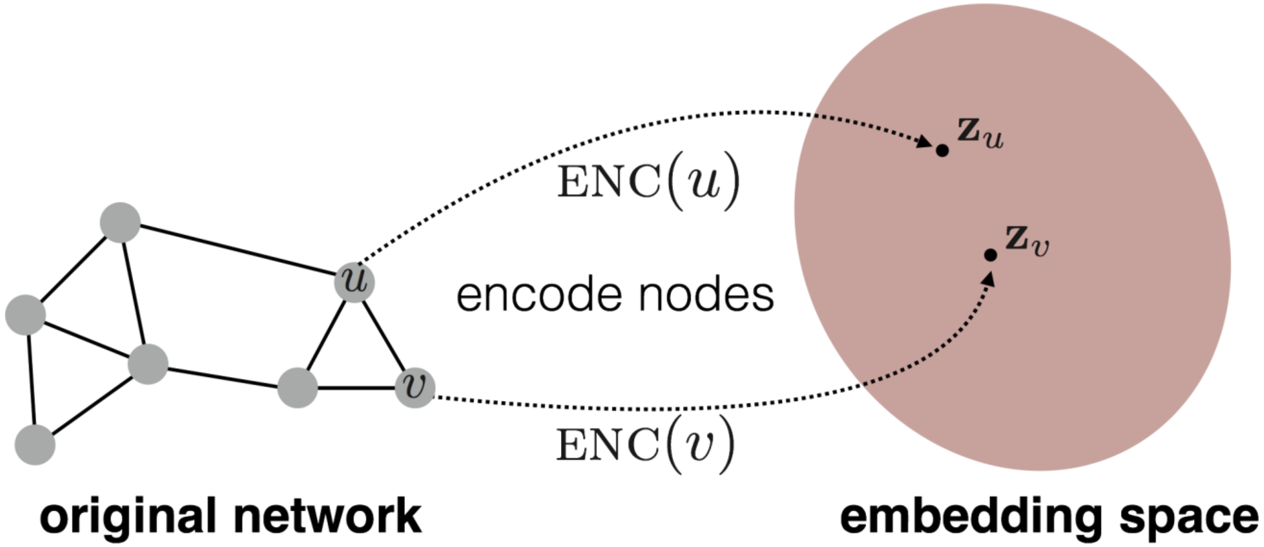
  (1) Convergence are not guaranteed.

  (2) Cannot use node feature information.



ReCap: Embedding Nodes

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

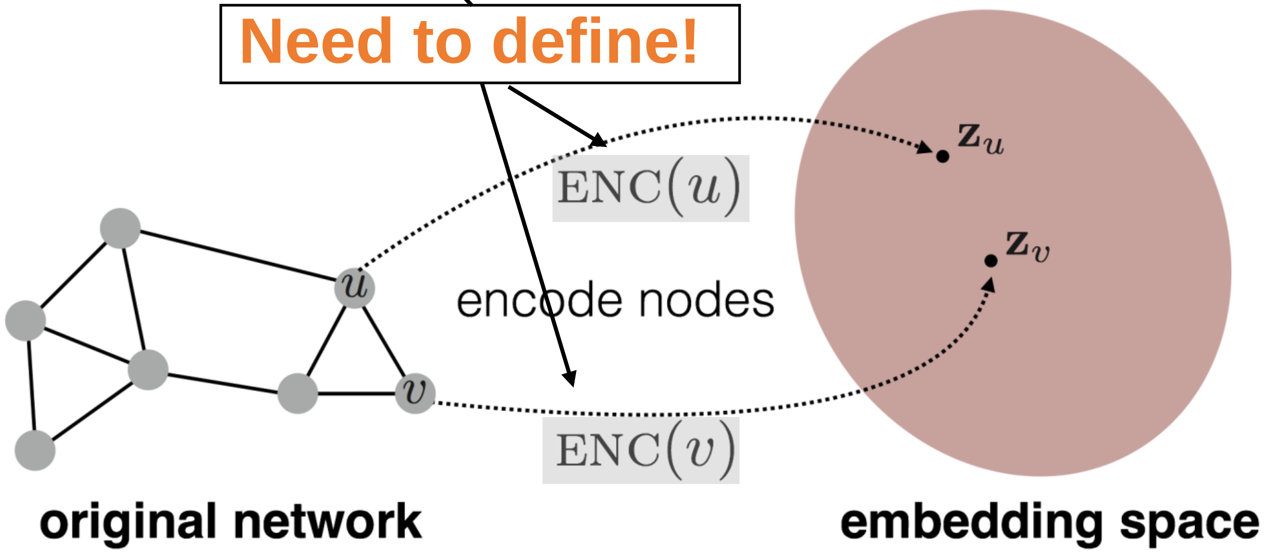


Representation Learning on Networks, snap.stanford.edu/proj/embeddings-www, WWW 2018

ReCap: Embedding Nodes

- **Goal:**

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



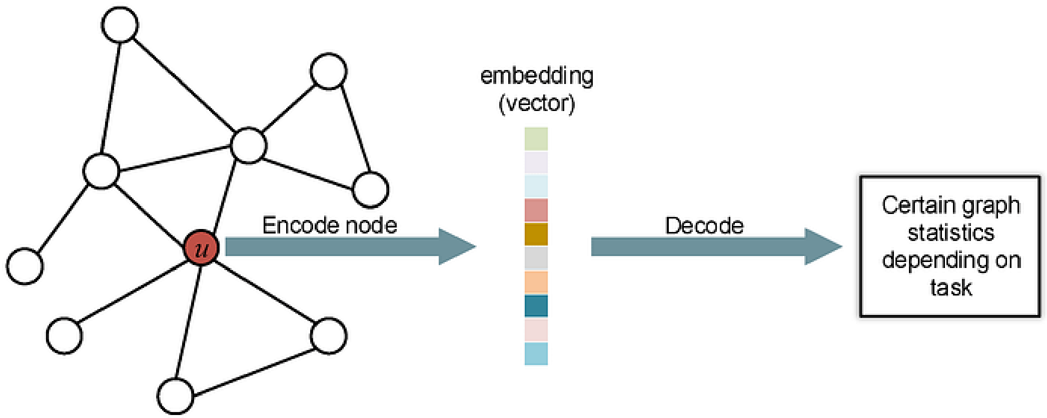
Representation Learning on Networks, snap.stanford.edu/proj/embeddings-www, WWW 2018

ReCap: Two Key Components

- Encoder: Mapping nodes → embeddings (d-dimensional vector, ENC(v) = Z_v)
- Decoder: Mapping embeddings → similarity score (dot product)
- Define a node similarity function:
  - Whether 2 nodes are close in the graph, and how close are they?

Dot product between node embedding

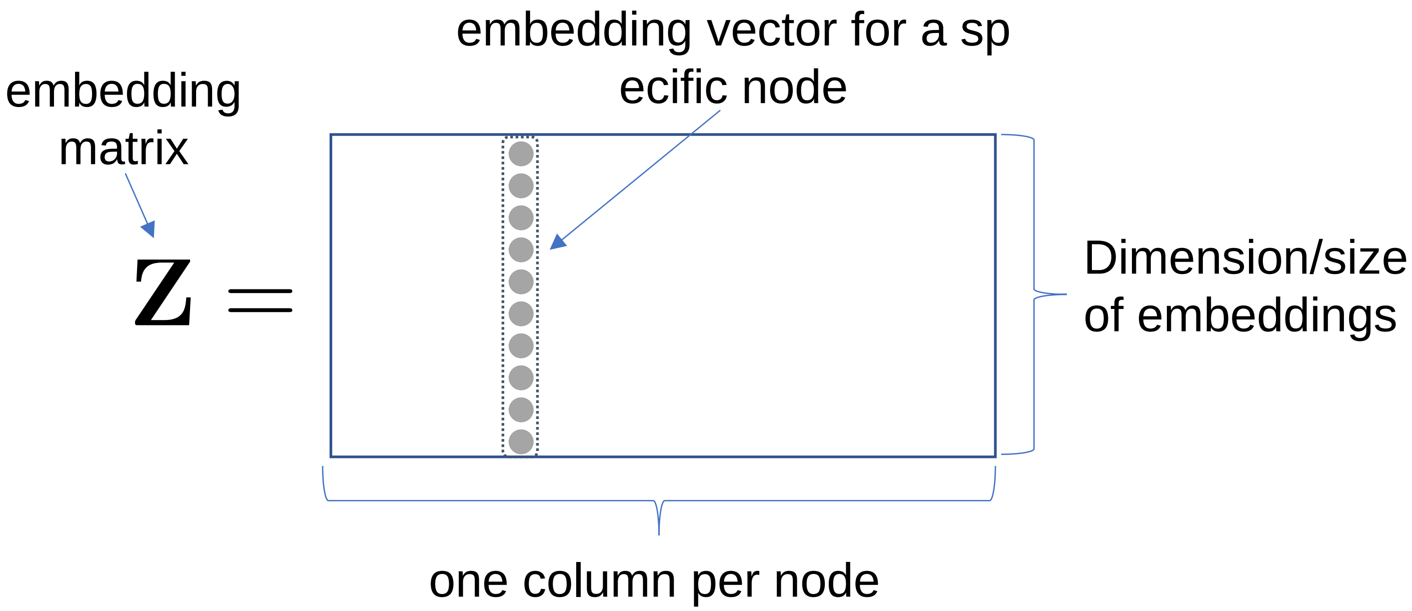
- Optimize → $$\underbrace{\text{similarity}(u,v)}_{\text{in the original network}} \approx \underbrace{\mathbf{z}_v^{\mathrm{T}}\mathbf{z}_u}_{\text{Similarity of the embedding}}$$
  - Maximize $\boldsymbol{z}_v^T\boldsymbol{z}_u$ for node pairs (u,v) that are similar.



https://medium.com/the-modern-scientist/graph-neural-networks-series-part-3-node-embedding-36613cc967d5

From “Shallow” to “Deep”

- ➢ So far, we have focused on “shallow” encoders, i.e. embedding lookups:



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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.

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

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

The Basics: Graph Neural Networks

- **Idea**: Propagate node features by exchanging info between adjacent nodes.
- Message:
  - Prepare message that will be passed to another nodes
- Aggregate and Update
  - Aggregate the coming messages
  - Update node with the aggregated message

Based on material from:

Hamilton et al. 2017. Representation Learning on Graphs: Methods and Applications. IEEE Data Engineering Bulletin on Graph Systems.

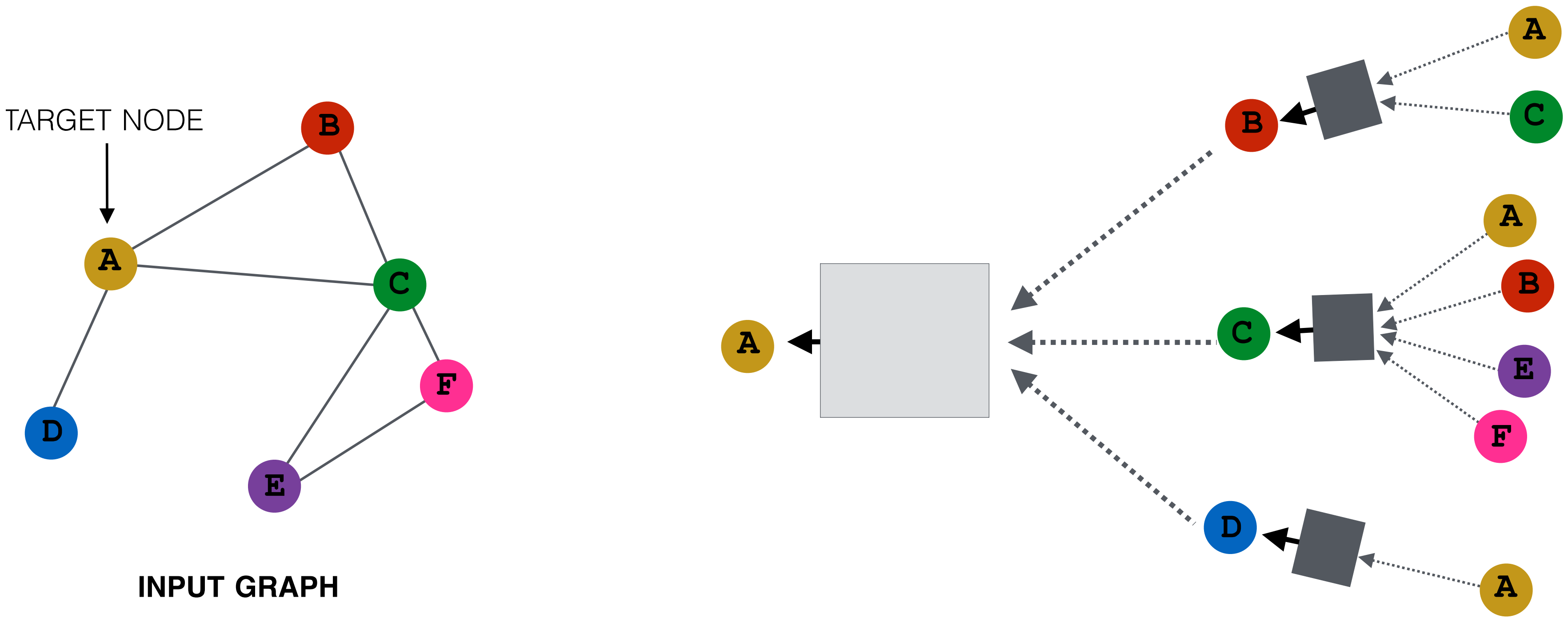
Scarselli et al. 2005. The Graph Neural Network Model. IEEE Transactions on Neural Networks.

Graph Neural Networks: Setup

- Assume we have a graph G:
  - V is the node set.
  - v: a node in V; N(v): the set of neighbors of v.
  - A is the adjacency matrix (assume binary).
  - $X \in R^{N \times d}$ 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, vector of constant 1).

Neighborhood Aggregation

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



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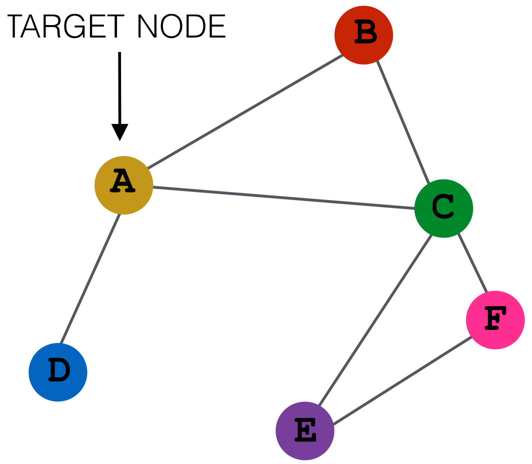
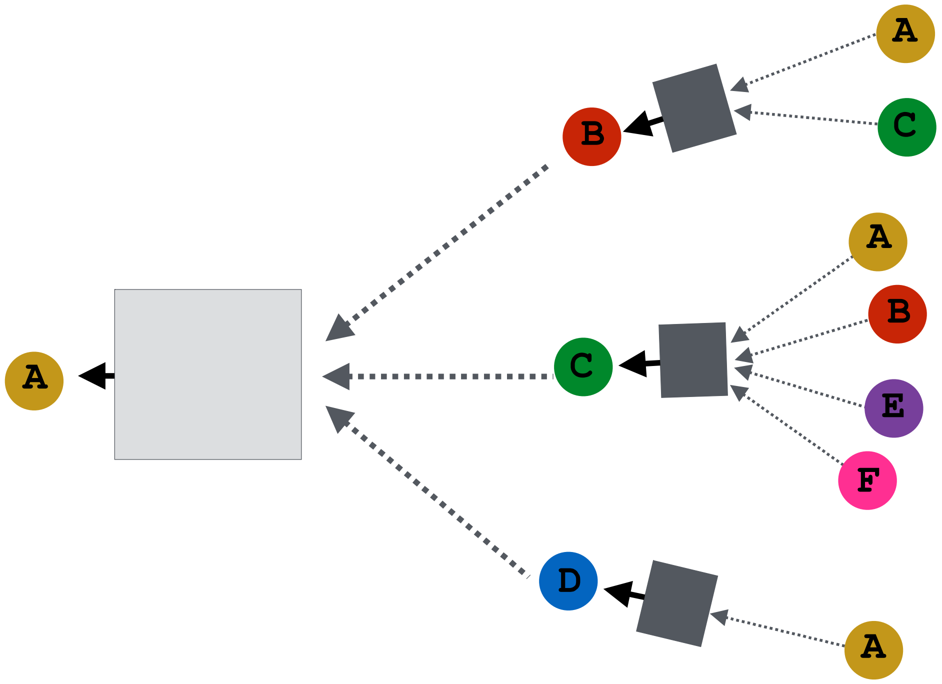
Neighborhood Aggregation

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



INPUT GRAPH



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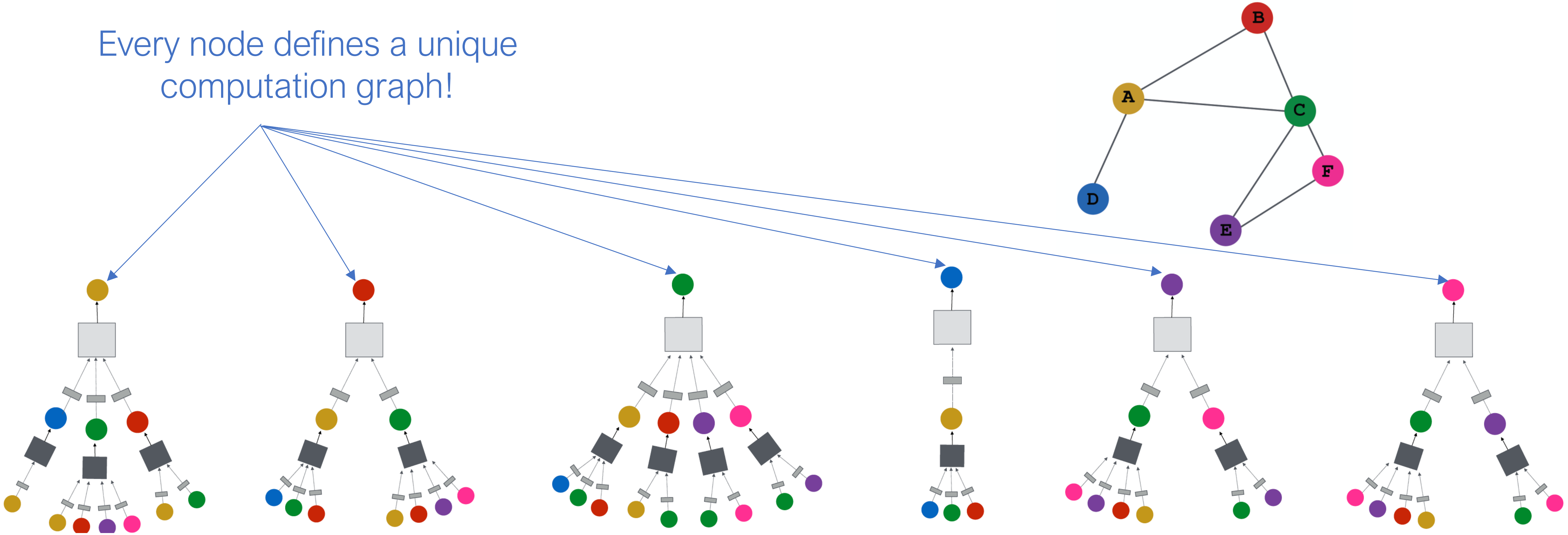
Neighborhood Aggregation

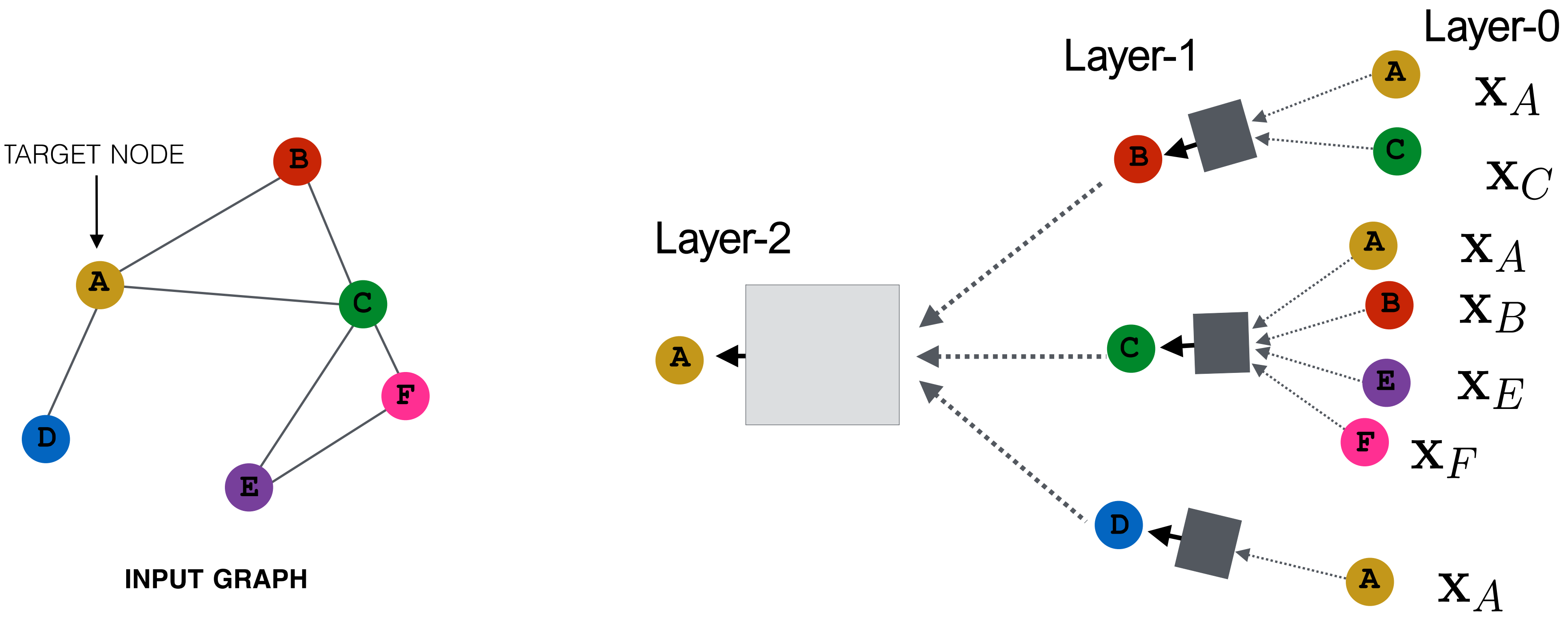
- Intuition: Network neighborhood defines a computation graph.



Every node defines a unique computation graph!

Neighborhood Aggregation

- Nodes have embeddings at each layer.
- Model can be arbitrary depth.
- “layer-0” embedding of node u is its input feature, i.e. x_u



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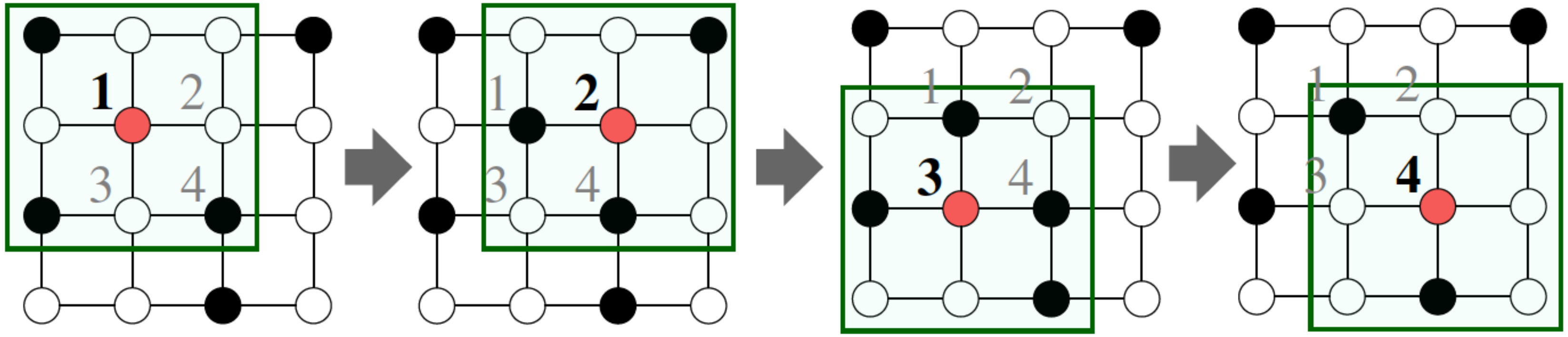
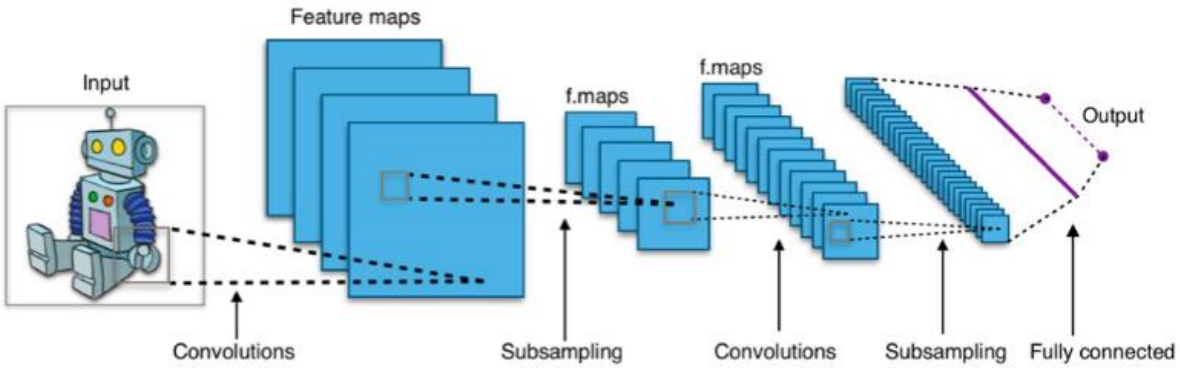
Neighborhood “Convolutions”

- Neighborhood aggregation can be viewed as a center-surround filter.
  - Same as CNN on an image:

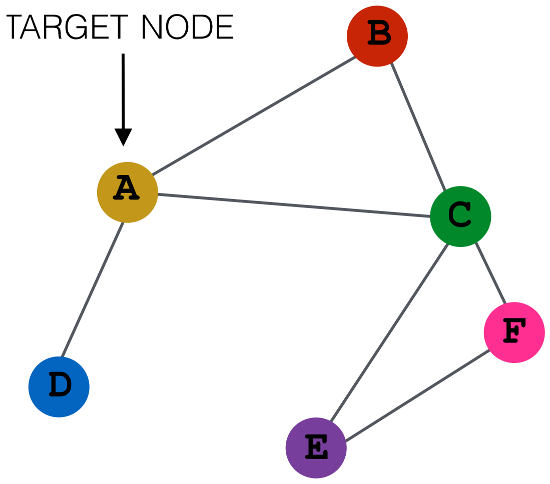




- Mathematically related to spectral graph convolutions.

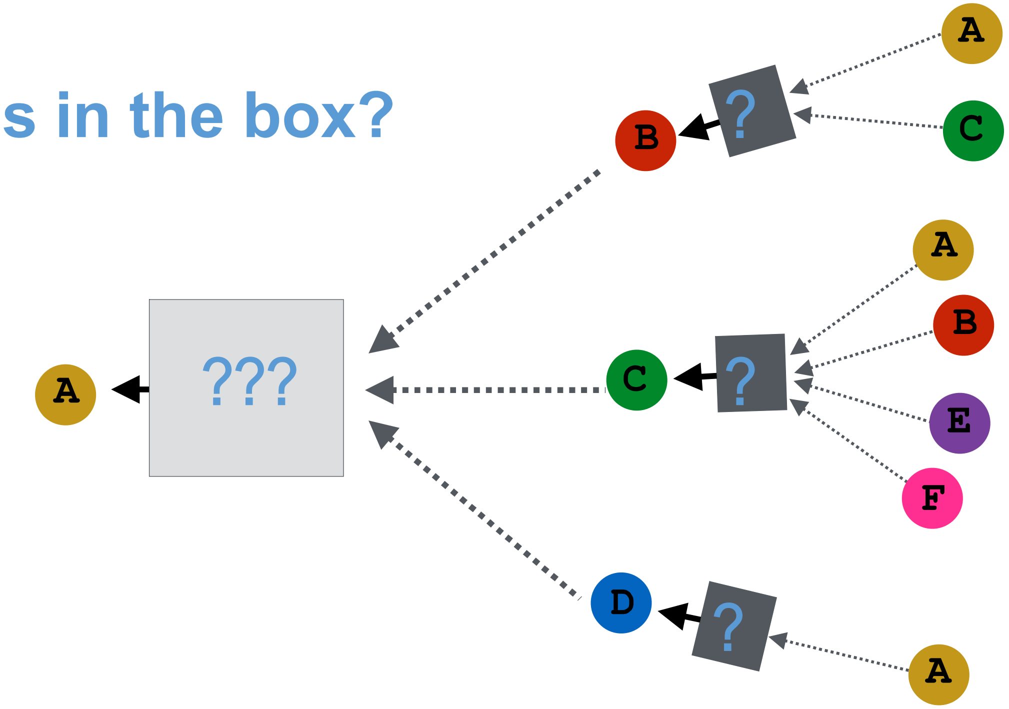
Neighborhood Aggregation

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



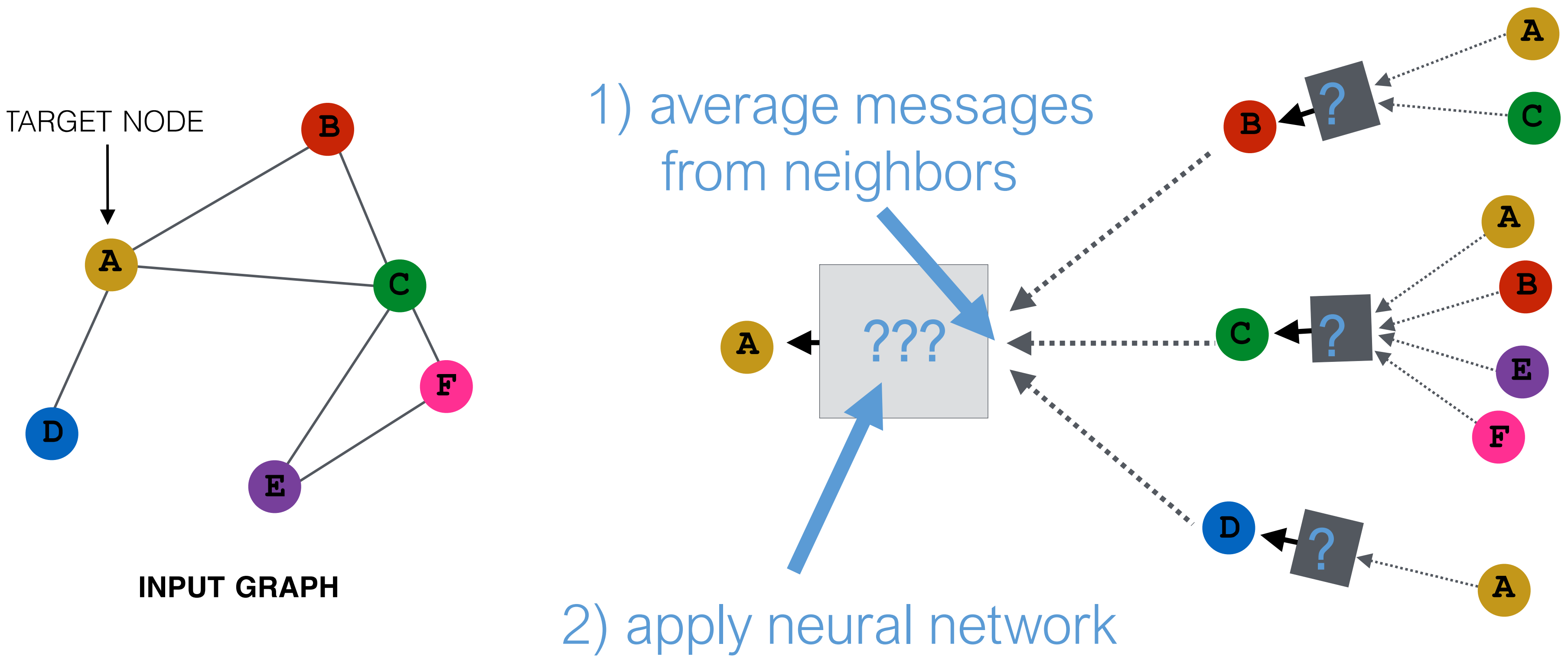
INPUT GRAPH

what's in the box?



Neighborhood Aggregation

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



Neighborhood Aggregation: Mathematics

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

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

Initial “layer 0” embeddings are equal to node features

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|} + \mathbf{B}_k \mathbf{h}_v^{k-1}\right), \quad \forall k > 0$$

previous layer embedding of v

kth layer embedding of v

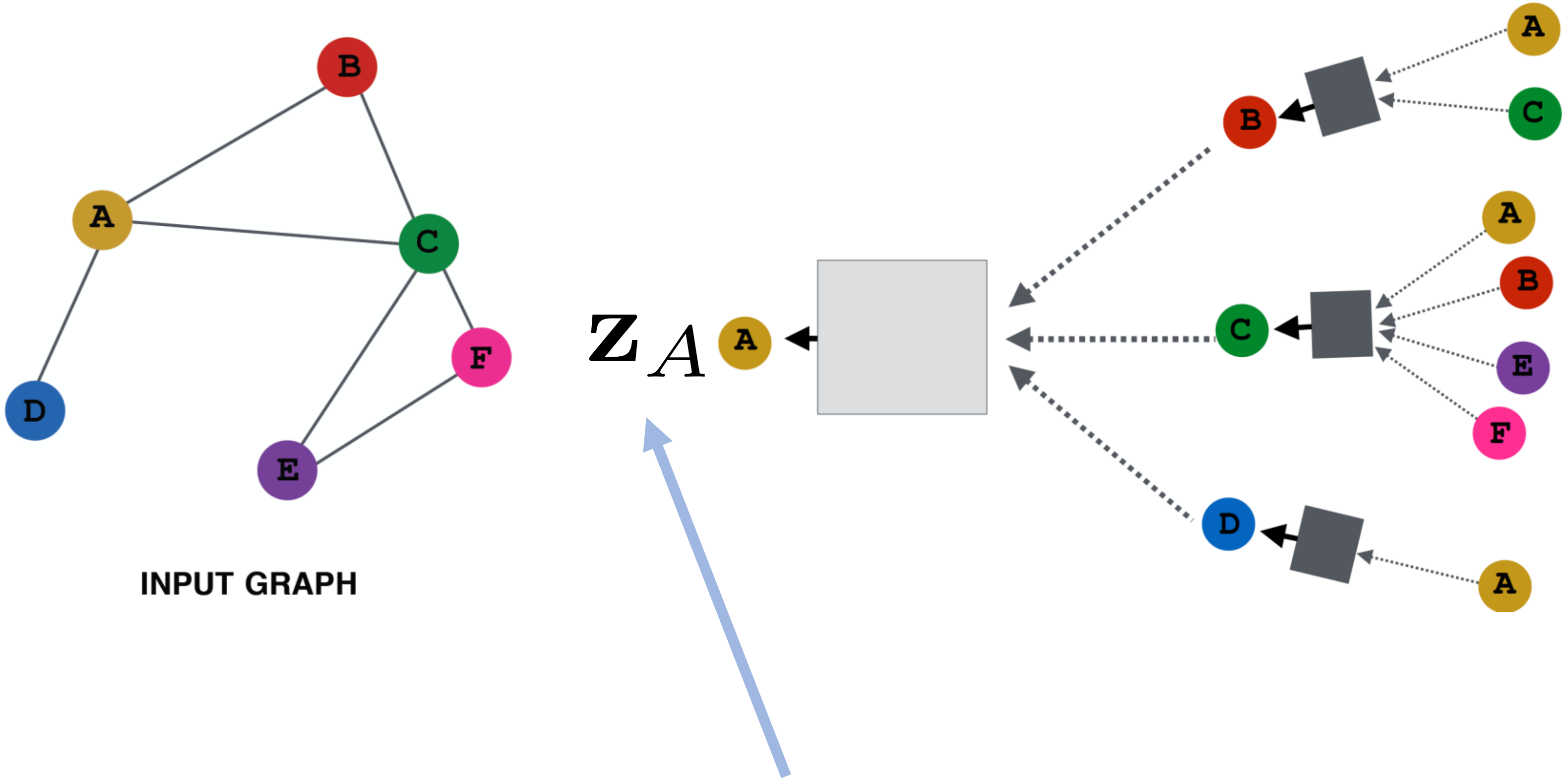
non-linearity (e.g., ReLU or tanh)

average of neighbor’s previous layer embeddings

Representation Learning on Networks, snap.stanford.edu/proj/embeddings-www, WWW 2018

Training the Model

- ➢ How do we train the model to generate “high-quality” embeddings?



Need to define a loss function on the embeddings, $\mathcal{L}(z_u)$**!**

Training the Model

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

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

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

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

- 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 based on:
  - Random walks (node2vec, DeepWalk).
  - Graph factorization.
  - i.e., train the model so that “similar” nodes have similar embeddings.

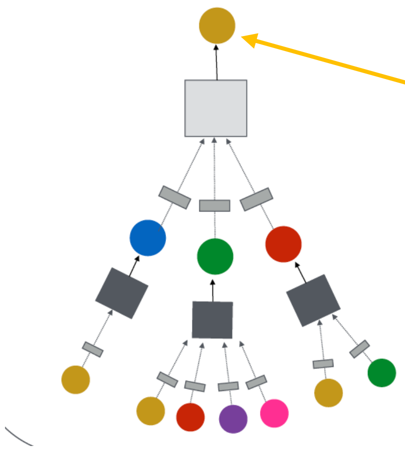
Overview of Model

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

classification weights

Human or bot?

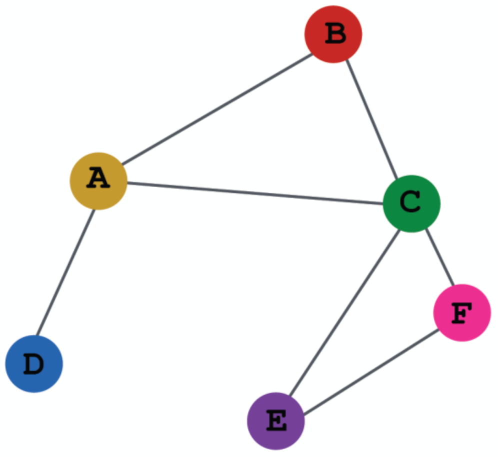
$$\mathcal{L} = \sum_{v \in V} y_v \log(\sigma(\mathbf{z}_v^\top \boldsymbol{\theta})) + (1 - y_v) \log(1 - \sigma(\mathbf{z}_v^\top \boldsymbol{\theta}))$$



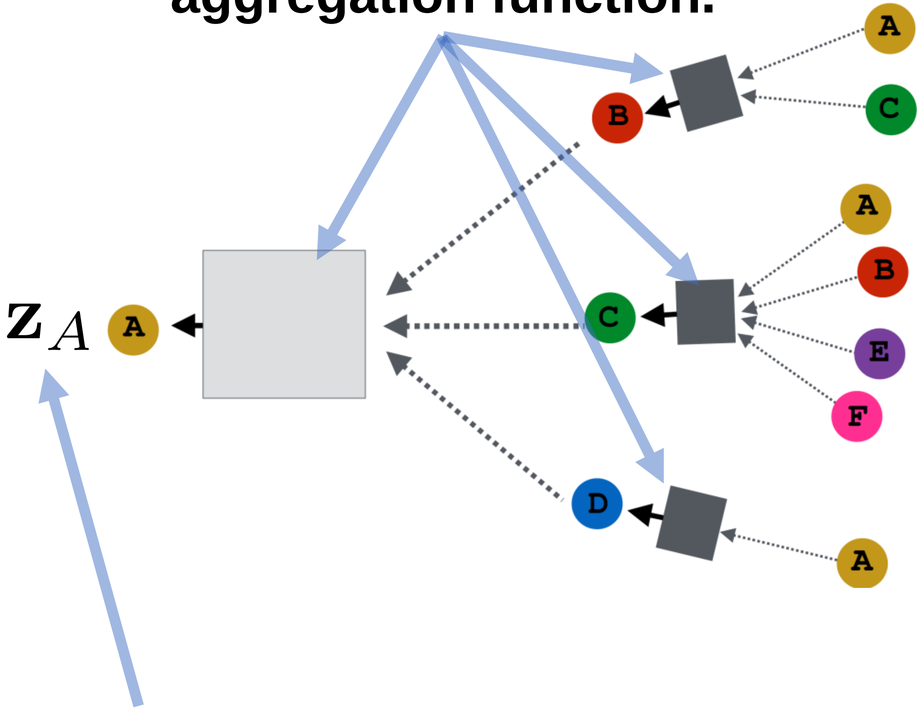
output node embedding

node class label

Overview of Model Design



INPUT GRAPH

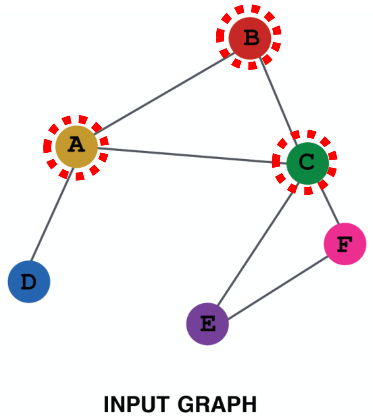


1) Define a neighborhood aggregation function.

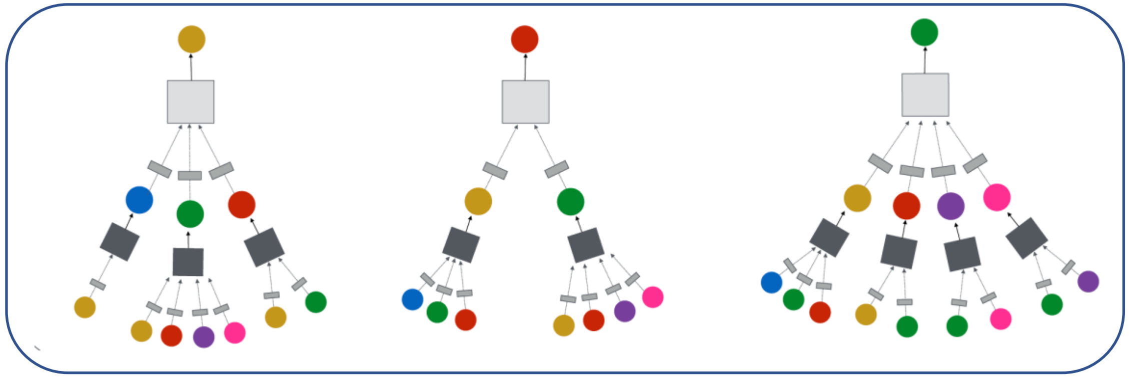
2) Define a loss function on the embeddings, $L(z_u)$

Representation Learning on Networks, snap.stanford.edu/proj/embeddings-www, WWW 2018

Overview of Model Design



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



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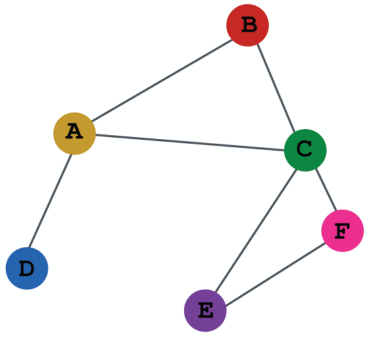
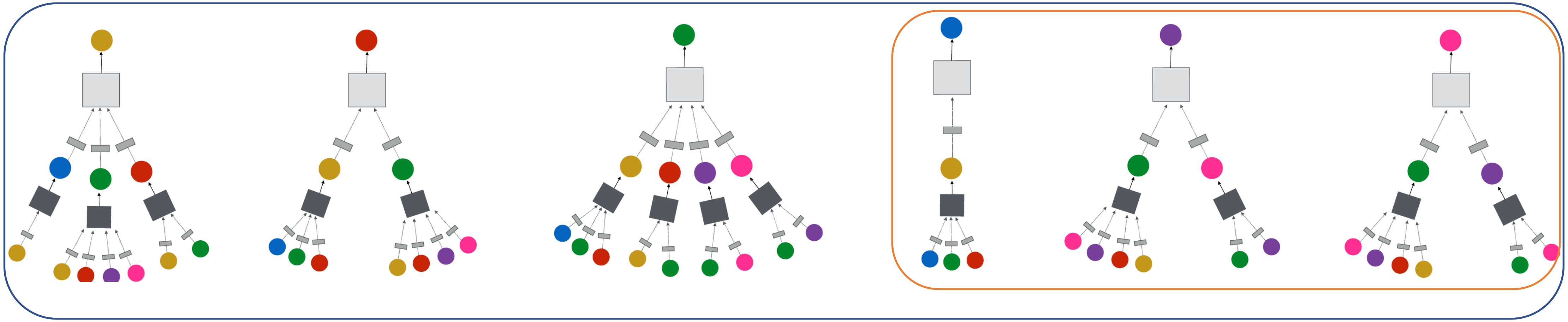
Overview of Model Design



INPUT GRAPH

4) Generate embeddings for nodes as needed

Even for nodes we never trained on!!!!



Graph Convolutional Networks

- GCN are slight variation on the neighborhood aggregation idea.

Basic Neighborhood Aggregation

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|} + \mathbf{B}_k \mathbf{h}_v^{k-1}\right), \ \forall k > 0$$

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

Kipf et al., 2017. Semi-supervised Classification with Graph Convolutional Networks. ICLR

Graph Convolutional Networks

- Empirically, 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

Kipf et al., 2017. Semi-supervised Classification with Graph Convolutional Networks. ICLR

Graph Convolutional Networks: 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

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

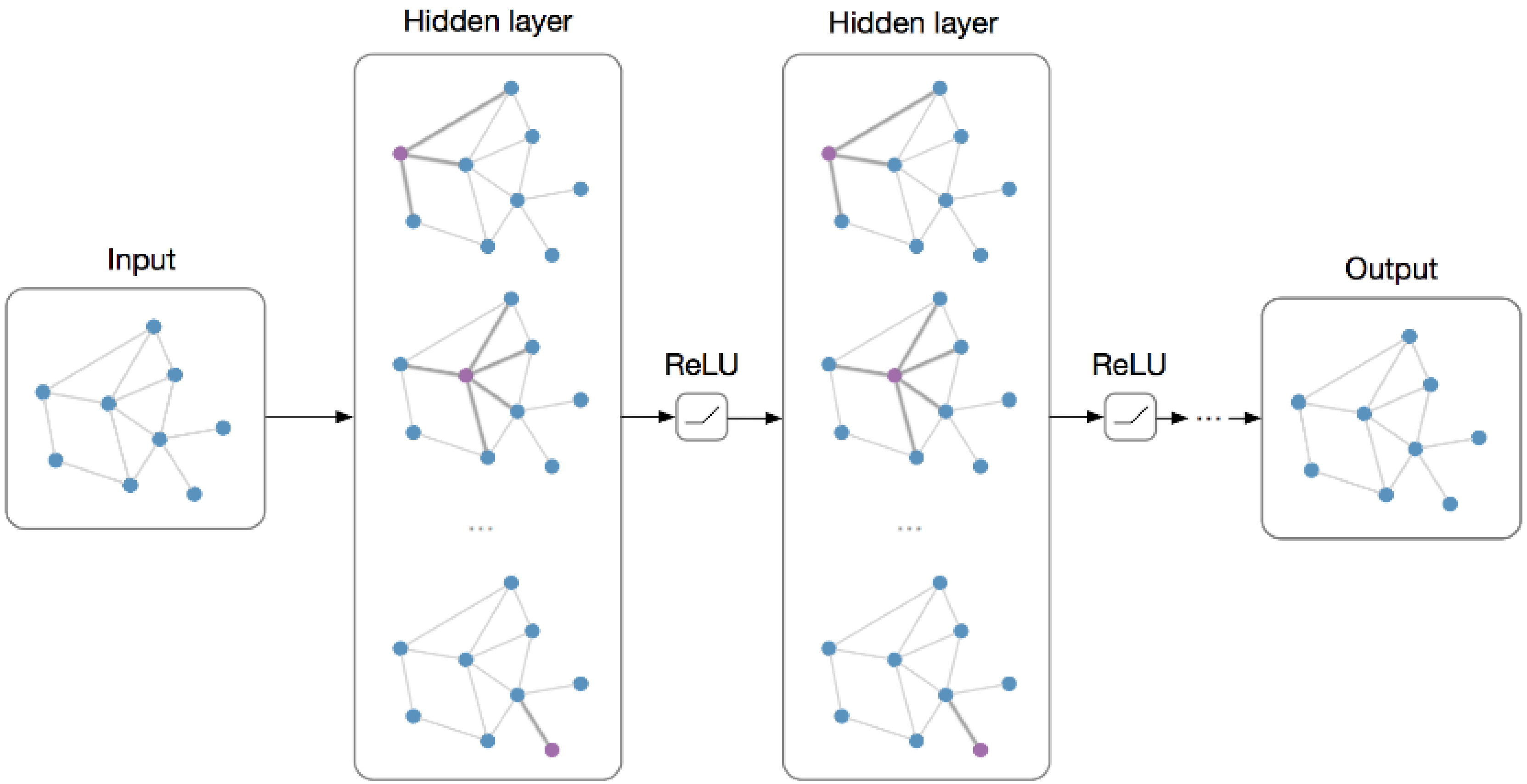
$$\mathbf{D}_{ii} = \sum_j \mathbf{A}_{i,j}$$

- O(|E|) time complexity overall.

Kipf et al., 2017. Semi-supervised Classification with Graph Convolutional Networks. ICLR

Graph Convolutional Networks

- Architecture model design:



Kipf et al., 2017. Semi-supervised Classification with Graph Convolutional Networks. ICLR

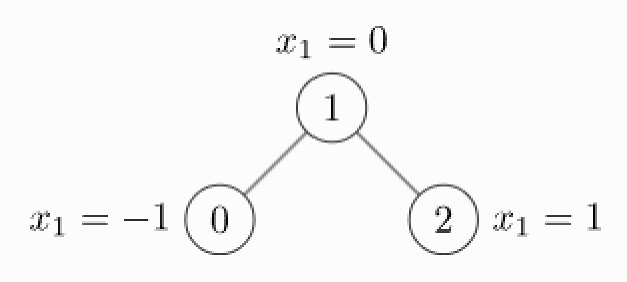
Graph Neural Network Libraries: Introduction

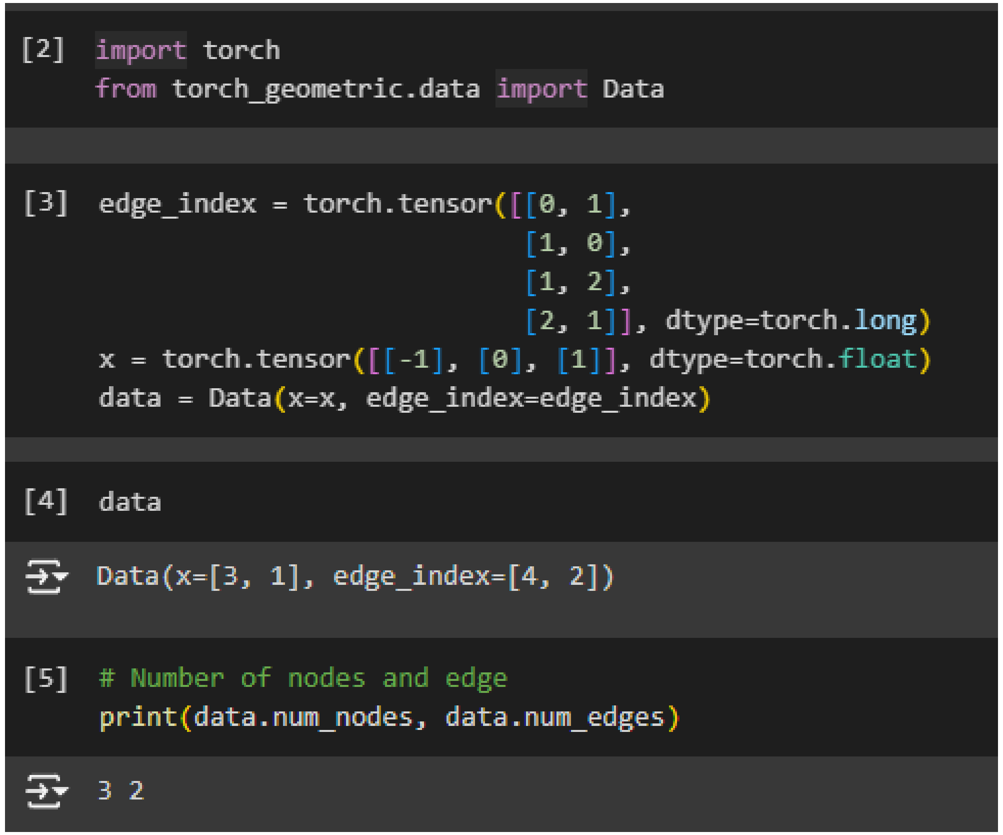
- PyTorch Geometric
  - PyG is a library built upon PyTorch to easily write and train Graph Neural Networks (GNNs) for a wide range of applications related to structured data.
  - PyG consists of various methods for deep learning on graphs from a variety of published papers.
- DGL (Deep Graph Library)
  - DGL is a Python package built for easy implementation of graph neural network model family, on top of existing DL frameworks
  - It has a Diverse Ecosystem, including bioinformatics and cheminformatics, and many others.
- Note that:
  - Both libraries already contain a lot of useful datasets.
  - Both libraries only represent a graph under edge index.

PyTorch Geometric: Creating graph datasets

- Construct a simplified Graph
  - Note that PyG only represent Graph with **edge index**

E.g., a simple example of an unweighted and undirected graph with three nodes and four edges. Each node contains exactly one feature





```
[2]  import torch
     from torch_geometric.data import Data
```

```
[3]  edge_index = torch.tensor([[0, 1],
                                [1, 0],
                                [1, 2],
                                [2, 1]], dtype=torch.long)
     x = torch.tensor([[-1], [0], [1]], dtype=torch.float)
     data = Data(x=x, edge_index=edge_index)
```

```
[4]  data
```

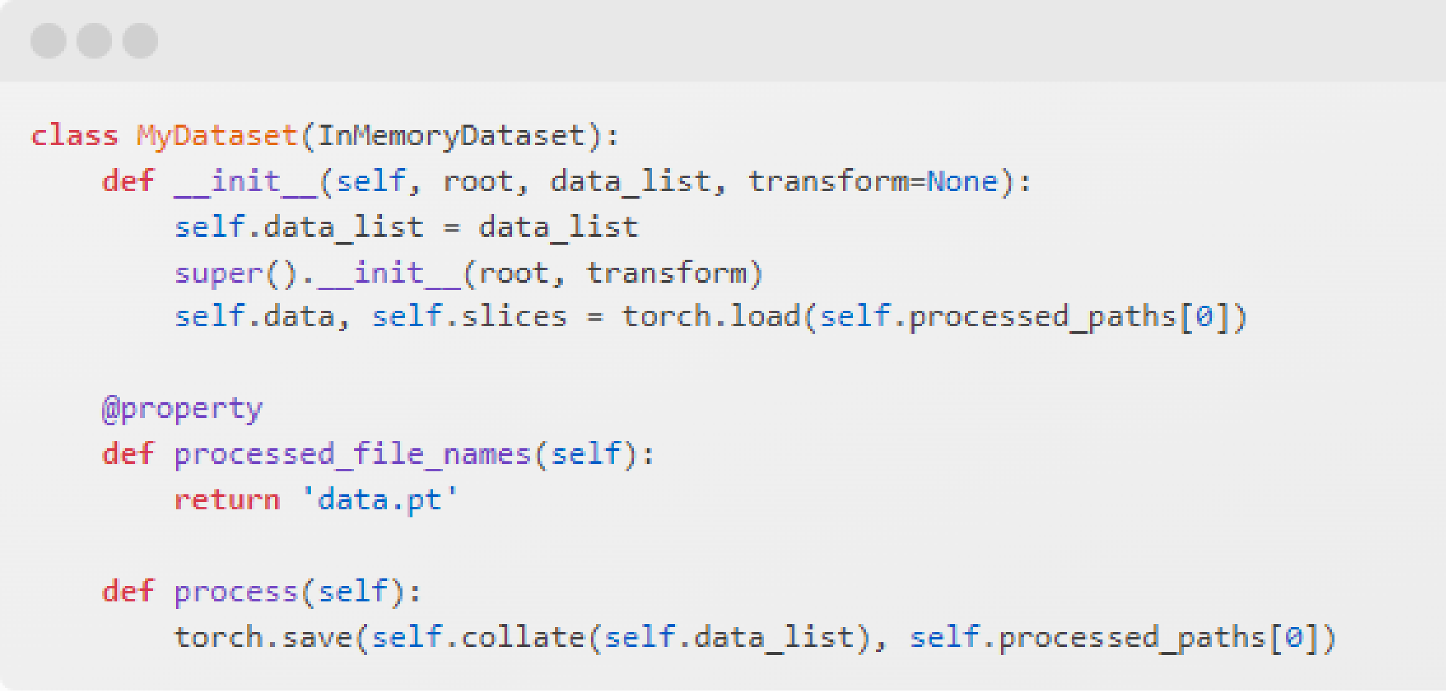
```
Data(x=[3, 1], edge_index=[4, 2])
```

```
[5]  # Number of nodes and edge
     print(data.num_nodes, data.num_edges)
```

```
3 2
```

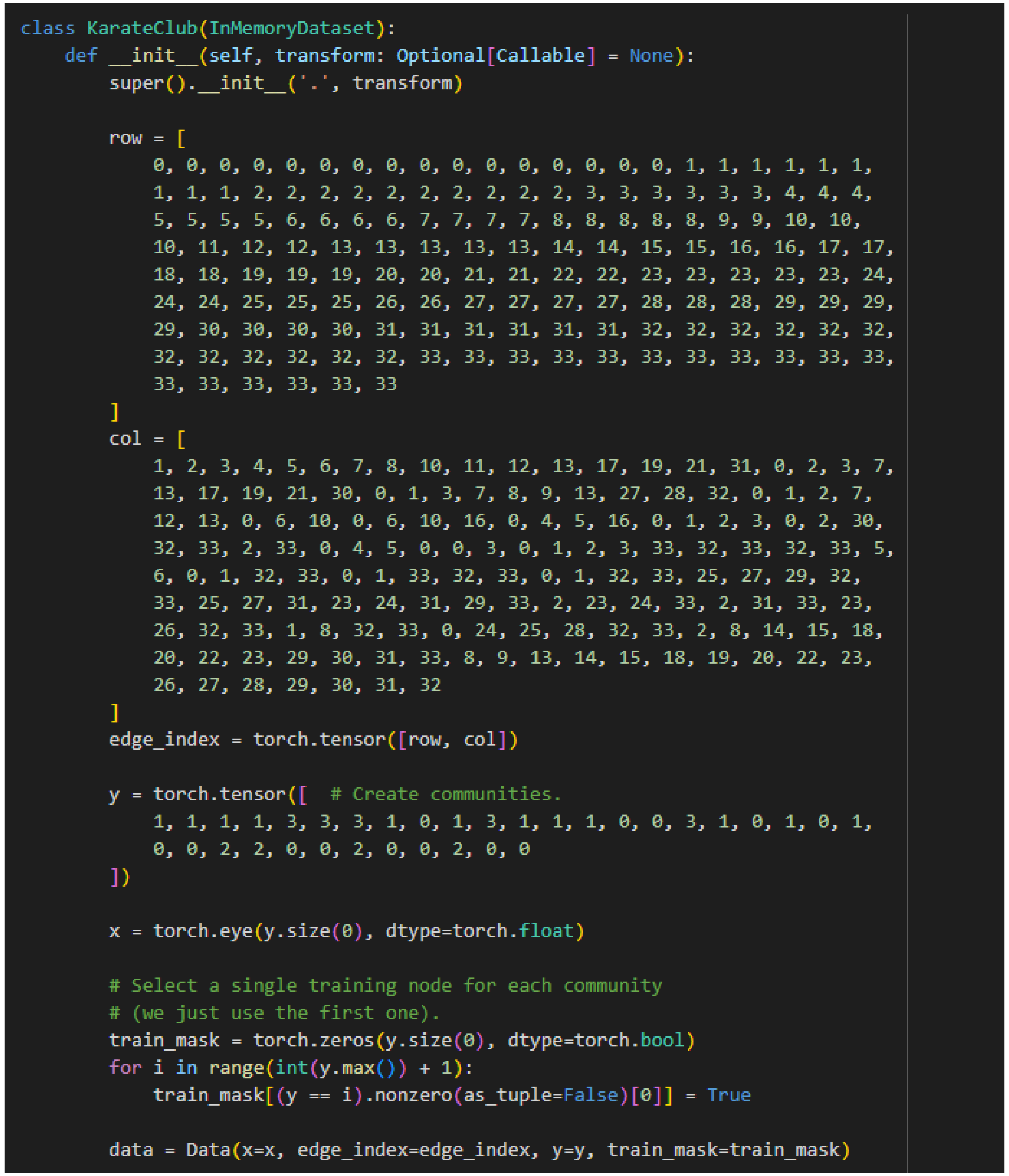
PyTorch Geometric: Creating our own Graph Datasets

- Although PyG already contains a lot of useful datasets, we can create our own dataset with self-recorded or non-publicly available data.

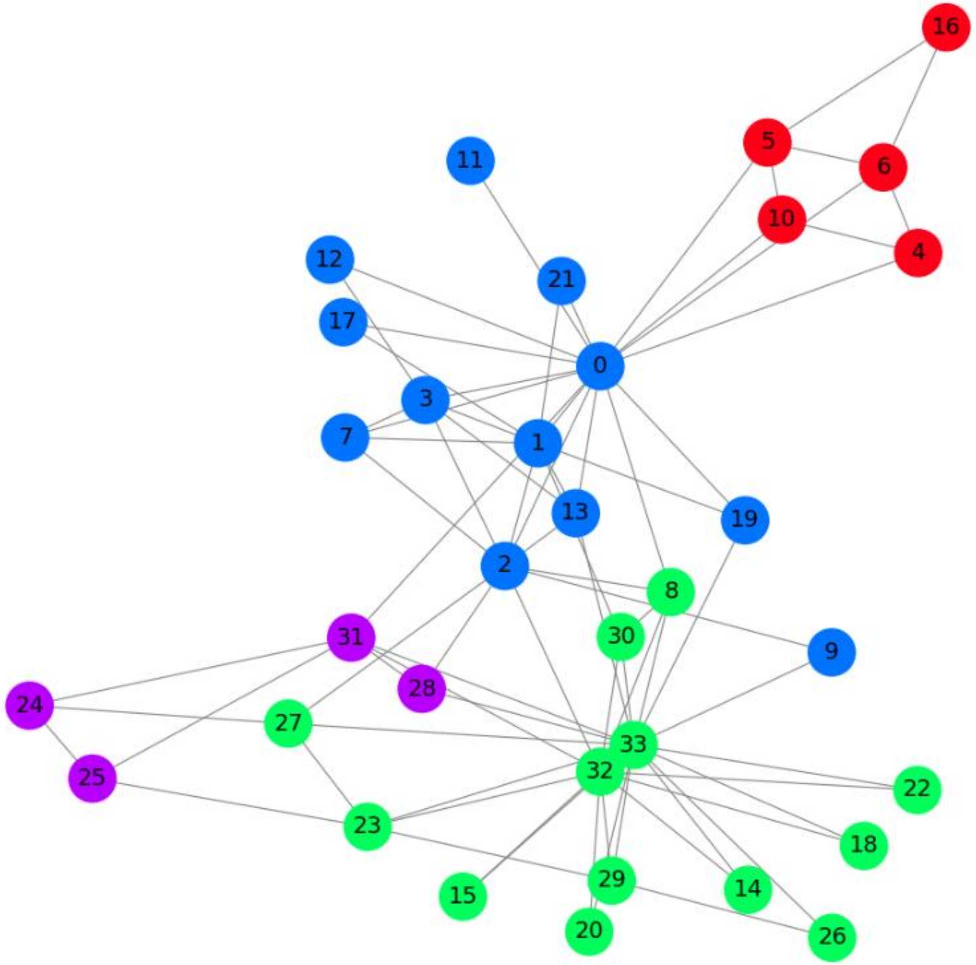


```python
class MyDataset(InMemoryDataset):
    def __init__(self, root, data_list, transform=None):
        self.data_list = data_list
        super().__init__(root, transform)
        self.data, self.slices = torch.load(self.processed_paths[0])

    @property
    def processed_file_names(self):
        return 'data.pt'

    def process(self):
        torch.save(self.collate(self.data_list), self.processed_paths[0])
```

PyTorch Geometric: Creating Graph Datasets with Karate Graph



```
class KarateClub(InMemoryDataset):
    def __init__(self, transform: Optional[Callable] = None):
        super().__init__('.', transform)

        row = [
            0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1,
            1, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 3, 3, 3, 3, 3, 3, 4, 4, 4,
            5, 5, 5, 5, 6, 6, 6, 6, 7, 7, 7, 7, 8, 8, 8, 8, 8, 9, 9, 10, 10,
            10, 11, 12, 12, 13, 13, 13, 13, 13, 14, 14, 15, 15, 16, 16, 17, 17,
            18, 18, 19, 19, 19, 20, 20, 21, 21, 22, 22, 23, 23, 23, 23, 23, 24,
            24, 24, 25, 25, 25, 26, 26, 27, 27, 27, 27, 28, 28, 28, 29, 29, 29,
            29, 30, 30, 30, 30, 31, 31, 31, 31, 31, 31, 32, 32, 32, 32, 32, 32,
            32, 32, 32, 32, 32, 32, 33, 33, 33, 33, 33, 33, 33, 33, 33, 33, 33,
            33, 33, 33, 33, 33, 33
        ]
        col = [
            1, 2, 3, 4, 5, 6, 7, 8, 10, 11, 12, 13, 17, 19, 21, 31, 0, 2, 3, 7,
            13, 17, 19, 21, 30, 0, 1, 3, 7, 8, 9, 13, 27, 28, 32, 0, 1, 2, 7,
            12, 13, 0, 6, 10, 0, 6, 10, 16, 0, 4, 5, 16, 0, 1, 2, 3, 0, 2, 30,
            32, 33, 2, 33, 0, 4, 5, 0, 0, 3, 0, 1, 2, 3, 33, 32, 33, 32, 33, 5,
            6, 0, 1, 32, 33, 0, 1, 33, 32, 33, 0, 1, 32, 33, 25, 27, 29, 32,
            33, 25, 27, 31, 23, 24, 31, 29, 33, 2, 23, 24, 33, 2, 31, 33, 23,
            26, 32, 33, 1, 8, 32, 33, 0, 24, 25, 28, 32, 33, 2, 8, 14, 15, 18,
            20, 22, 23, 29, 30, 31, 33, 8, 9, 13, 14, 15, 18, 19, 20, 22, 23,
            26, 27, 28, 29, 30, 31, 32
        ]
        edge_index = torch.tensor([row, col])

        y = torch.tensor([  # Create communities.
            1, 1, 1, 1, 3, 3, 3, 1, 0, 1, 3, 1, 1, 1, 0, 0, 3, 1, 0, 1, 0, 1,
            0, 0, 2, 2, 0, 0, 2, 0, 0, 2, 0, 0
        ])

        x = torch.eye(y.size(0), dtype=torch.float)

        # Select a single training node for each community
        # (we just use the first one).
        train_mask = torch.zeros(y.size(0), dtype=torch.bool)
        for i in range(int(y.max()) + 1):
            train_mask[(y == i).nonzero(as_tuple=False)[0]] = True

        data = Data(x=x, edge_index=edge_index, y=y, train_mask=train_mask)
```



Q A

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