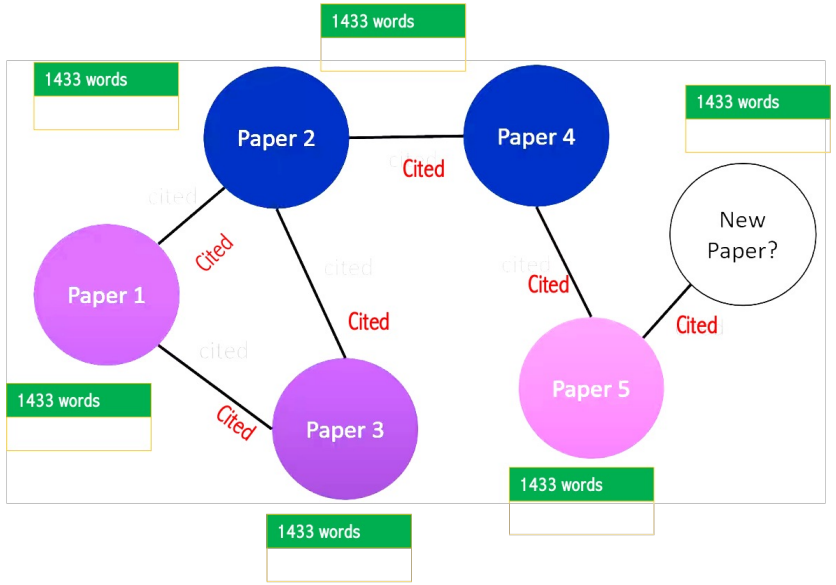
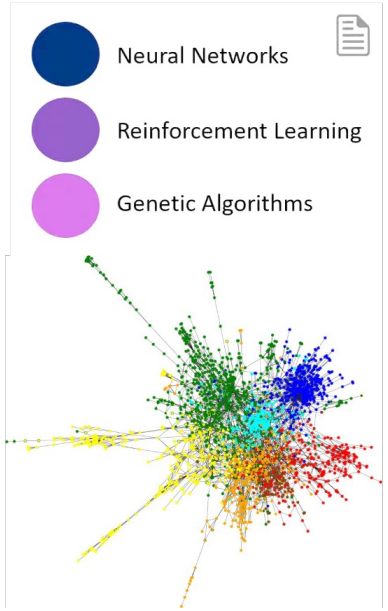
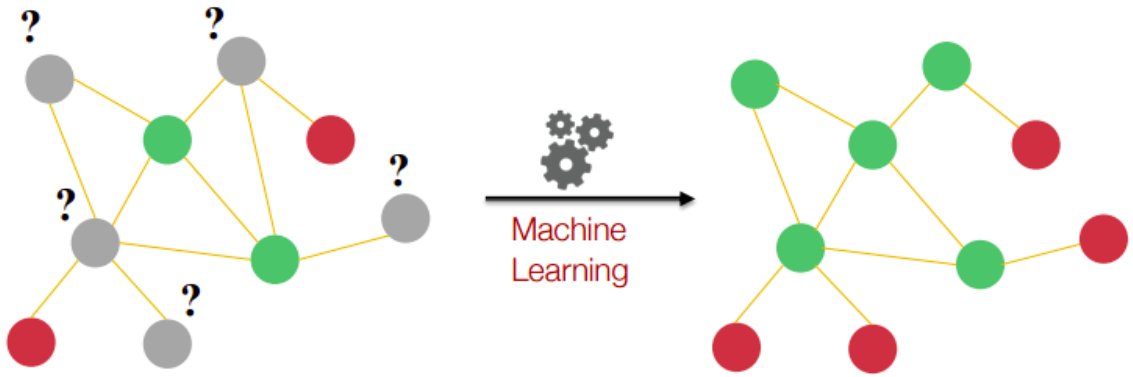
AI VIETNAM
All-in-One Course

Introduction to Graph Neural Network
(Node Classification: Cora Citation Dataset)







Vinh Dinh Nguyen
PhD in Computer Science

Outline

- Objective
- Introduction to Graph Data
- Graph Data with Neural Network
- Node Classification Problem: Cora Citation Dataset
- Summary

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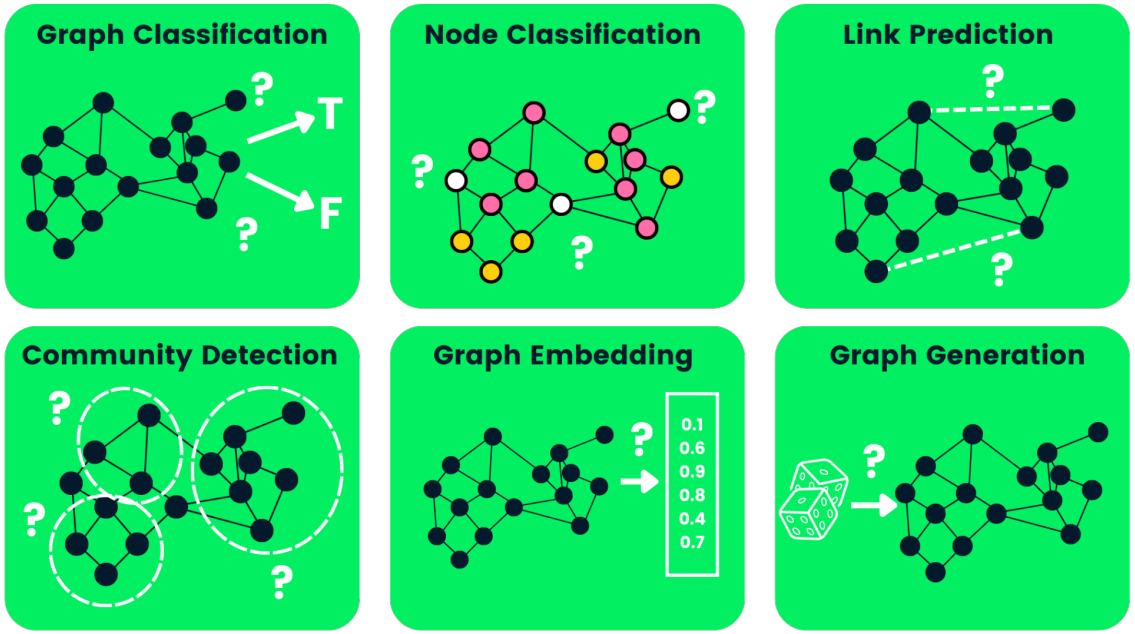
Objective



1. What is Graph Data Around Us
2. Understand Graph Neural Network
3. Understand Graph Convolutional Neural Network
4. Node Classification with Cora Citation Dataset

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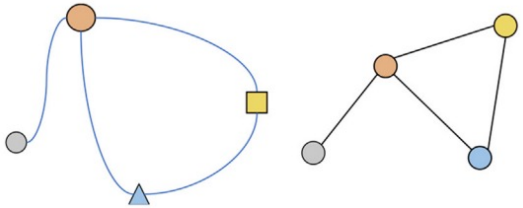
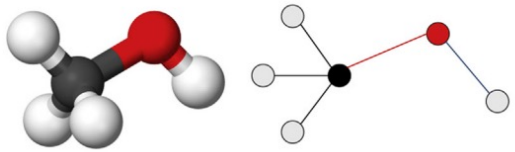
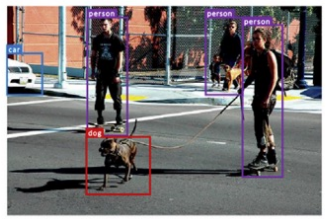
Applications of GNNs

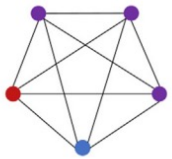


(a) Physics

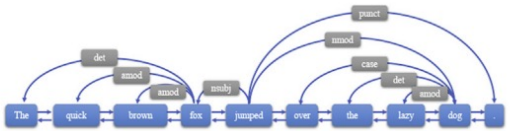


(b) Molecule

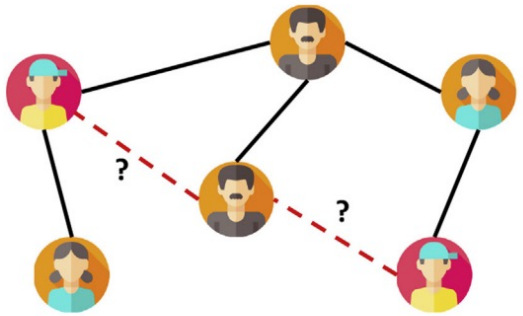




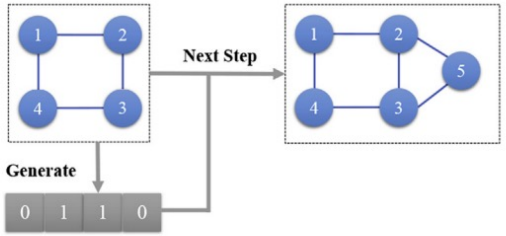
(c) Image



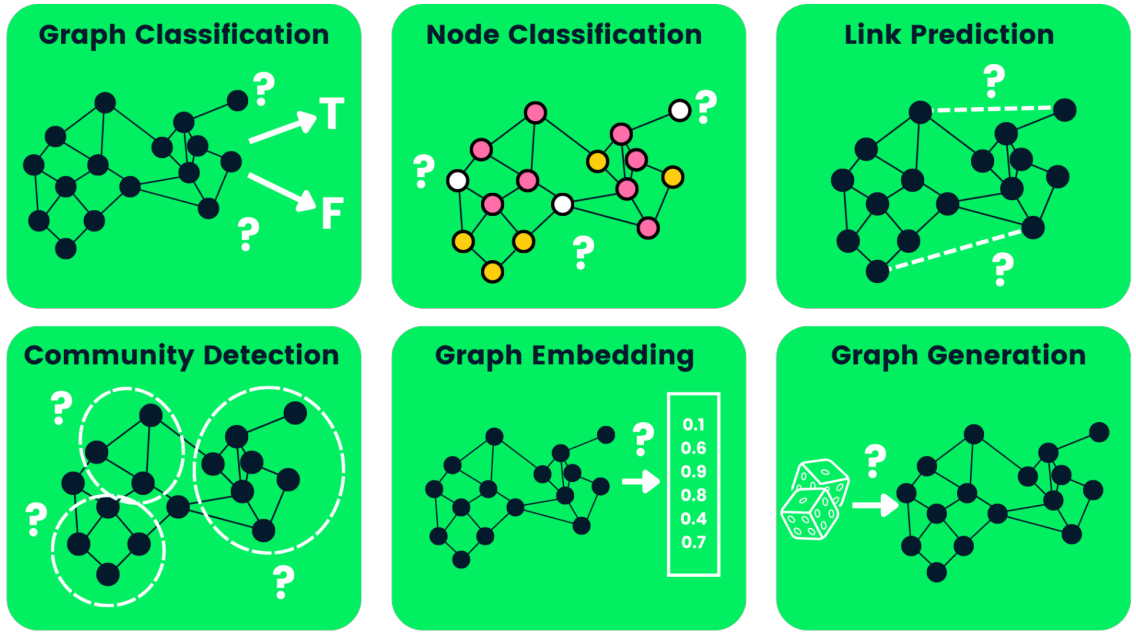
(d) Text



(e) Social Network

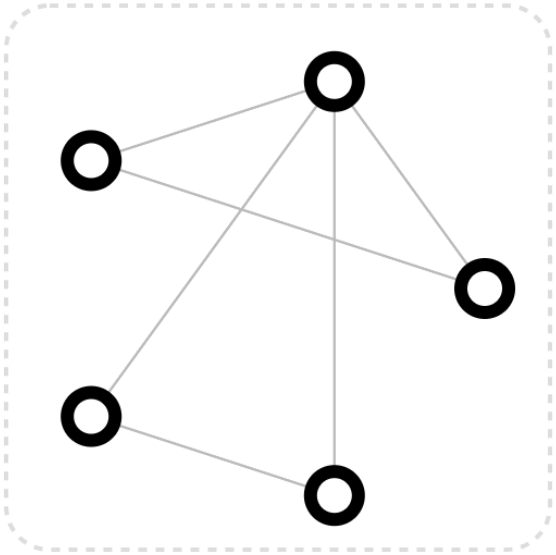


(f) Generation

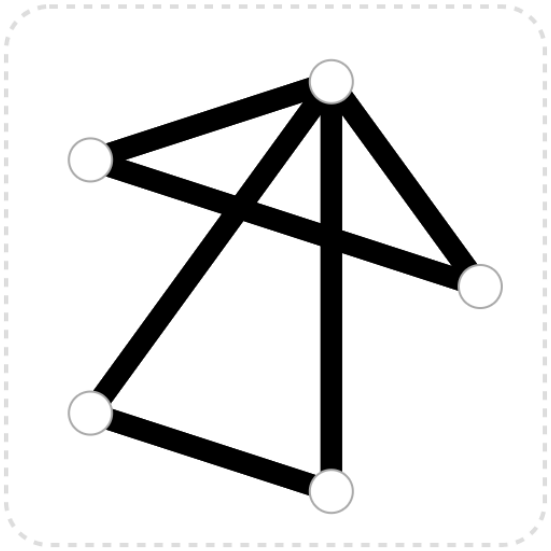


Graph Definition

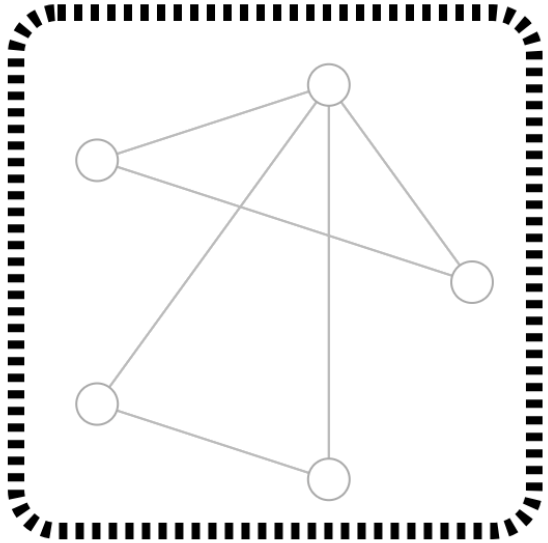
A graph represents the relations (edges) between a collection of entities (nodes).



V Vertex (or node) attributes
e.g., node identity, number of neighbors

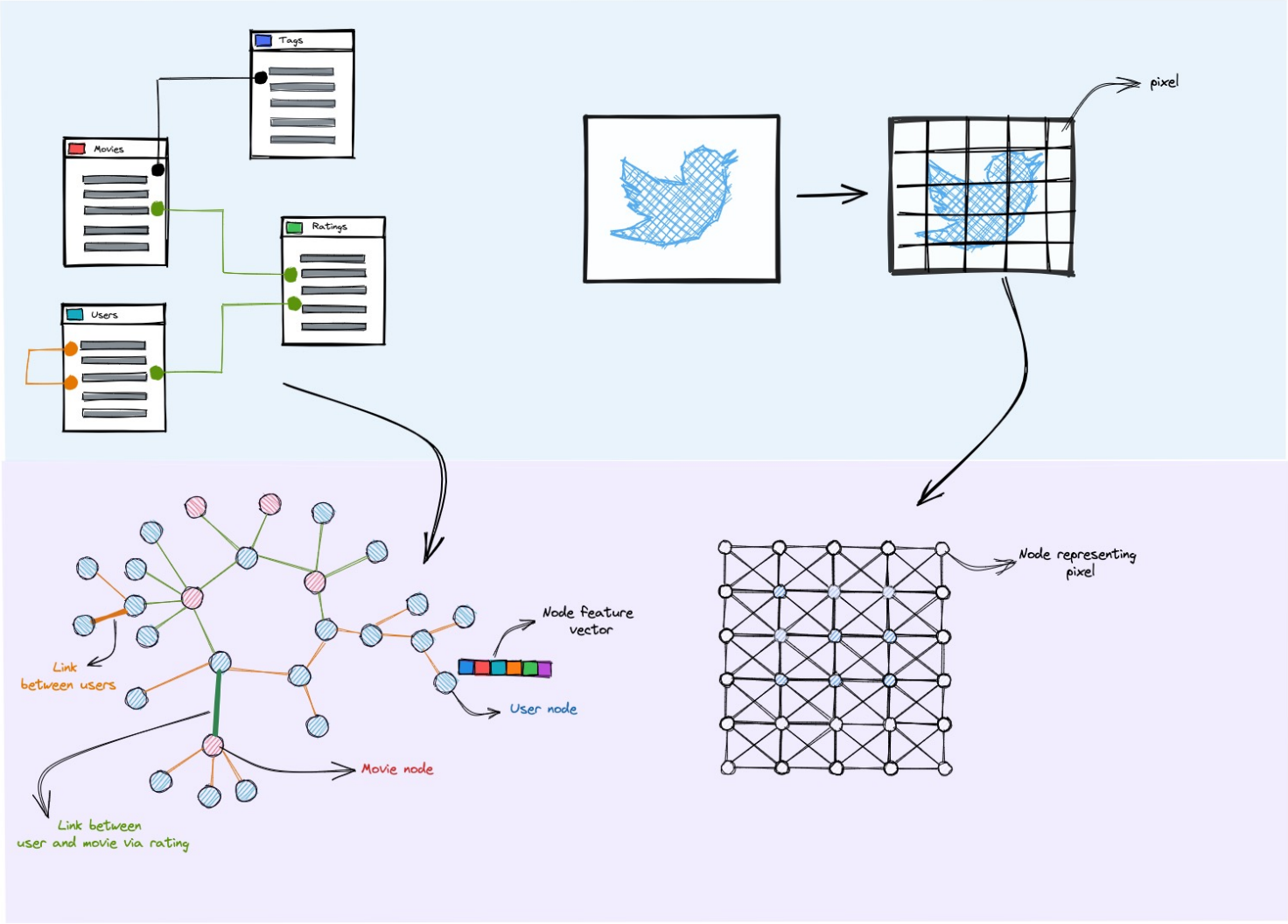


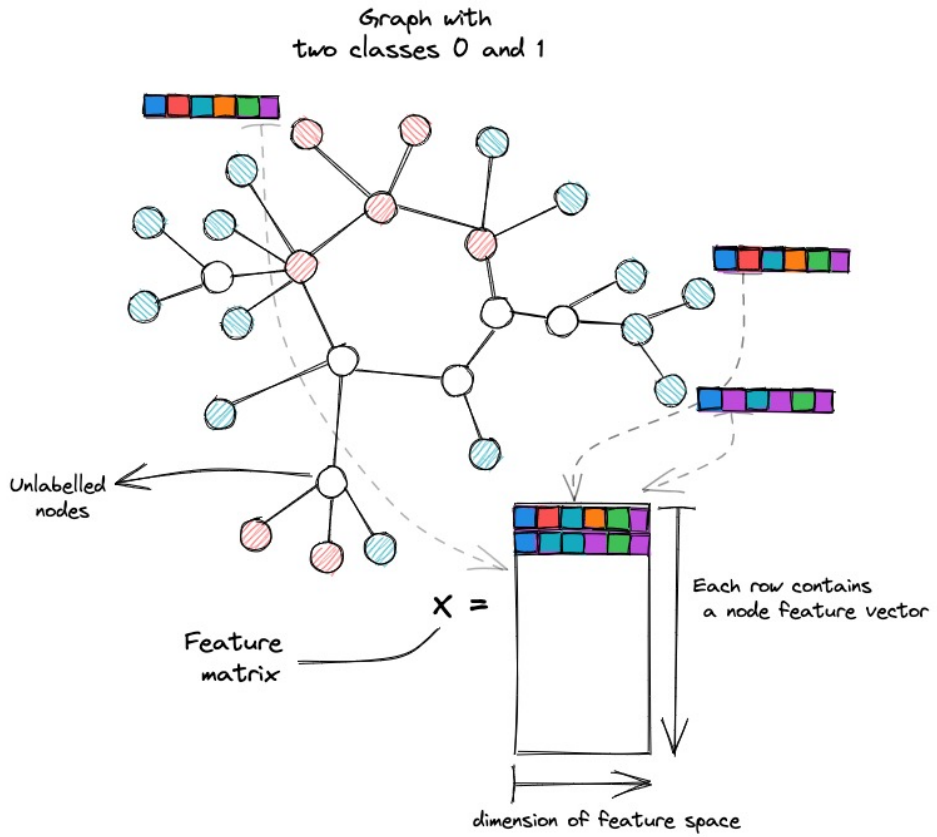
E Edge (or link) attributes and directions
e.g., edge identity, edge weight



U Global (or master node) attributes
e.g., number of nodes, longest path

Graphs are everywhere

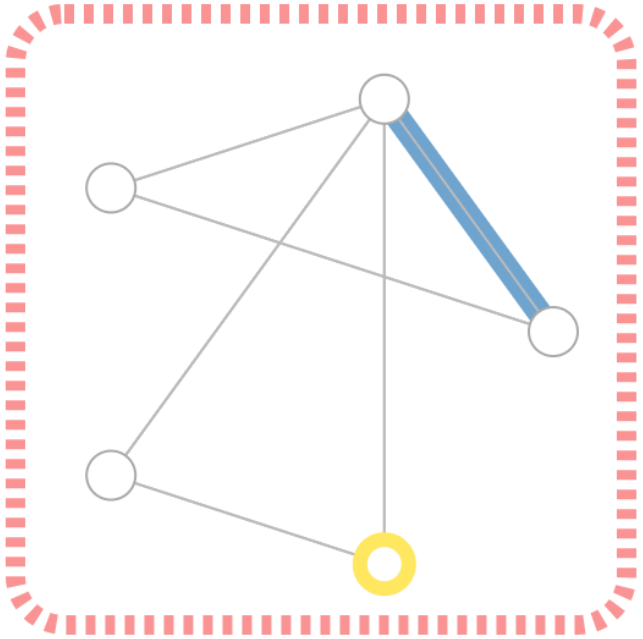




https://towardsdatascience.com/over-smoothing-issue-in-graph-neural-network-bddc8fbc2472

Graph Definition

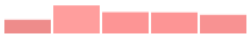
To further describe each node, edge or the entire graph, we can store information in each of these pieces of the graph



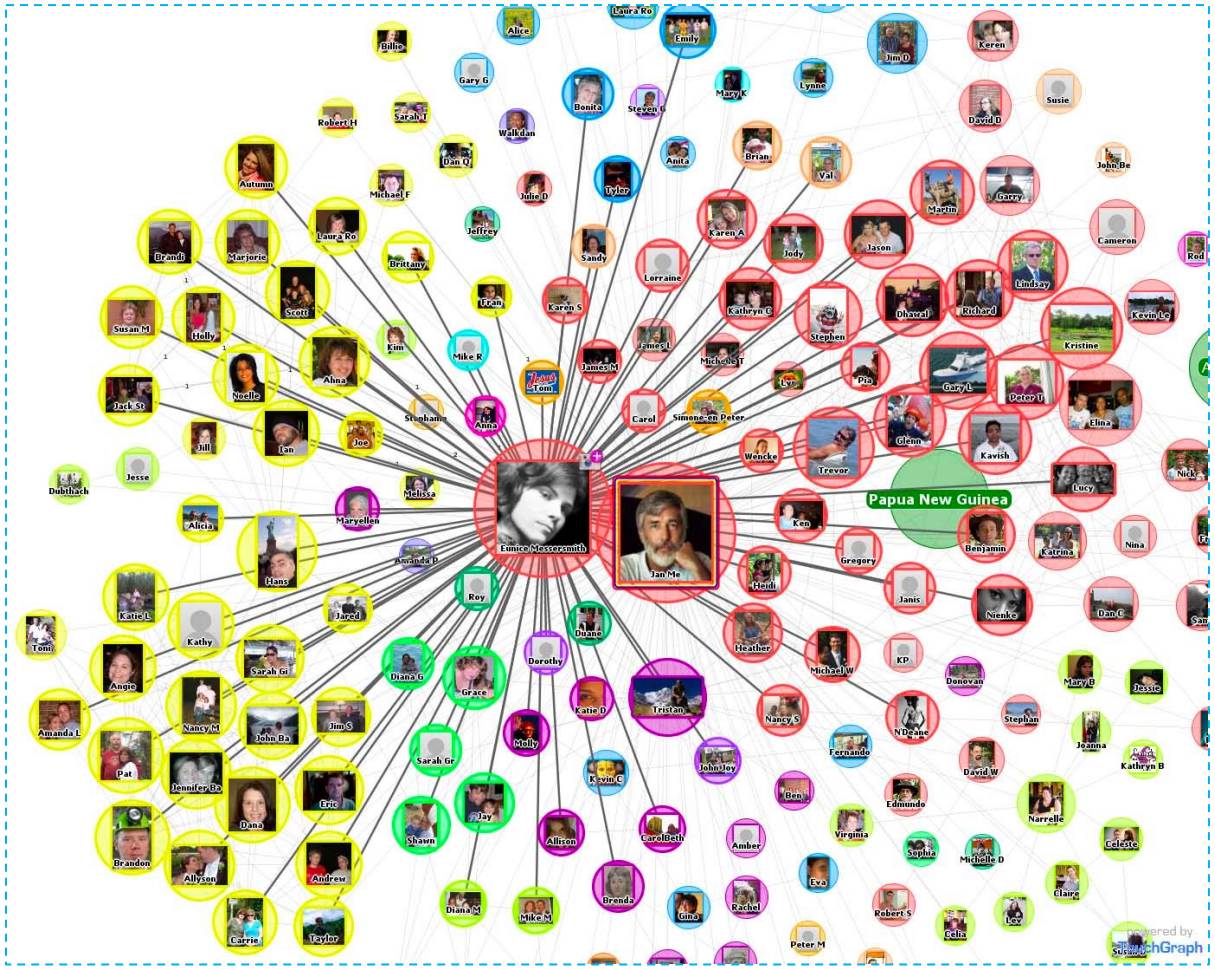
Vertex (or node) embedding

Edge (or link) attributes and embedding

Global (or master node) embedding



Graphs and where to find them



Social networks

Two types of data that you might not think could be modeled as graphs:

Image

Graphs are all around us

Text

Image as Graphs

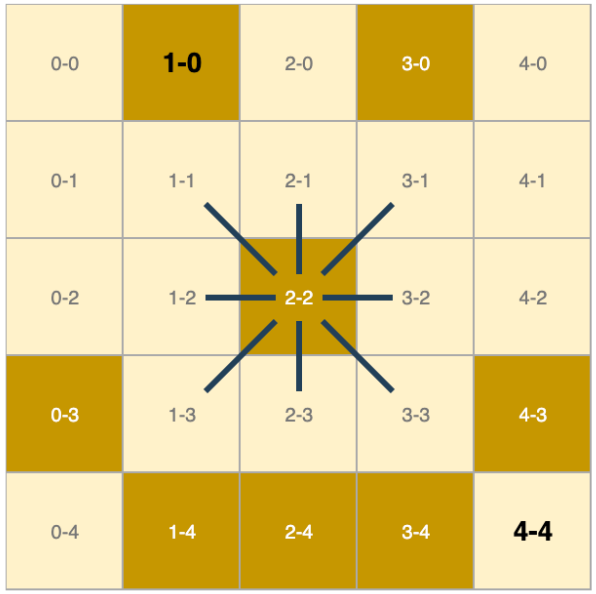
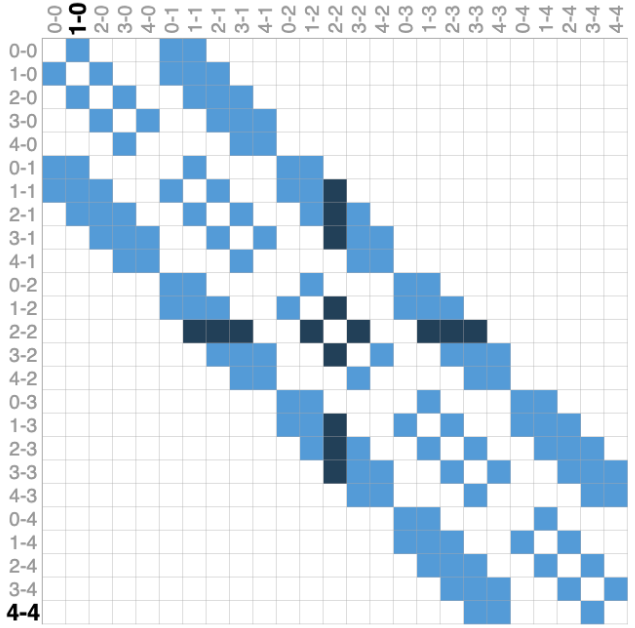
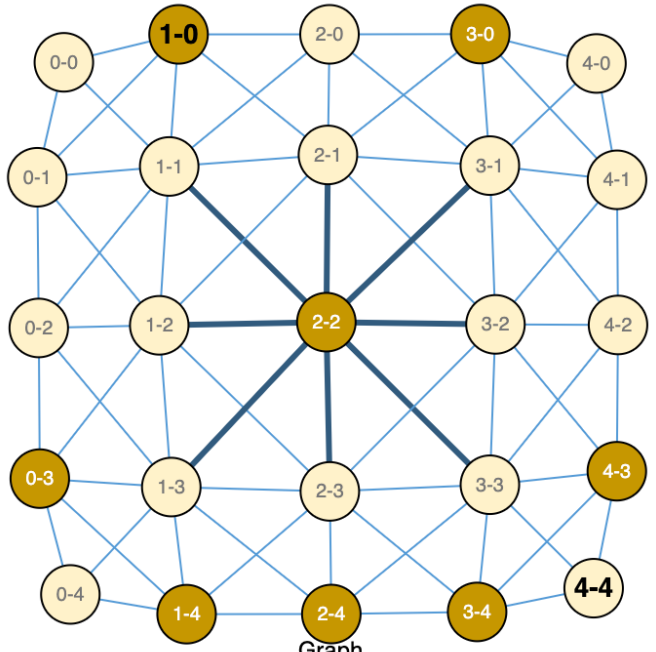


Image Pixels



Adjacency Matrix

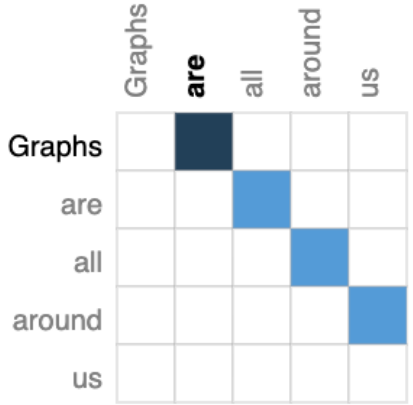


Graph

Another way to think of images is as graphs with regular structure, where each pixel represents a node and is connected via an edge to adjacent pixels. Each non-border pixel has exactly 8 neighbors, and the information stored at each node is a 3-dimensional vector representing the RGB value of the pixel.

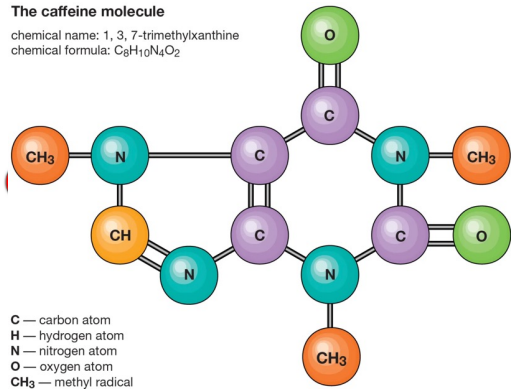
Source: https://distill.pub/2021/gnn-intro/

Text as Graphs

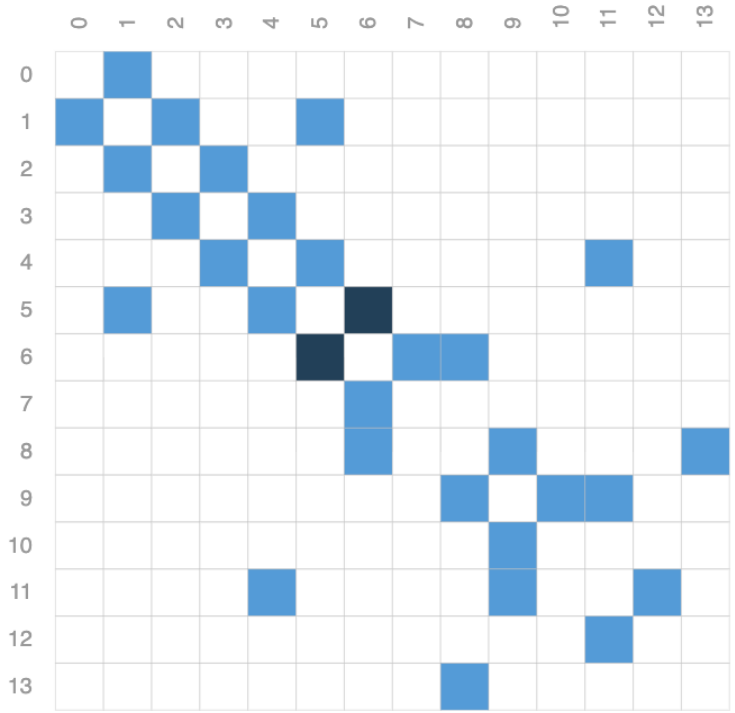


We can digitize text by associating indices to each character, word, or token, and representing text as a sequence of these indices. This creates a simple directed graph, where each character or index is a node and is connected via an edge to the node that follows it.

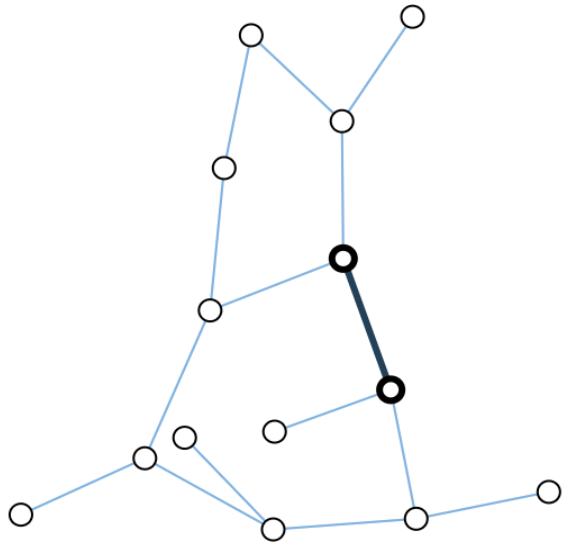
Other Graph Data



Cafeine molecule



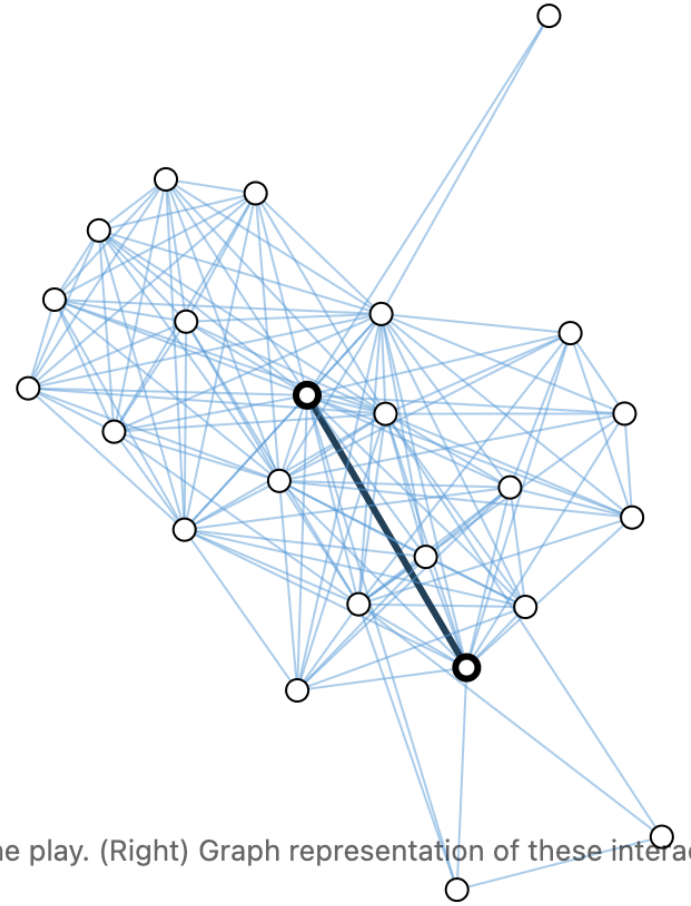
Adjacency matrix



Grap model

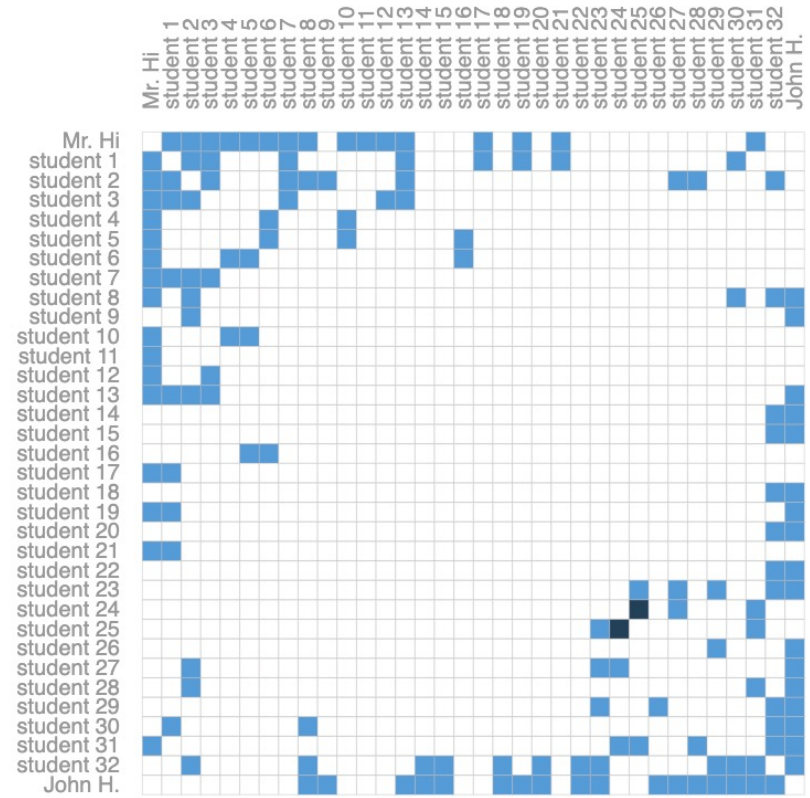
Molecules as graphs

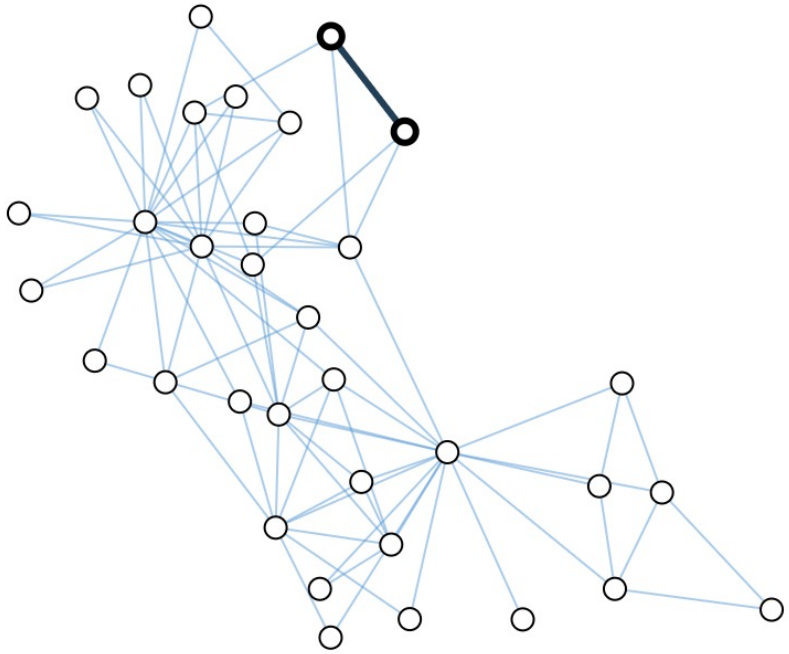
Other Graph Data



(Left) Image of a scene from the play "Othello". (Center) Adjacency matrix of the interaction between characters in the play. (Right) Graph representation of these interactions.

Other Graph Data





(Left) Image of karate tournament. (Center) Adjacency matrix of the interaction between people in a karate club. (Right) Graph representation of these interactions.

Other Graph Data

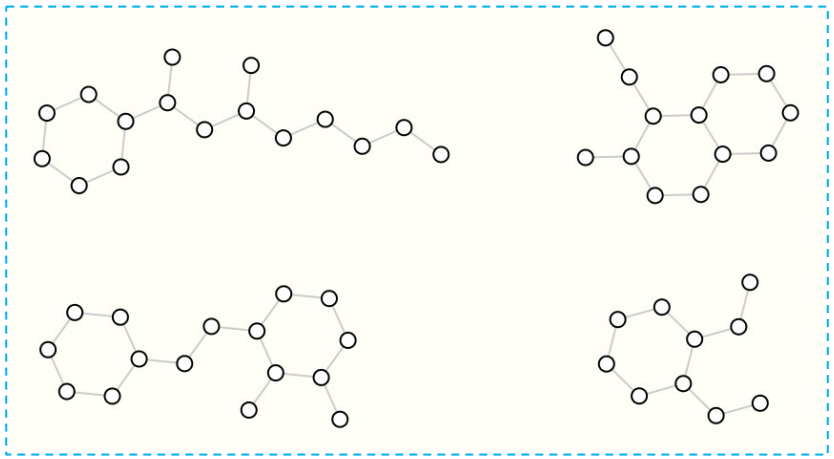
					Edges per node (degree)		
Dataset	**Domain**	**graphs**	**nodes**	**edges**	**min**	**mean**	**max**
karate club	Social network	1	34	78		4.5	17
qm9	Small molecules	134k	≤ 9	≤26	1	2	5
Cora	Citation network	1	23,166	91,500	1	7.8	379
Wikipedia links, English	Knowledge graph	1	12M	378M		62.24	1M

Summary statistics on graphs found in the real world. Numbers are dependent on featurization decisions.

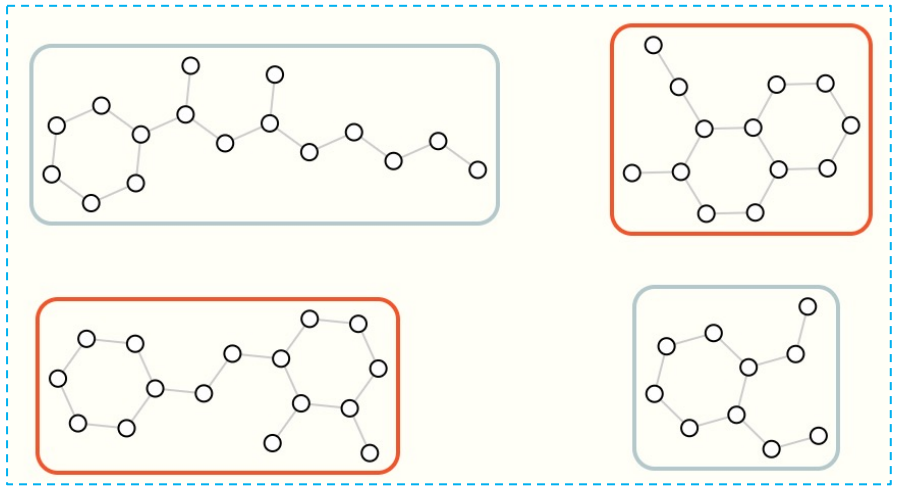
Tasks on Graph Data

Graph-level task

Similar to image classification problems



Input: graphs



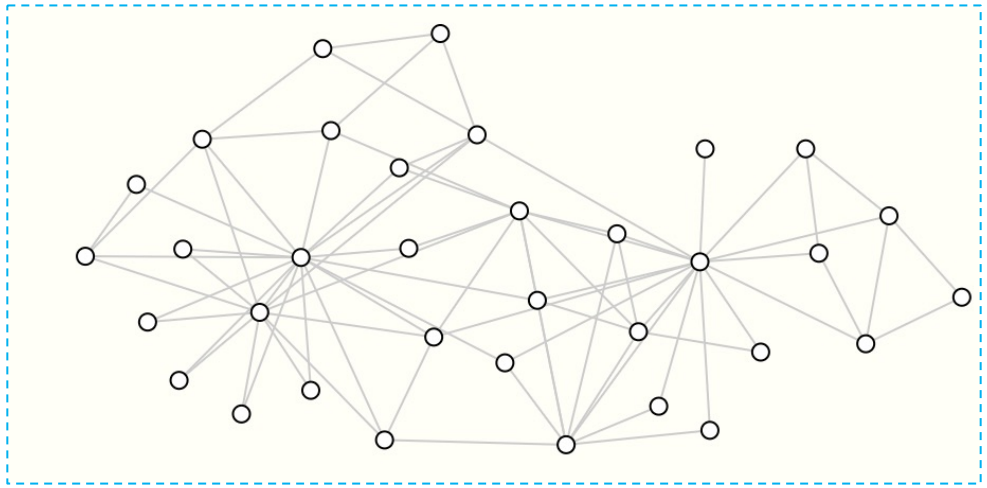
Output: labels for each graph, (e.g., "does the graph contain two rings?")

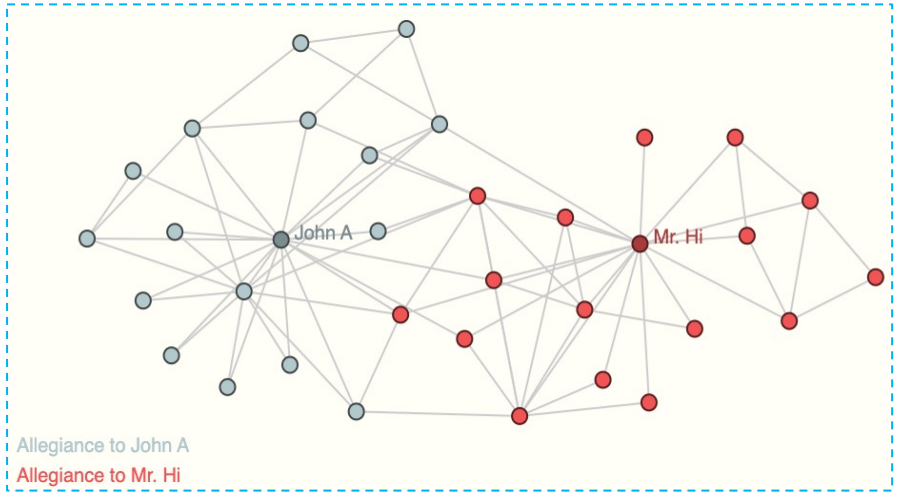
In a graph-level task, our goal is to predict the property of an entire graph. For example, for a molecule represented as a graph, we might want to predict what the molecule smells like, or whether it will bind to a receptor implicated in a disease.

Tasks on Graph Data

Node-level task

Similar to image segmentation problems





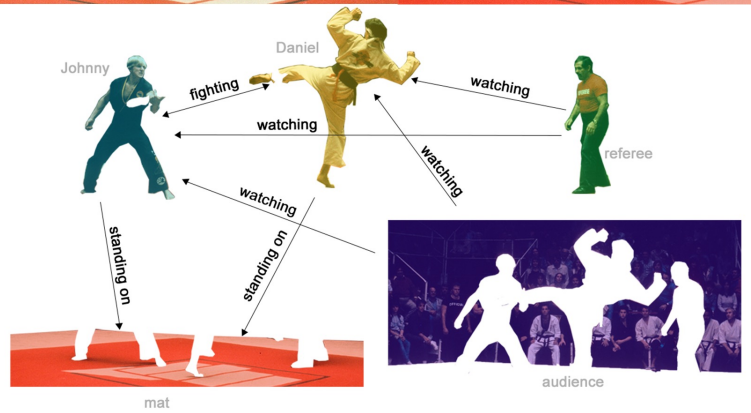
Input: graph with unlabled nodes

Output: graph node labels

Node-level tasks are concerned with predicting the identity or role of each node within a graph.

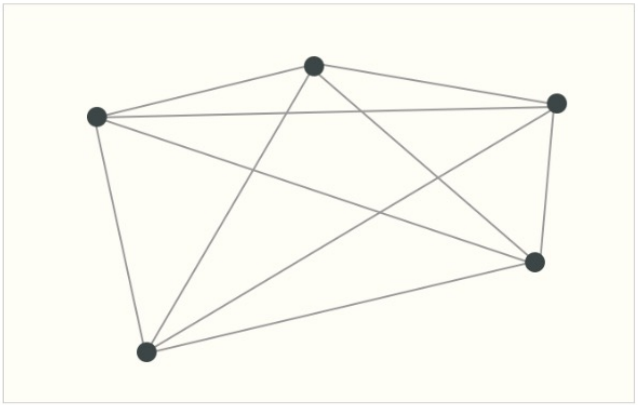
Tasks on Graph Data

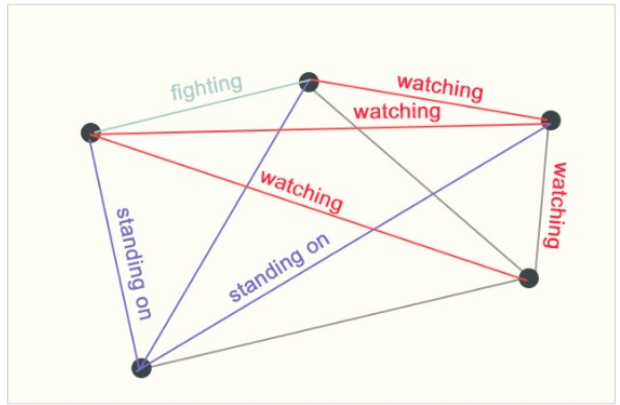
Edge-level task



Similar to image scene understanding

Node-level tasks are concerned with predicting the identity or role of each node within a graph.

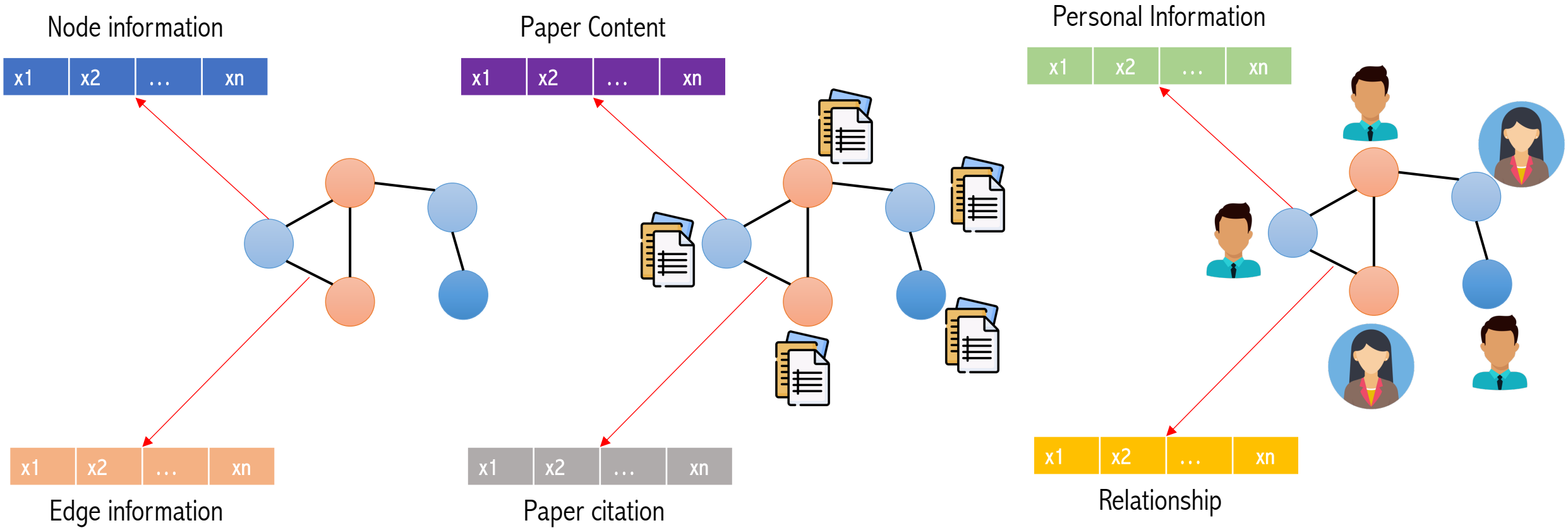




Input: fully connected graph, unlabeled edges

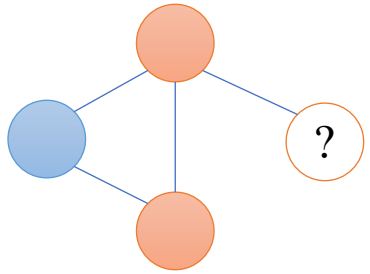
Output: labels for edges

A Simple Graph



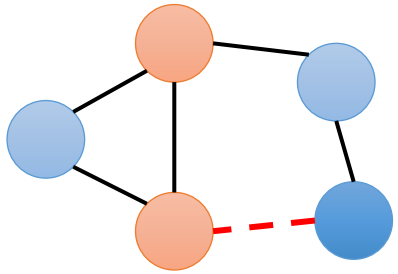
Example

Nodel level prediction



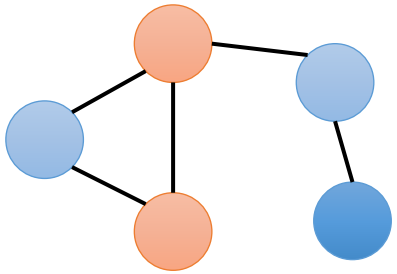
Does this student smoke?
(unlable node)

Edge level predictions
(Link prediction)



Next Youtube
Video?

Graph Level
Predictions



Is this molecule a suitable
drug?

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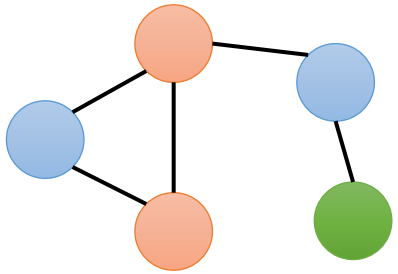
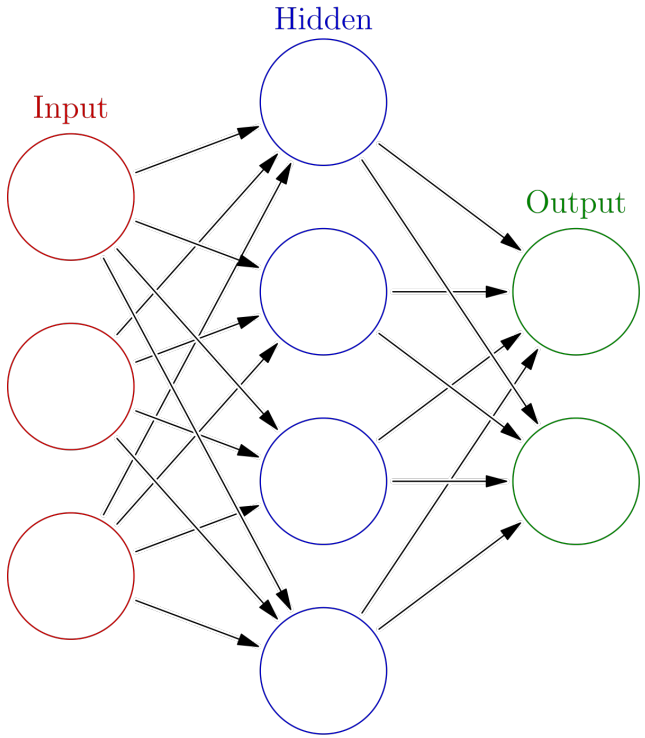
Graph Data with Neural Network

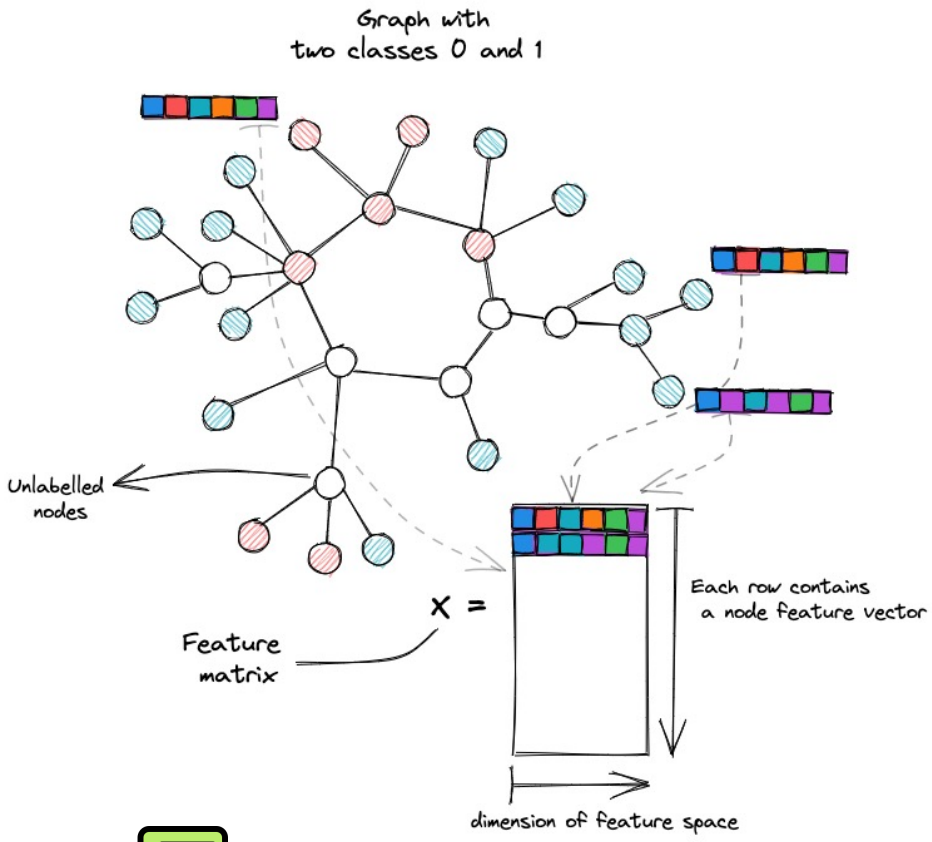


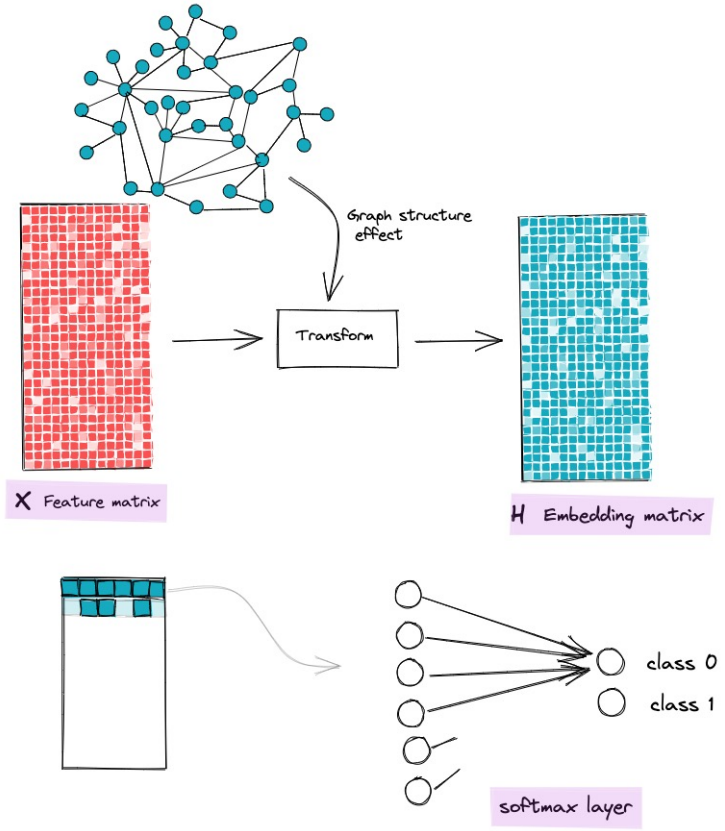
G(V,E)



So, how do we go about solving these different graph tasks with neural networks? The first step is to think about how we will represent graphs to be compatible with neural networks.

Graph Data with Neural Network

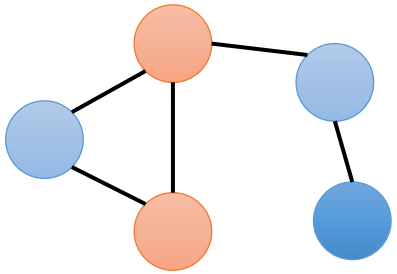


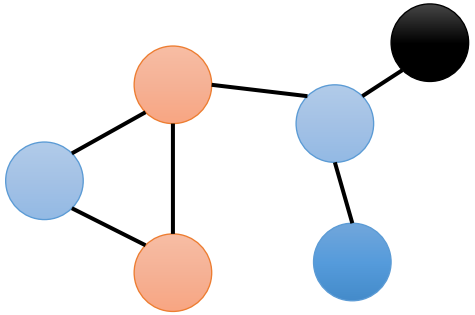


The goal of GNN is to transform node features to features that are aware of the graph structure

Problem with Graph Data

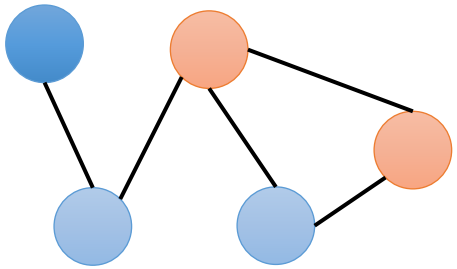
Difference in Size and Shape



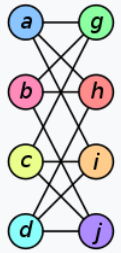
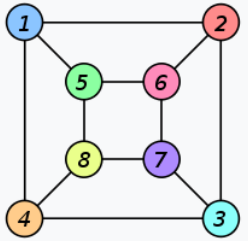


How to handel arbitrary input graph shape?

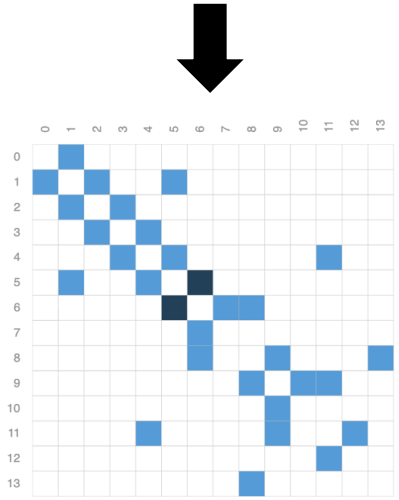
Isomorphism



Permutaton invariant

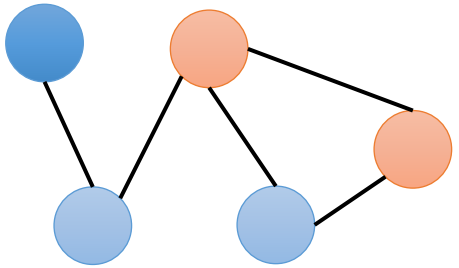
Graph G	Graph H	An isomorphism between G and H
		$f(a) = 1$ $f(b) = 6$ $f(c) = 8$ $f(d) = 3$ $f(g) = 5$ $f(h) = 2$ $f(i) = 4$ $f(j) = 7$

Cannot use adjacency matrix as an input

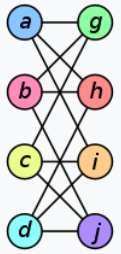
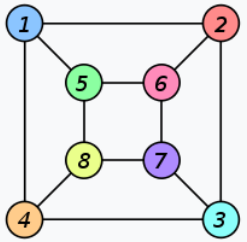


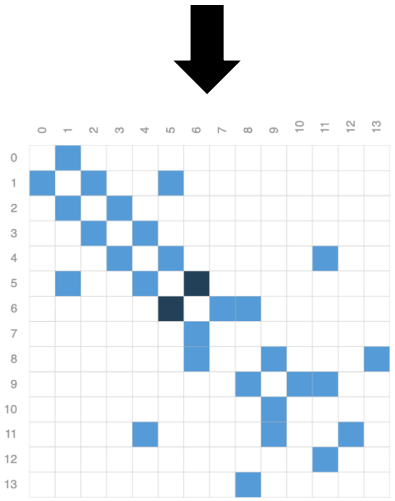
Problem with Graph Data

Isomorphism



Permutaton invariant

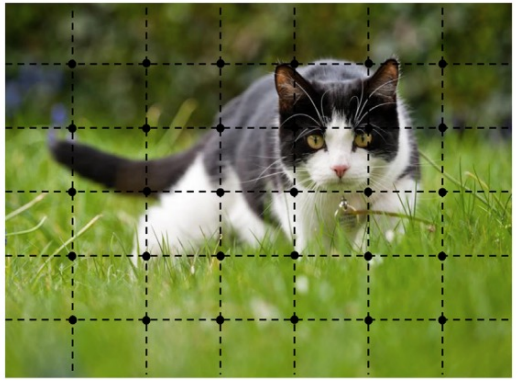
Graph G	Graph H	An isomorphism between G and H
		$f(a) = 1$ $f(b) = 6$ $f(c) = 8$ $f(d) = 3$ $f(g) = 5$ $f(h) = 2$ $f(i) = 4$ $f(j) = 7$



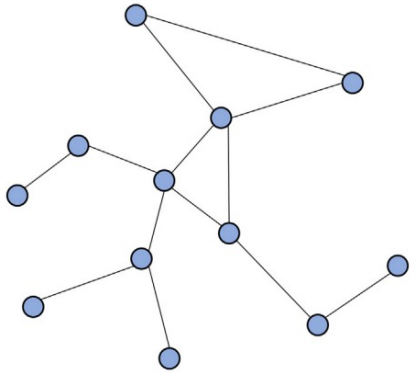
Cannot use adjacency matrix as an input

Grid Structure

Information between nodes



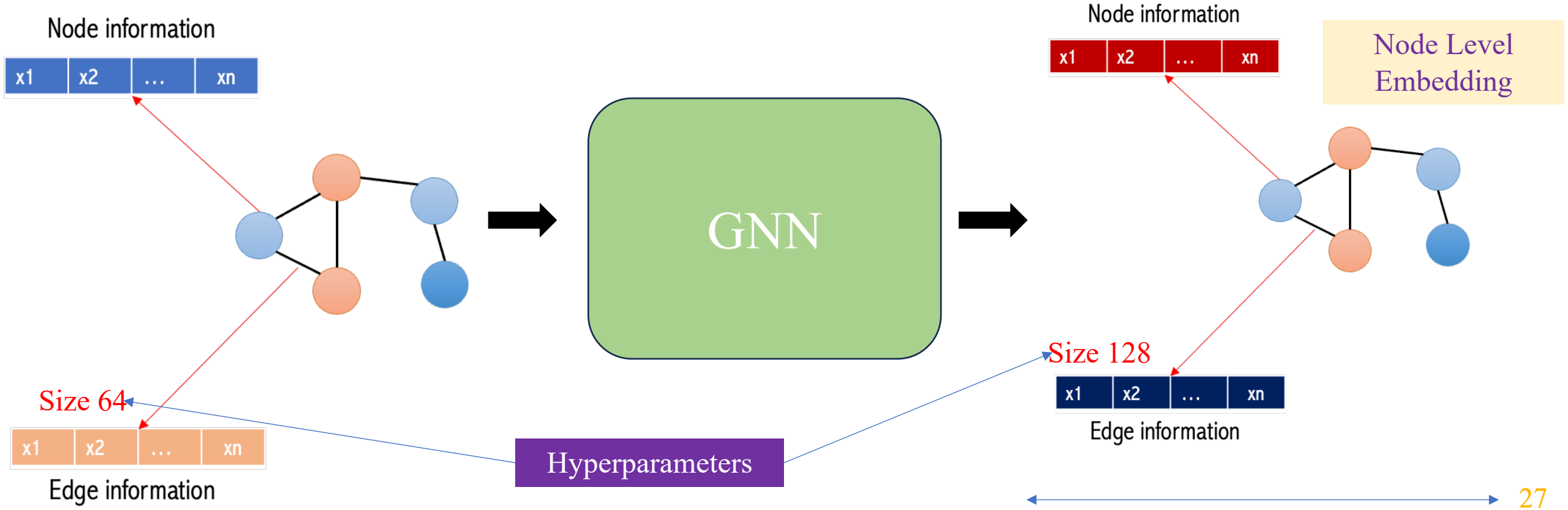
Eulidean space



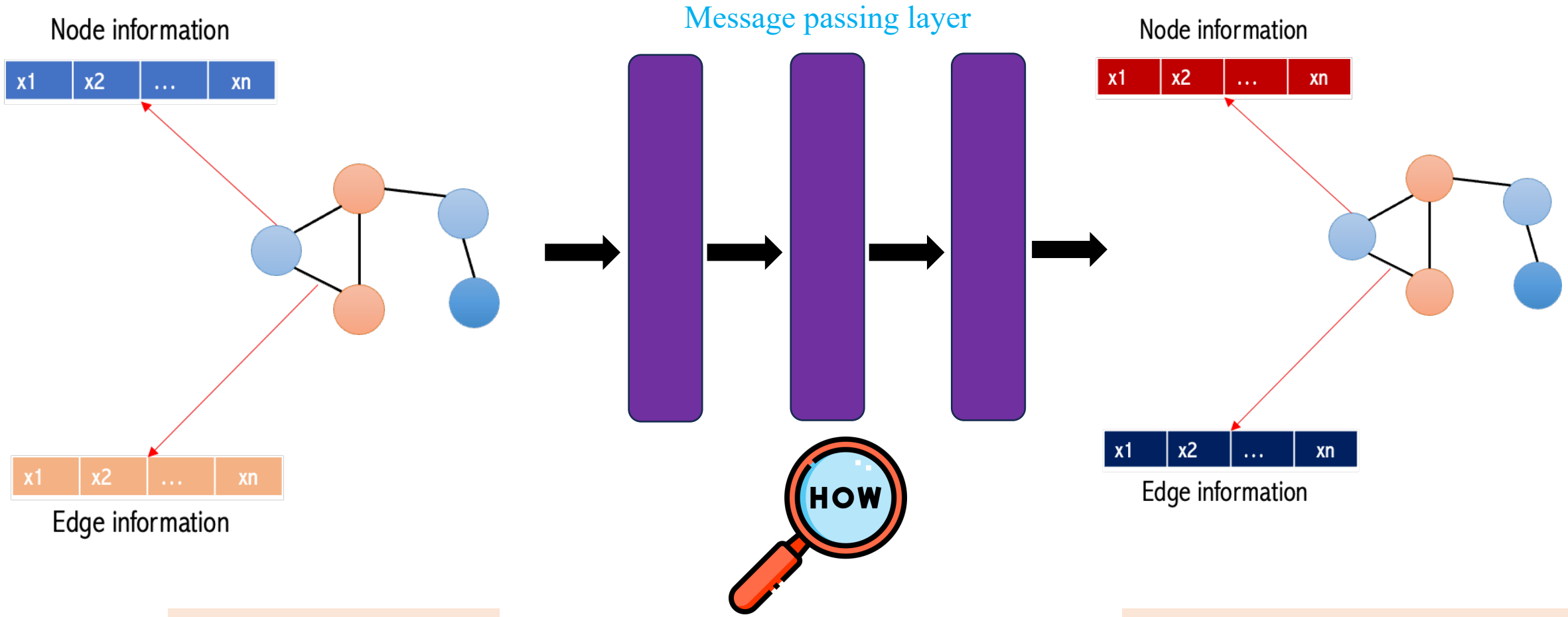
Non-Euclidean space

Fundamental Idea of GNNs

Learning a for neural network suitable representation of graph data
<Representation Learning>>

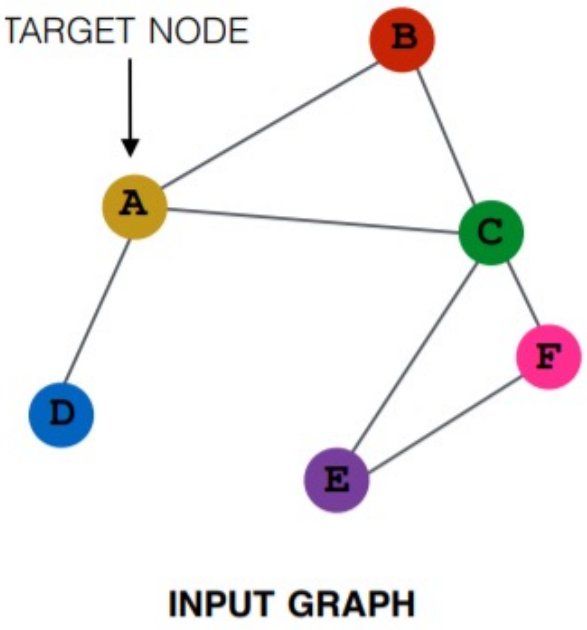


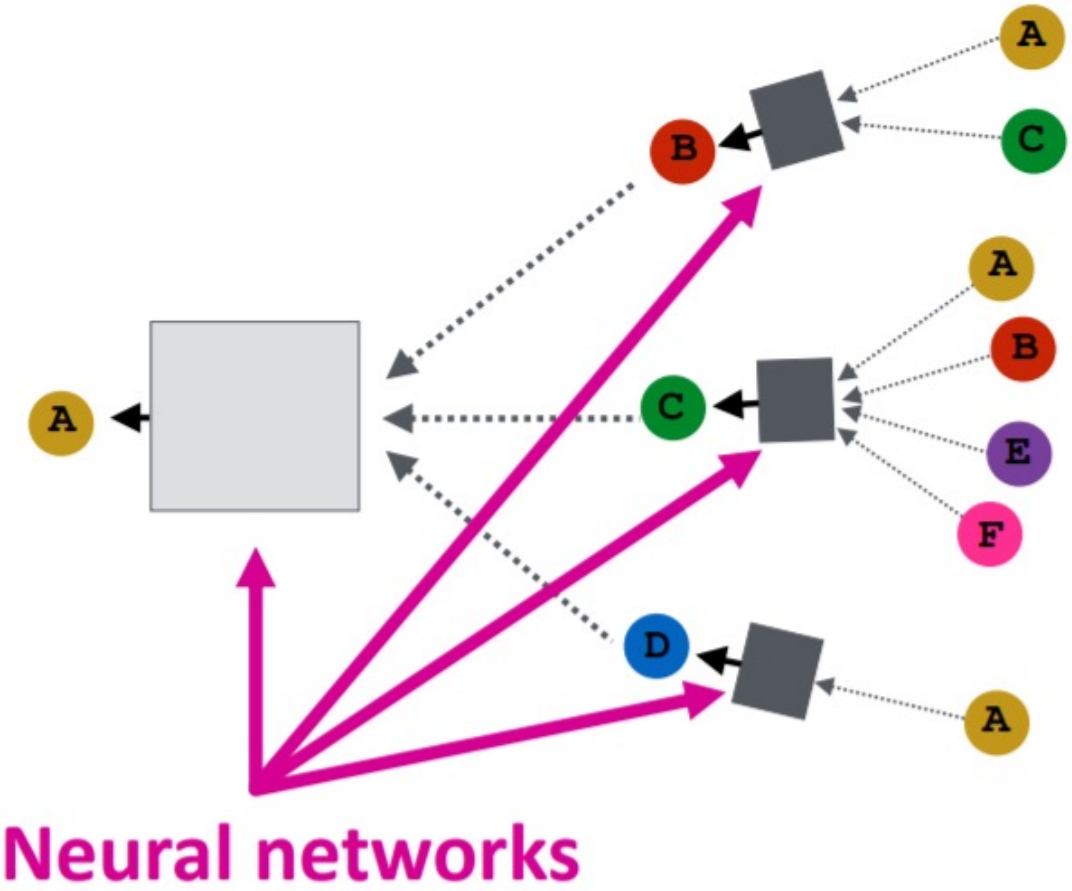
How do Graph Neural Network Work?



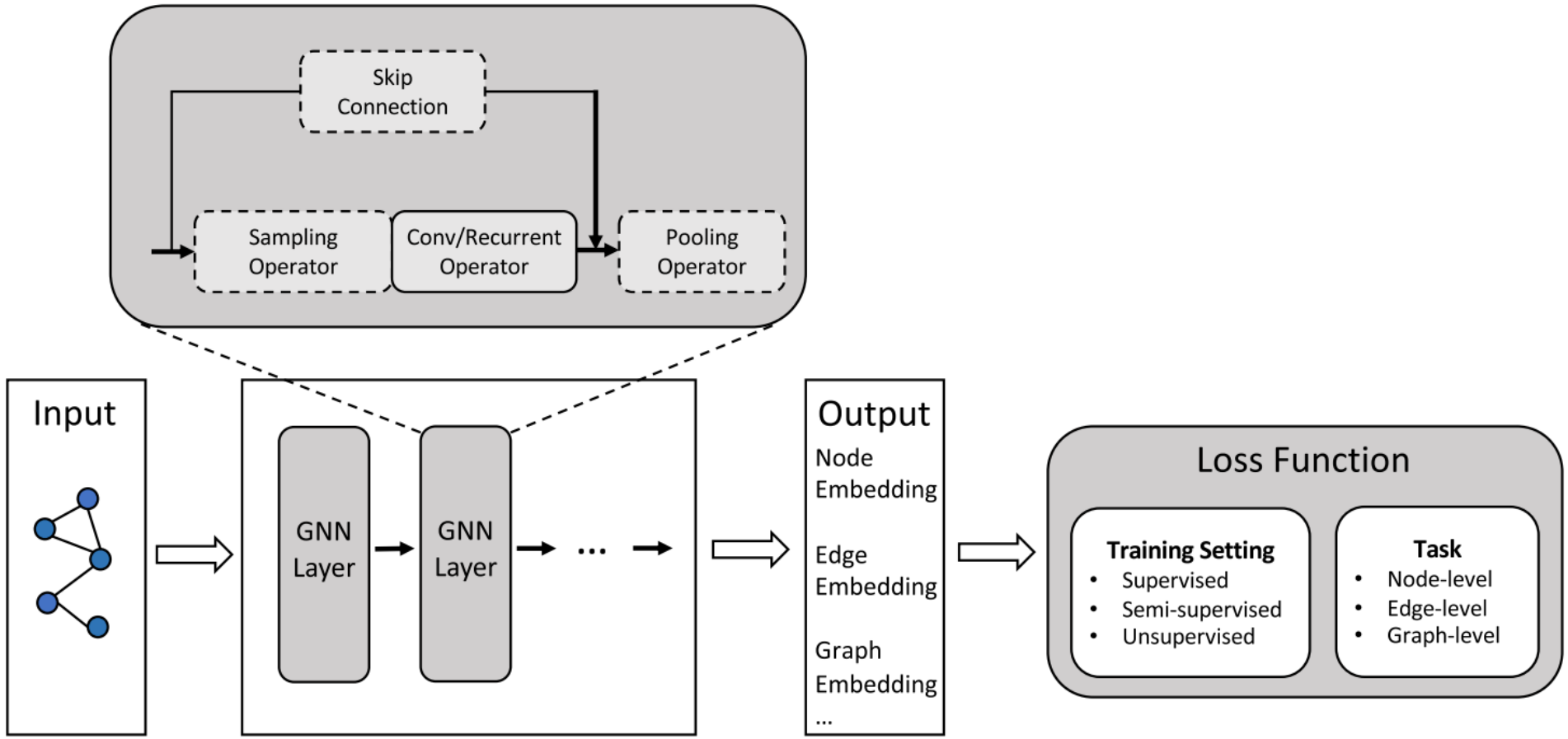
Edge and Node Information → 1.Sample Neighborhood 2. Aggregation 3. Update → Node Level Embedding Information

How do Graph Neural Network Work?





How do Graph Neural Network Work?



1. Find graph structure.

2. Specify graph type and scale.

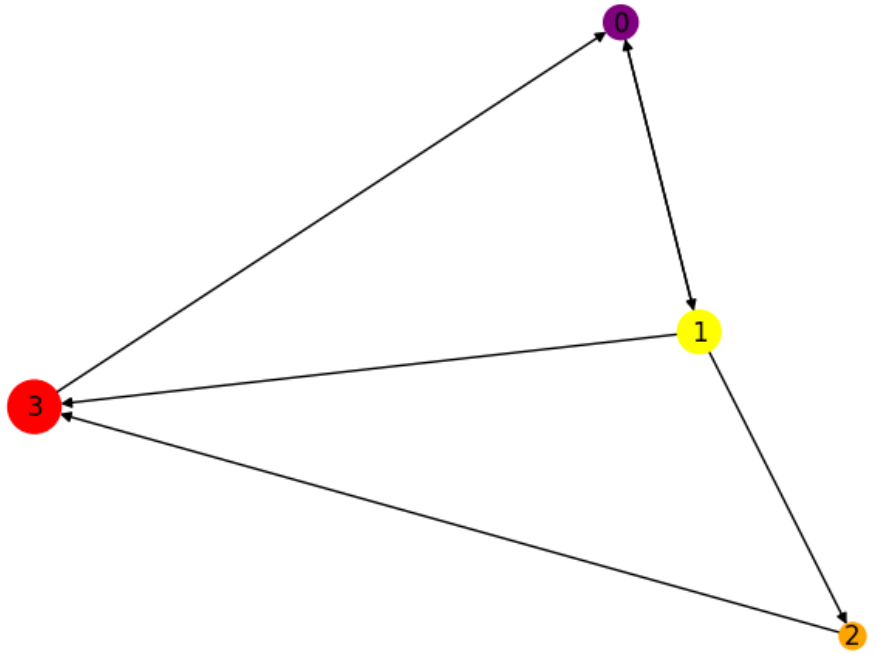
4. Build model using computational modules.

3. Design loss function.

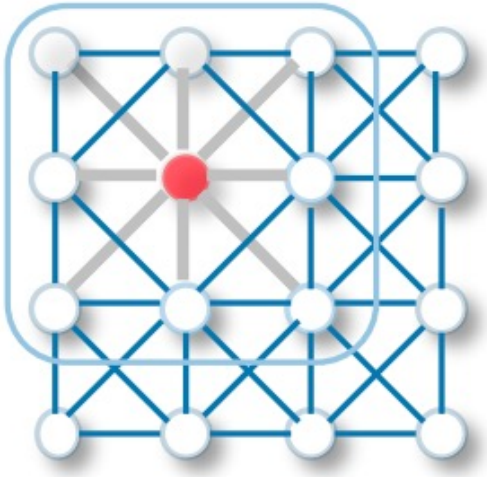
https://arxiv.org/pdf/1812.08434.pdf

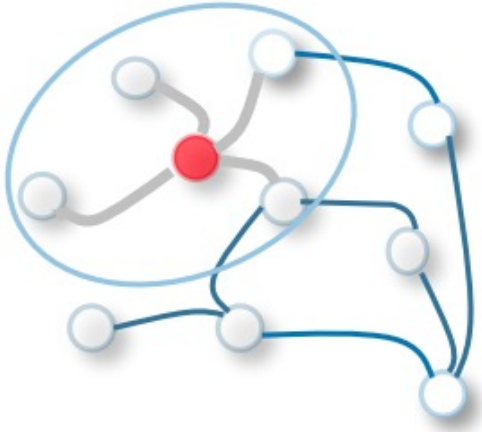
Create a graph using NetworkX

```
import networkx as nx
H = nx.DiGraph()

#adding nodes
H.add_nodes_from([
  (0, {"color": "purple", "size": 250}),
  (1, {"color": "yellow", "size": 400}),
  (2, {"color": "orange", "size": 150}),
  (3, {"color": "red", "size": 600})
])

#adding edges
H.add_edges_from([
  (0, 1), (1, 2), (1, 0), (1, 3), (2, 3), (3,0)
])

node_colors = nx.get_node_attributes(H, "color").values()
colors = list(node_colors)
node_sizes = nx.get_node_attributes(H, "size").values()
sizes = list(node_sizes)

#Plotting Graph
nx.draw(H, with_labels=True, node_color=colors, node_size=sizes)
```



CNN Vs. GNN: Messsage Passing



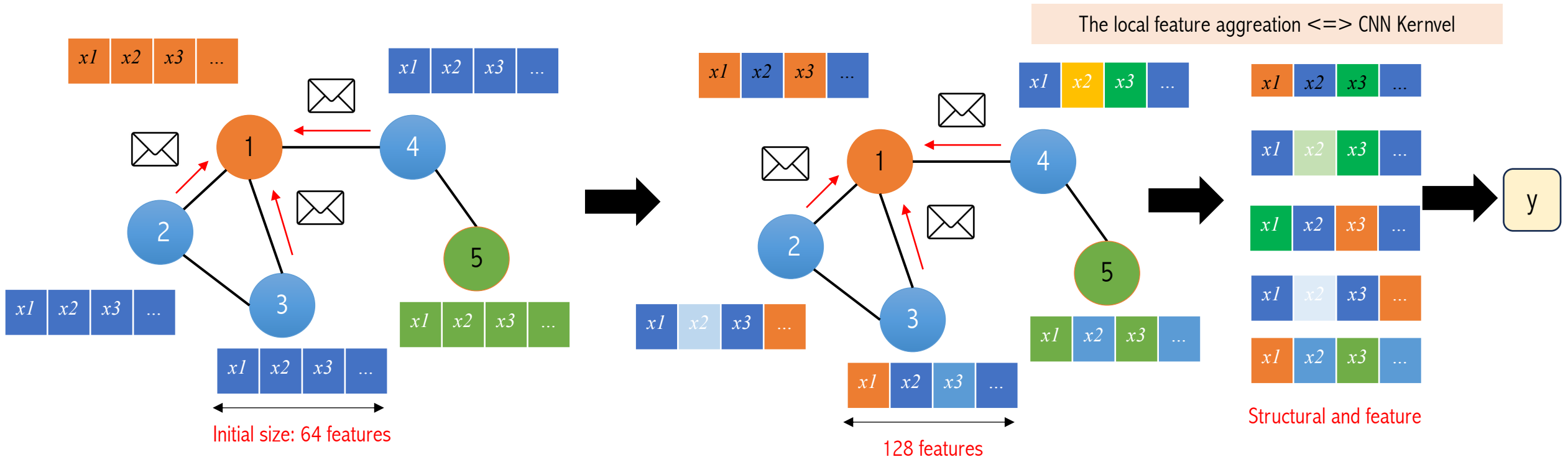


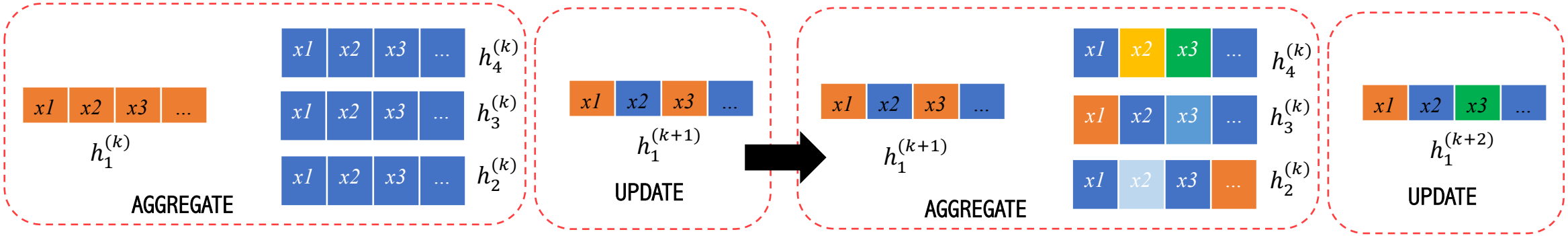
2D Convolution. Analogous to a graph, each pixel in an image is taken as a node where neighbors are determined by the filter size. The 2D convolution takes the weighted average of pixel values of the red node along with its neighbors. The neighbors of a node are ordered and have a fixed size

Graph Convolution. To get a hidden representation of the red node, one simple solution of the graph convolutional operation is to take the average value of the node features of the red node along with its neighbors. Different from image data, the neighbors of a node are unordered and variable in size

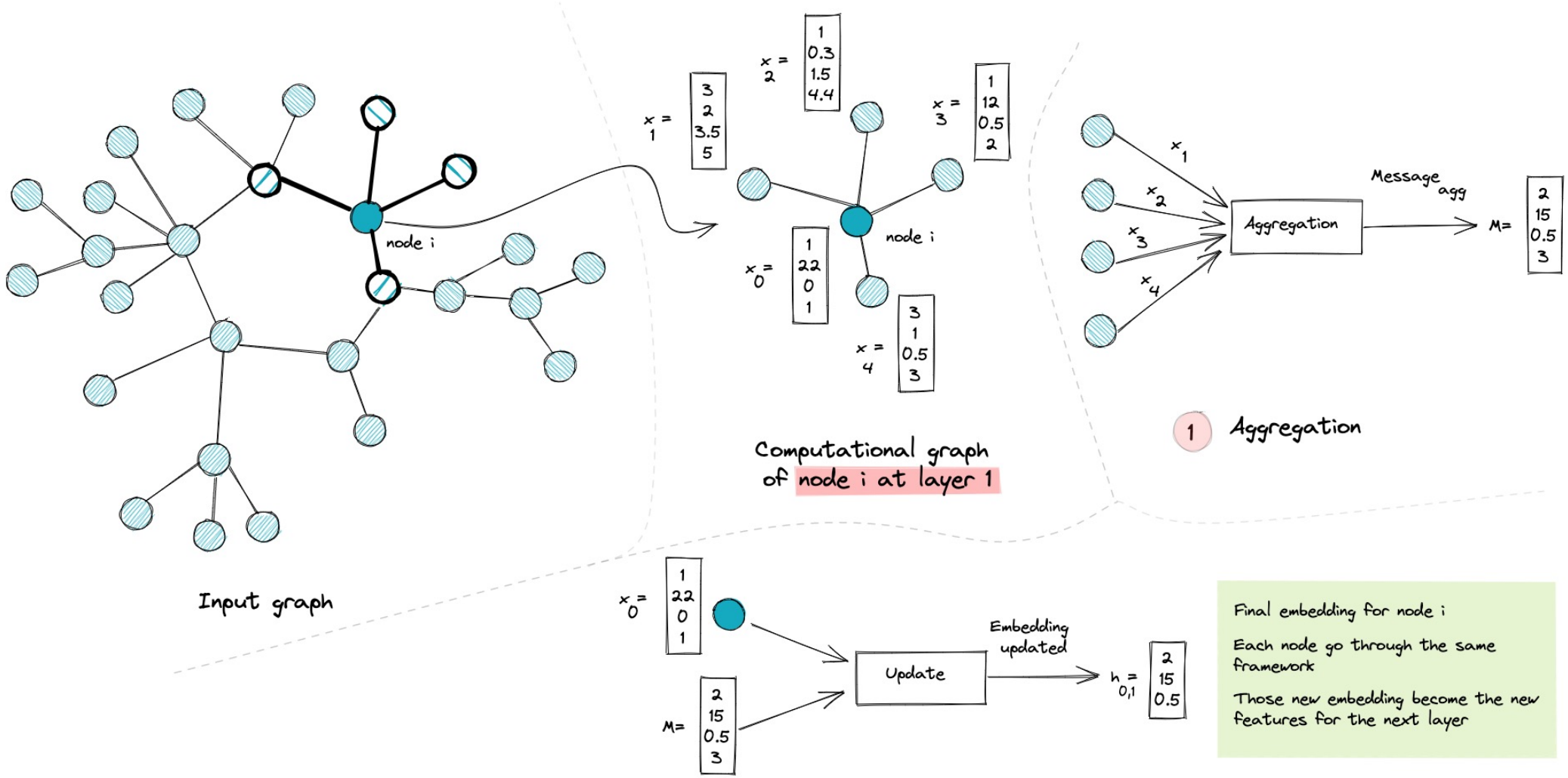
https://arxiv.org/pdf/1901.00596.pdf

Message Passing: Behind the Scene



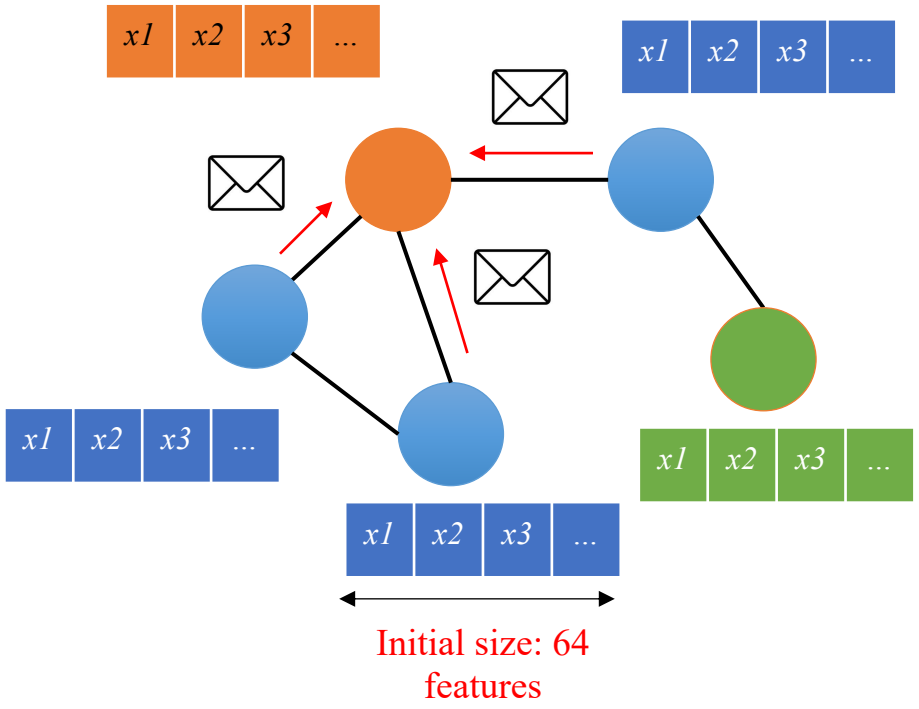


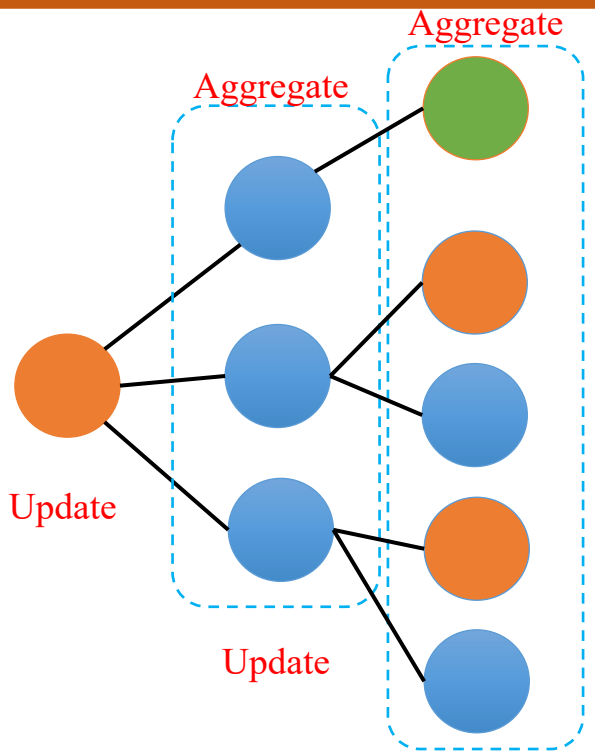
Graph: Example



https://towardsdatascience.com/over-smoothing-issue-in-graph-neural-network-bddc8fbc2472

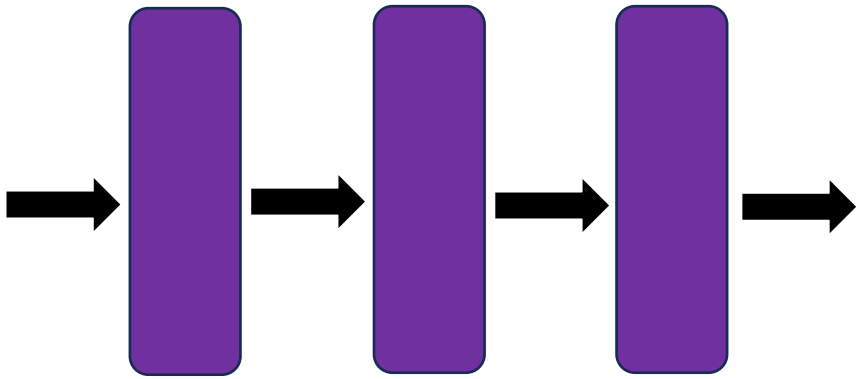
Computation Graph Representation





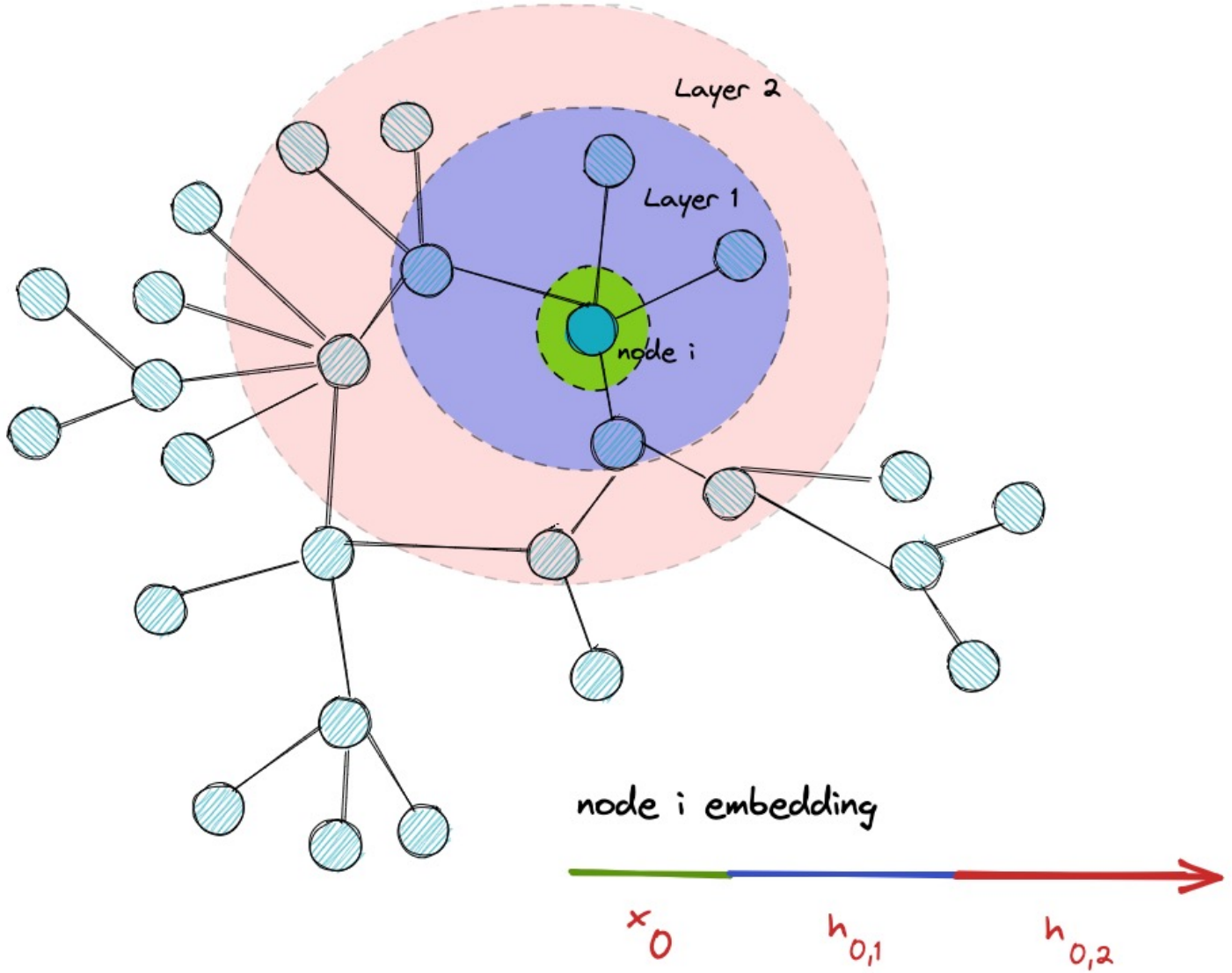
Computationnal Graph for Node v

The number of layers defined by how many neighborhood nodes

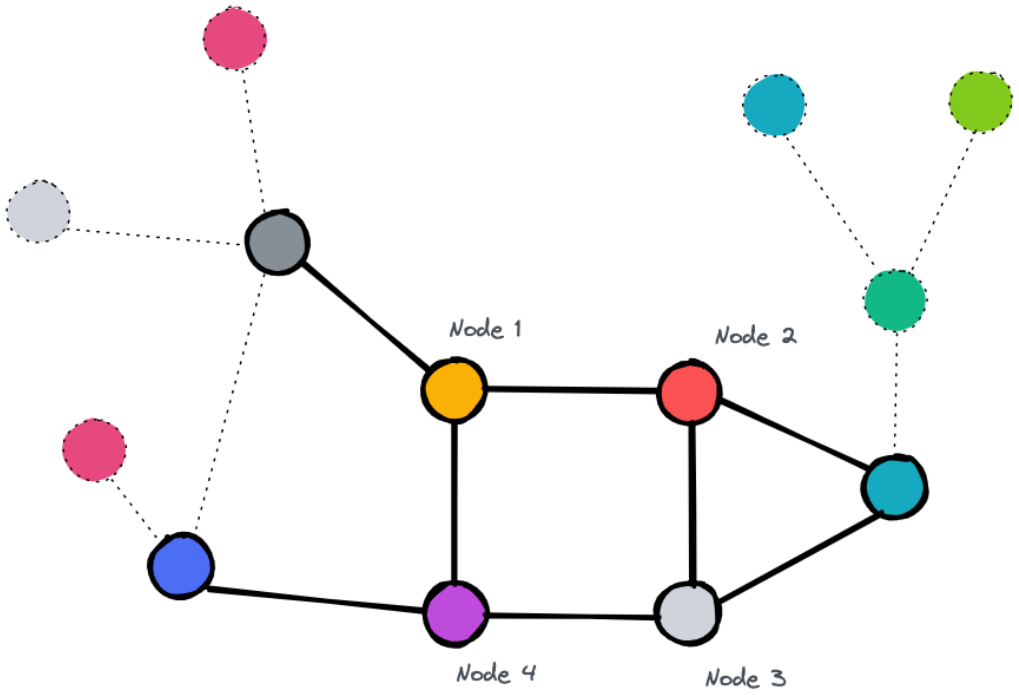


The number of MP-Layer is a hyper parameters

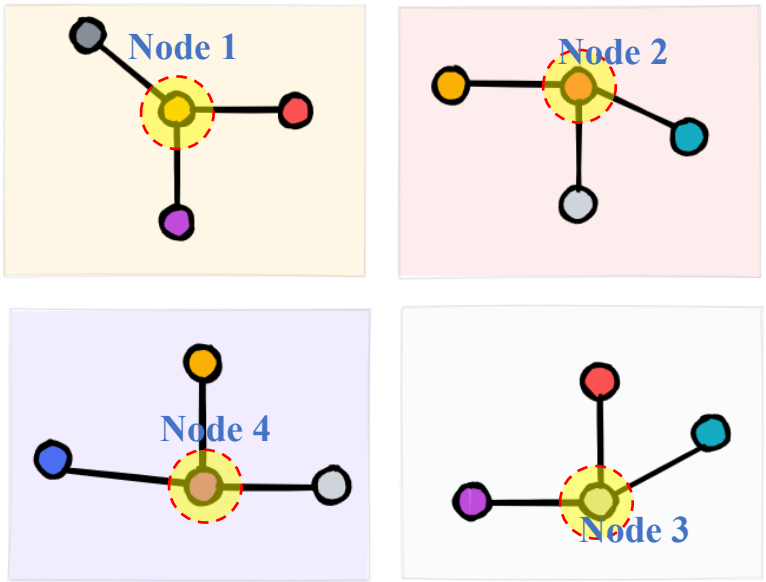
Graph: Example



Over-smoothing in GNN



Input graph

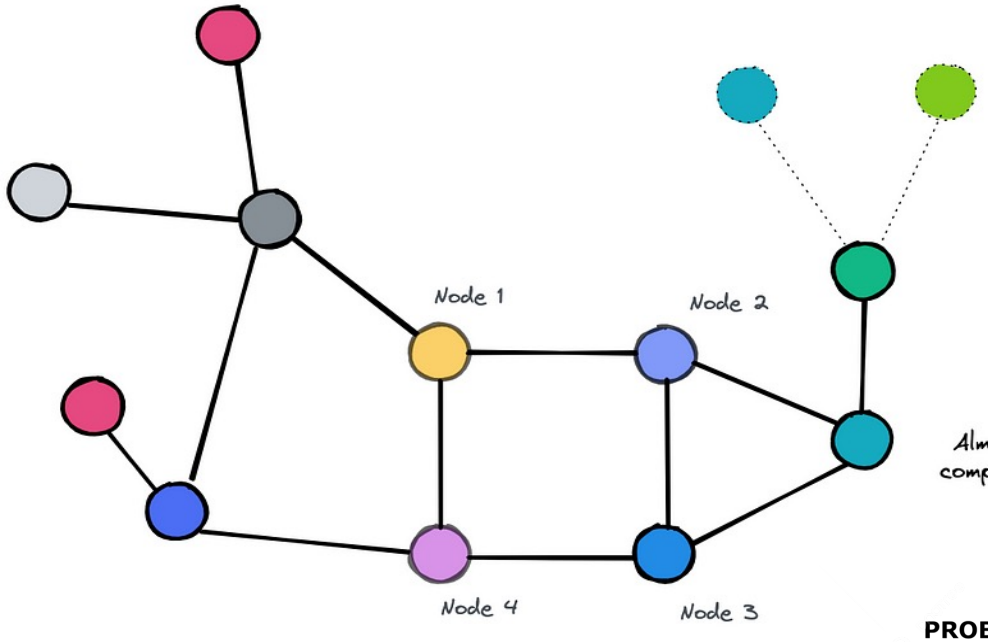


Computational graphs at layer 1

Node 2 and node 3 have almost access to the same information -> We can predict that their embeddings will be slightly similar.

Node 1 and Node 4, they interact with each other but have different neighbors -> We may predict that their new embeddings will be different.

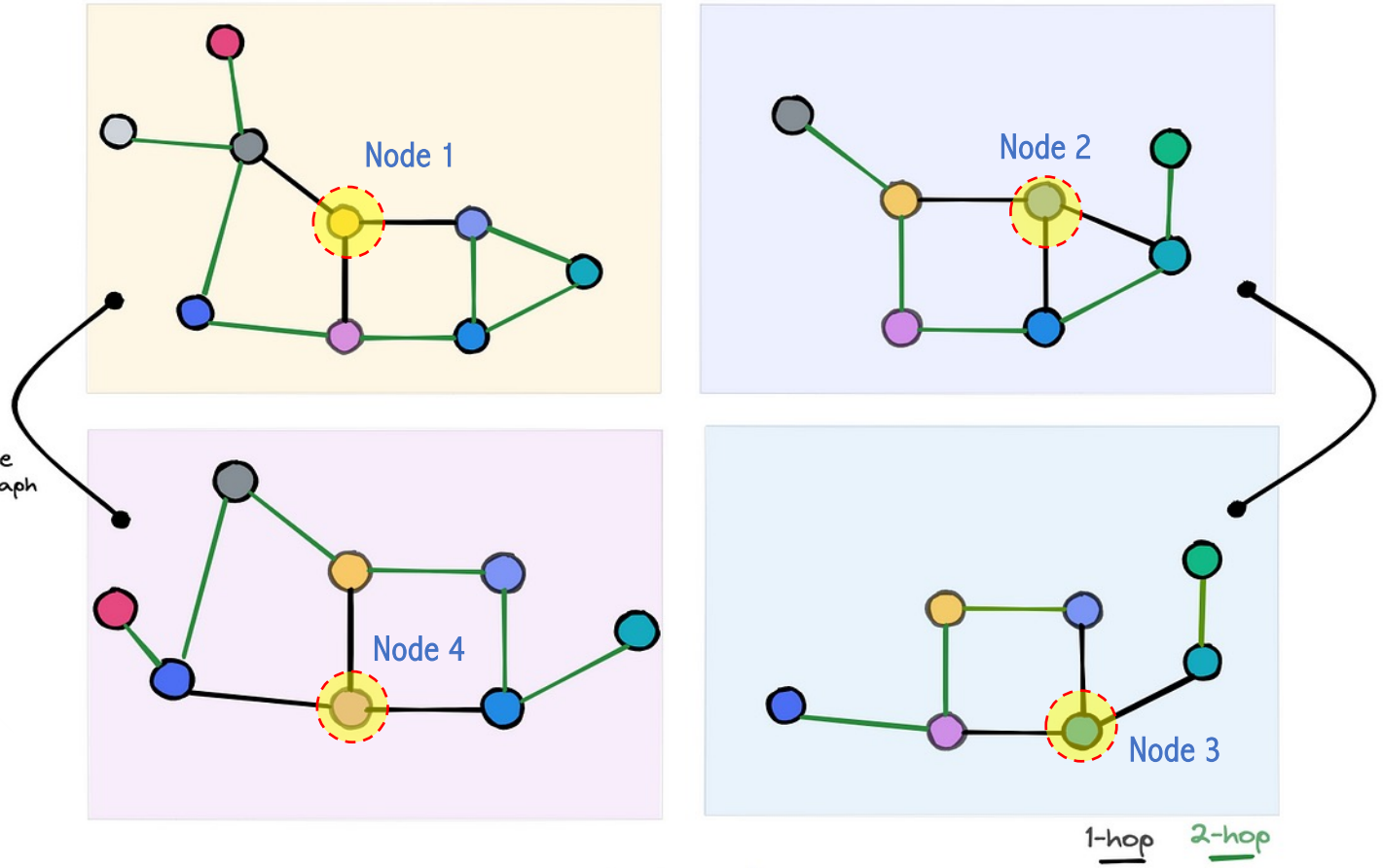
Over-smoothing in GNN



Updated graph

Almost the same computational graph

PROBLEM

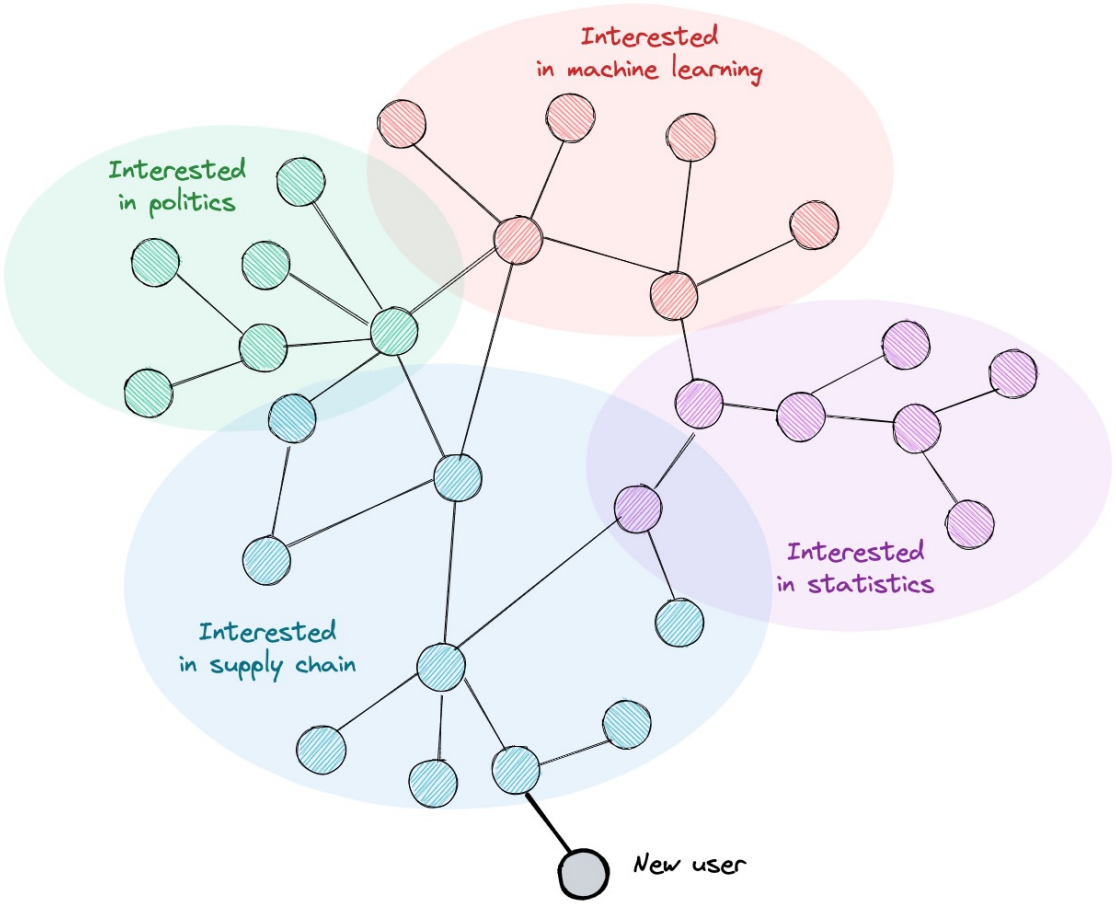


Computational graphs at layer 2

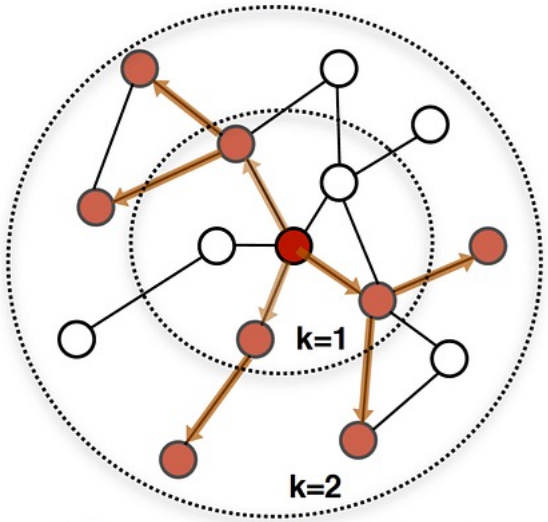
The computational graphs of nodes 1,4, and 2,3 are almost the same respectively

Over-smoothing in GNN

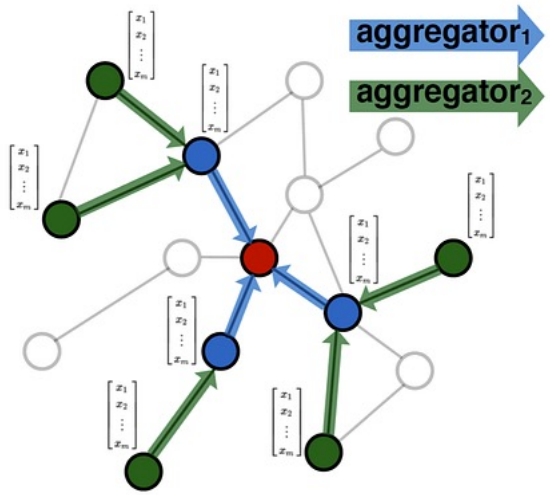
Graph Neural Networks, or GNNs, are really good at working with data that is organized in a graph structure. But sometimes, when we add more layers to a GNN architecture, it doesn't work as well as we would like. This is called over-smoothing.



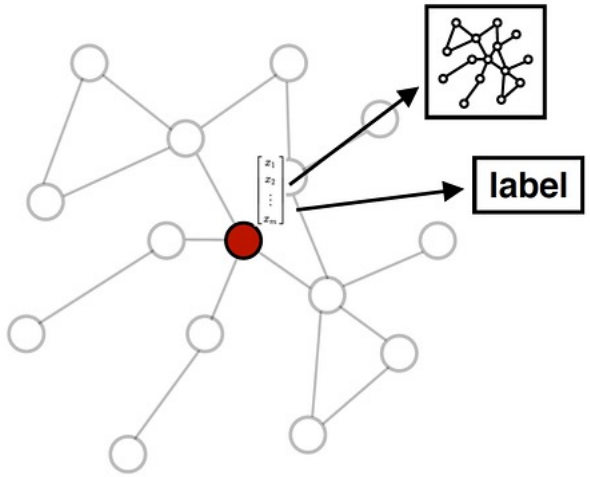
Why over-smoothing happens?



1. Sample neighborhood



2. Aggregate feature information from neighbors



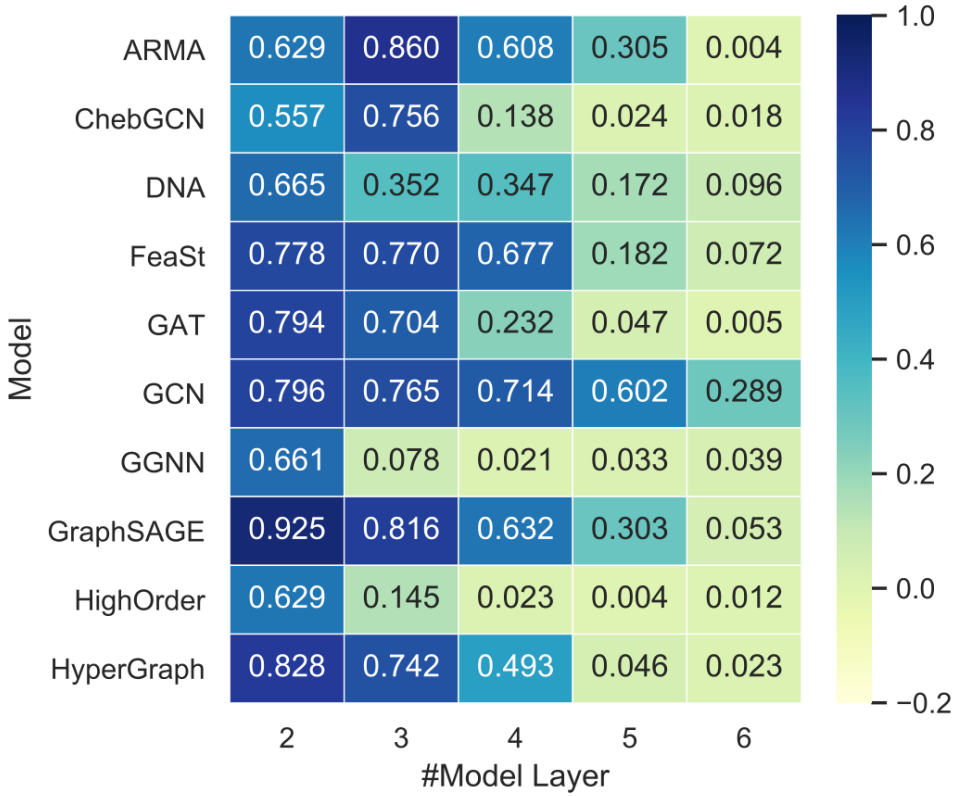
3. Predict graph context and label using aggregated information

Reason 1 → More number of layers (depth)
Reason 2 → Default nature of GNNs

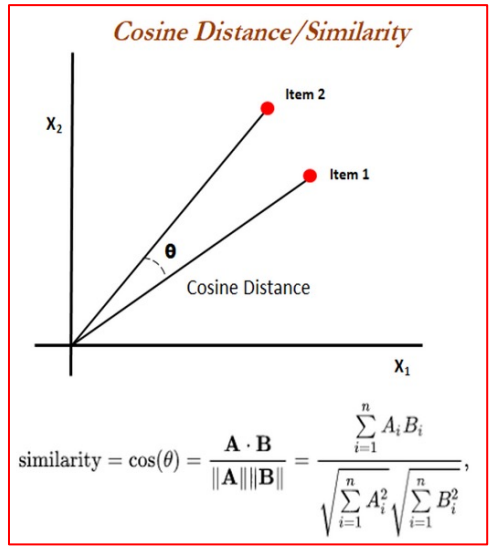
How to detect over-smoothing?

MAD computes the Mean Average Distance (MAD) between node representations (embeddings) in the graph

Metric 1: MAD(Mean Average Distance)



$$D_{ij} = 1 - \frac{\boldsymbol{H}_{i,:} \cdot \boldsymbol{H}_{j,:}}{|\boldsymbol{H}_{i,:}| \cdot |\boldsymbol{H}_{j,:}|} \qquad i, j \in [1, 2, \cdots, n],$$



Measuring and Relieving the Over-smoothing Problem for Graph Neural Networks from the Topological View

Deli Chen,[1] Yankai Lin,[2] Wei Li,[1] Peng Li,[2] Jie Zhou,[2] Xu Sun[1]
[1]MOE Key Lab of Computational Linguistics, School of EECS, Peking University
[2]Pattern Recognition Center, WeChat AI, Tencent Inc., China
{chendeli,liweitj47,xusun}@pku.edu.cn, {yankailin,patrickpli,withtomzhou}@tencent.com,

How to detect over-smoothing?

Metric 2 : MADGap

$$\text{MADGap} = \text{MAD}^{\text{rmt}} - \text{MAD}^{\text{neb}}, \quad (5)$$

where MAD^{rmt} is the MAD value of the remote nodes in the graph topology and MAD^{neb} is the MAD value of the neighbouring nodes.

It is based on the main hypothesis that when nodes interact, they have access to either important information from nodes of the same class or noise from nodes of other classes.

Measuring and Relieving the Over-smoothing Problem for Graph Neural Networks from the Topological View

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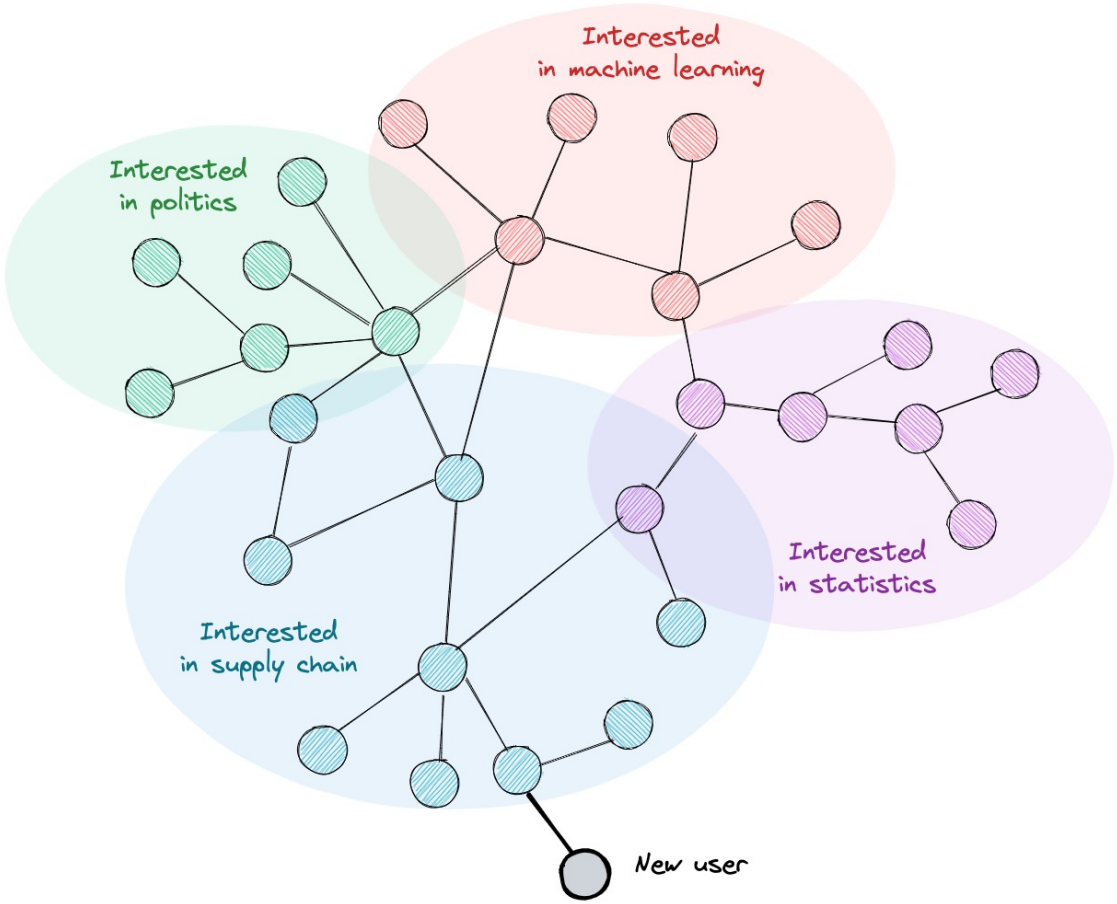
[2]Pattern Recognition Center, WeChat AI, Tencent Inc., China
{chendeli,liweitj47,xusun}@pku.edu.cn, {yankailin,patrickpli,withtomzhou}@tencent.com,

Over-smoothing in GNN



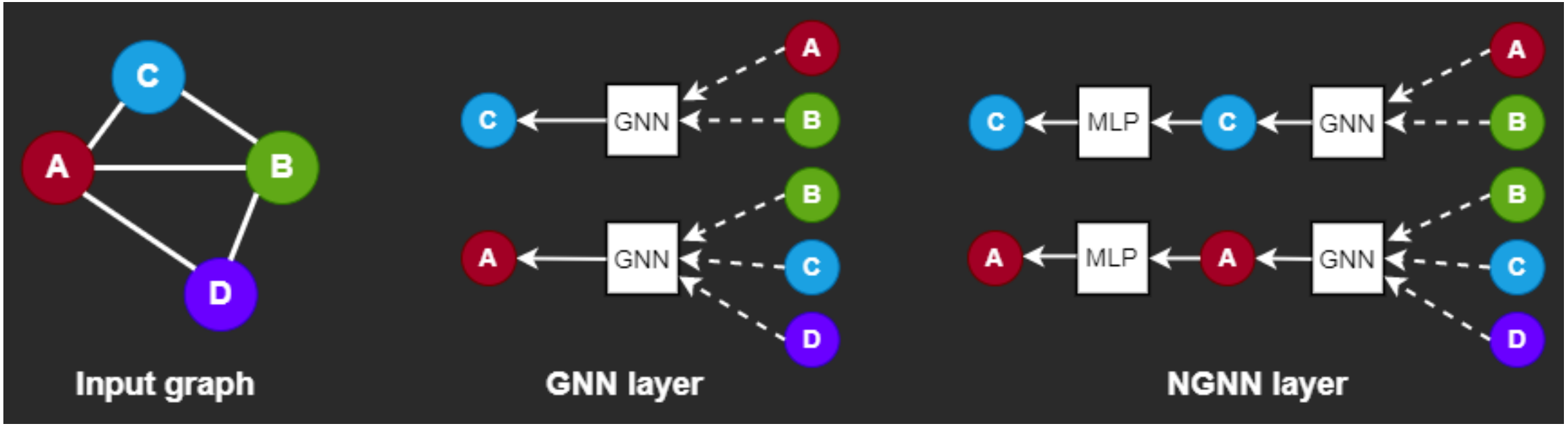
How to reduce the effect of over-smoothing.

We encounter a trade-off between a low-efficiency model and a model with more depth but less expressivity in terms of node representations

Imagine that we're dealing with a social network graph with thousands of nodes. Some new users just signed in to the platform and subscribed to their friend's profiles. Our goal is to find topic suggestions to fill their feed.

Over-smoothing in GNN

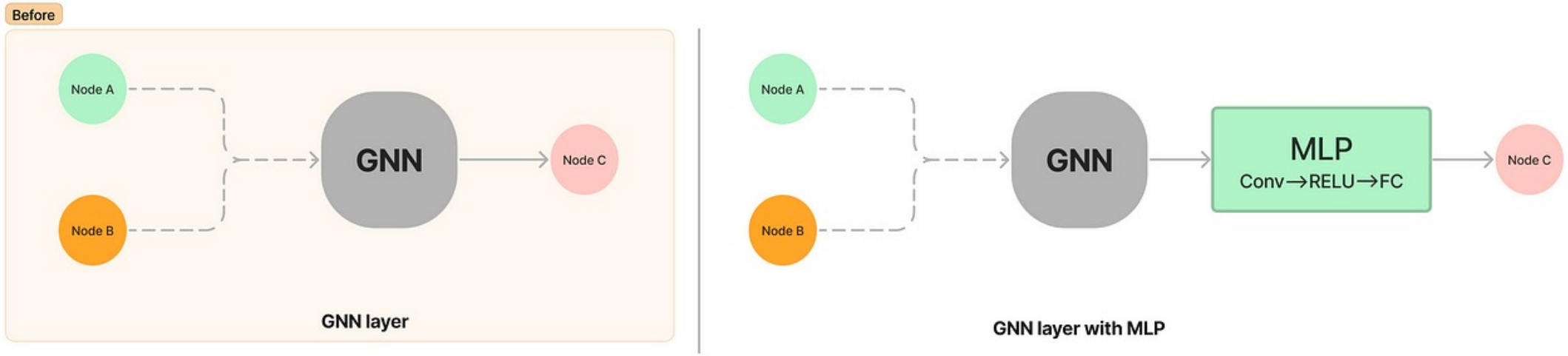
Solution ⟶ Inserting nonlinear feedforward neural network layer(s) within each GNN layer.



https://www.dgl.ai/blog/2022/11/28/ngnn.html

Over-smoothing in GNN

Solution ⟶ Inserting nonlinear feedforward neural network layer(s) within each GNN layer.



https://www.dgl.ai/blog/2022/11/28/ngnn.html

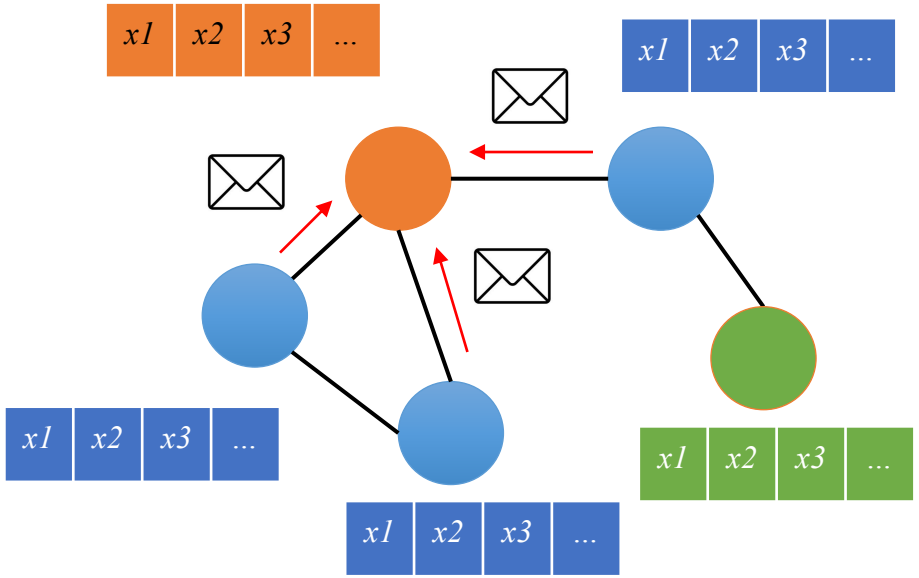
Over-smoothing in GNN

Solution ⟶ Inserting nonlinear feedforward neural network layer(s) within each GNN layer.

Dataset	Metric	Model		Performance
ogbn-proteins	ROC-AUC(%)	GraphSage+Cluster Sampling	Vanilla	67.45 ± 1.21
			+NGNN	**68.12 ± 0.96**
ogbn-products	Accuracy(%)	GraphSage	Vanilla	78.27 ± 0.45
			+NGNN	**79.88 ± 0.34**
		GAT+Neighbor Sampling	Vanilla	79.23 ± 0.16
			+NGNN	**79.67 ± 0.09**
ogbl-collab	hit@50(%)	GCN	Vanilla	49.52 ± 0.70
			+NGNN	**53.48 ± 0.40**
		GraphSage	Vanilla	51.66 ± 0.35
			+NGNN	**53.59 ± 0.56**
ogbl-ppa	hit@100(%)	SEAL-DGCNN	Vanilla	48.80 ± 3.16
			+NGNN	**59.71 ± 2.45**
		GCN	Vanilla	18.67 ± 1.32
			+NGNN	**36.83 ± 0.99**

https://www.dgl.ai/blog/2022/11/28/ngnn.html

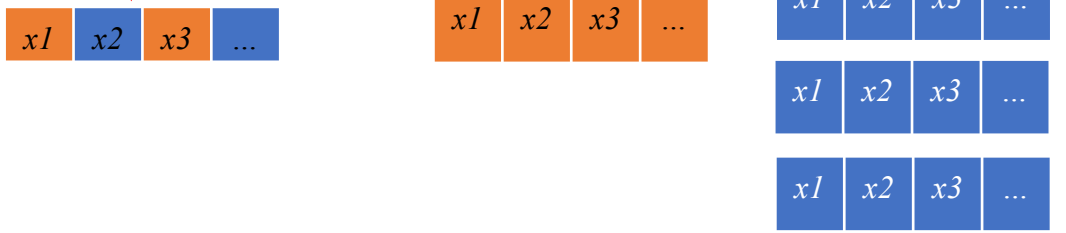
Message Passing: Math is Fun

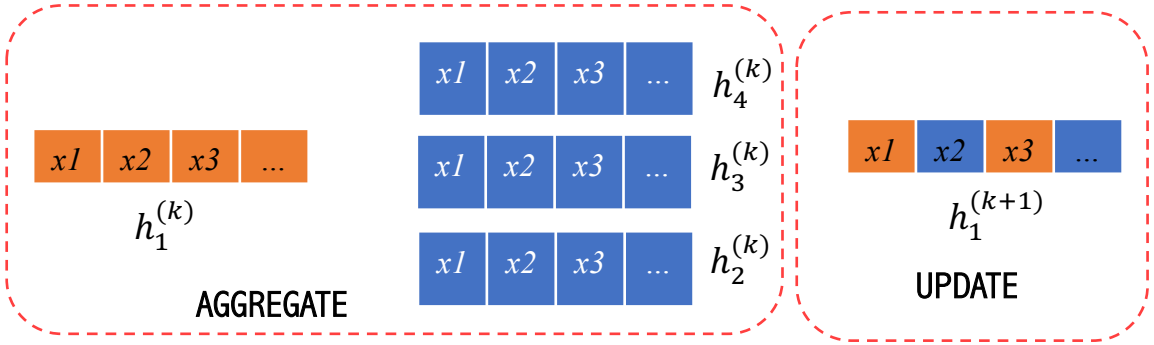


Mean
Max
Neural Network
Recurrent Neural Network

Mean
Max
Normalization Sum
Neural Network

$$h_u^{k+1} = UPDATE^{(k)}\left(h_u^{k+1}, AGGREGATE^{(k)}\left(\{h_V^k\}, \forall v \in \mathrm{N}(u)\right)\right)$$





Message Passing: Variants

Graph Convolutional Networks, Kipf and Welling [2016]

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

Self-loop

Sum of normalized neighbor embeddings

Multi-Layer-Perceptron as Aggregator, Zaheer et al. [2017]

$$\mathbf{m}_{\mathcal{N}(u)} = \mathrm{MLP}_\theta\left(\sum_{v \in N(u)} \mathrm{MLP}_\phi(\mathbf{h}_v)\right)$$

Aggregated message

trainable!

Send states through a MLP

Graph Attention Networks, Veličković et al. [2017]

$$\mathbf{m}_{\mathcal{N}(u)} = \sum_{v \in \mathcal{N}(u)} \alpha_{u,v} \mathbf{h}_v$$

Attention weights

$$\alpha_{u,v} = \frac{\exp\left(\mathbf{a}^\top [\mathbf{W}\mathbf{h}_u \oplus \mathbf{W}\mathbf{h}_v]\right)}{\sum_{v' \in \mathcal{N}(u)} \exp\left(\mathbf{a}^\top [\mathbf{W}\mathbf{h}_u \oplus \mathbf{W}\mathbf{h}_{v'}]\right)}$$

Gated Graph Neural Networks, Li et al. [2015]

$$\mathbf{h}_u^{(k)} = \mathrm{GRU}(\mathbf{h}_u^{(k-1)}, \mathbf{m}_{\mathcal{N}(u)}^{(k)})$$

Recurrent update of the state

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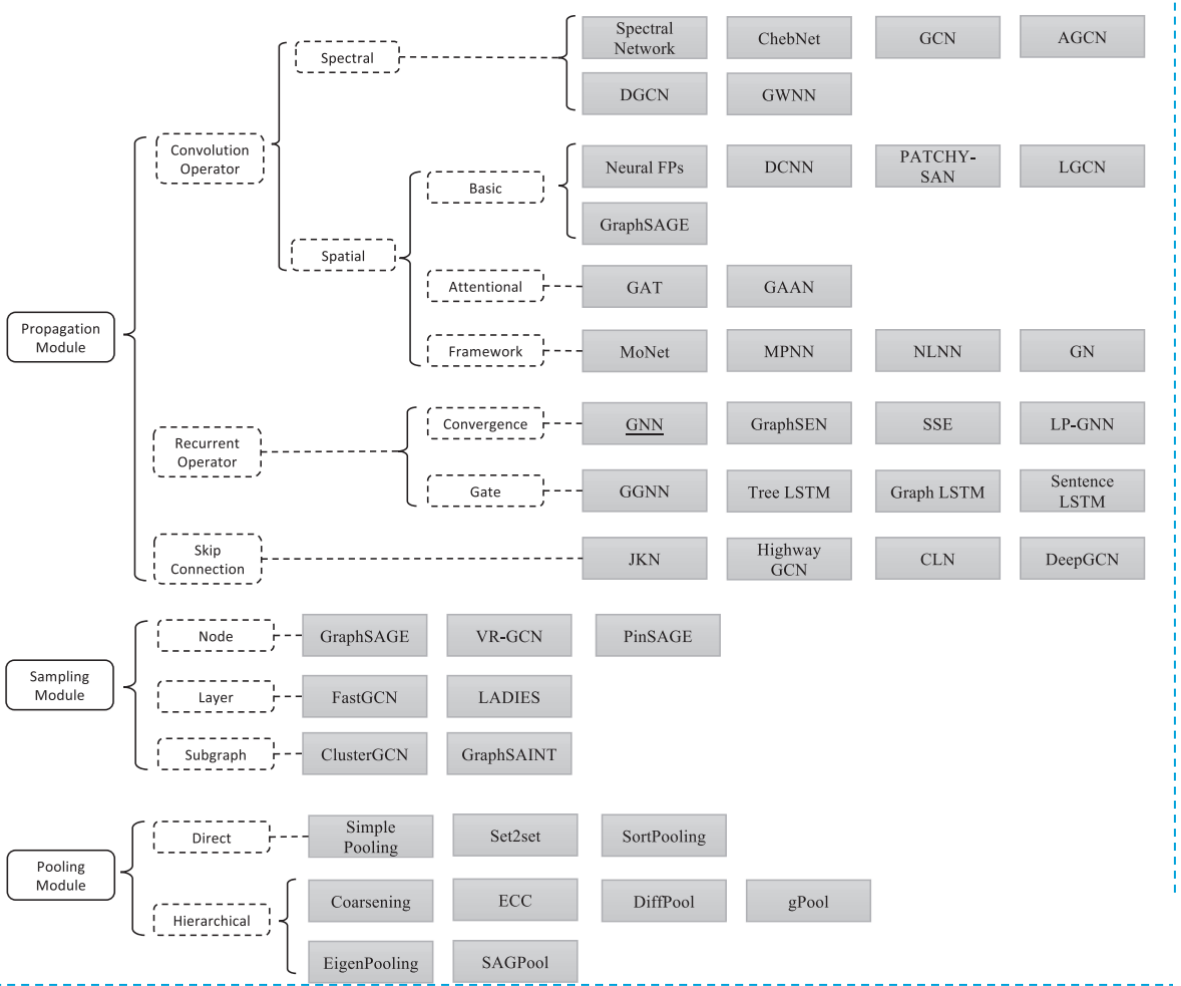
Message Passing: Variants



Different variants of recurrent operators.

Variant	Aggregator	Updater
GGNN	$\mathbf{h}^t_{\mathcal{N}_v} = \sum_{k\in\mathcal{N}_v} \mathbf{h}^{t-1}_k + \mathbf{b}$	$\mathbf{z}^t_v = \sigma(\mathbf{W}^z\mathbf{h}^t_{\mathcal{N}_v} + \mathbf{U}^z\mathbf{h}^{t-1}_v)$ $\mathbf{r}^t_v = \sigma(\mathbf{W}^r\mathbf{h}^t_{\mathcal{N}_v} + \mathbf{U}^r\mathbf{h}^{t-1}_v)$ $\tilde{\mathbf{h}}^t_v = \tanh(\mathbf{W}\mathbf{h}^t_{\mathcal{N}_v} + \mathbf{U}(\mathbf{r}^t_v \odot \mathbf{h}^{t-1}_v))$ $\mathbf{h}^t_v = (1-\mathbf{z}^t_v)\odot\mathbf{h}^{t-1}_v + \mathbf{z}^t_v \odot \tilde{\mathbf{h}}^t_v$
Tree LSTM (Child sum)	$\mathbf{h}^{ti}_{\mathcal{N}_v} = \sum_{k\in\mathcal{N}_v} \mathbf{U}^i\mathbf{h}^{t-1}_k$ $\mathbf{h}^{tf}_{\mathcal{N}_v k} = \mathbf{U}^f\mathbf{h}^{t-1}_k$ $\mathbf{h}^{to}_{\mathcal{N}_v} = \sum_{k\in\mathcal{N}_v} \mathbf{U}^o\mathbf{h}^{t-1}_k$ $\mathbf{h}^{tu}_{\mathcal{N}_v} = \sum_{k\in\mathcal{N}_v} \mathbf{U}^u\mathbf{h}^{t-1}_k$	$\mathbf{i}^t_v = \sigma(\mathbf{W}^i\mathbf{x}^t_v + \mathbf{h}^{ti}_{\mathcal{N}_v} + \mathbf{b}^i)$ $\mathbf{f}^t_{vk} = \sigma(\mathbf{W}^f\mathbf{x}^t_v + \mathbf{h}^{tf}_{\mathcal{N}_v k} + \mathbf{b}^f)$ $\mathbf{o}^t_v = \sigma(\mathbf{W}^o\mathbf{x}^t_v + \mathbf{h}^{to}_{\mathcal{N}_v} + \mathbf{b}^o)$ $\mathbf{u}^t_v = \tanh(\mathbf{W}^u\mathbf{x}^t_v + \mathbf{h}^{tu}_{\mathcal{N}_v} + \mathbf{b}^u)$ $\mathbf{c}^t_v = \mathbf{i}^t_v \odot \mathbf{u}^t_v + \sum_{k\in\mathcal{N}_v} \mathbf{f}^t_{vk} \odot \mathbf{c}^{t-1}_k$ $\mathbf{h}^t_v = \mathbf{o}^t_v \odot \tanh(\mathbf{c}^t_v)$
Tree LSTM (N-ary)	$\mathbf{h}^{ti}_{\mathcal{N}_v} = \sum_{l=1}^{K} \mathbf{U}^i_l\mathbf{h}^{t-1}_{vl}$ $\mathbf{h}^{tf}_{\mathcal{N}_v k} = \sum_{l=1}^{K} \mathbf{U}^f_{kl}\mathbf{h}^{t-1}_{vl}$ $\mathbf{h}^{to}_{\mathcal{N}_v} = \sum_{l=1}^{K} \mathbf{U}^o_l\mathbf{h}^{t-1}_{vl}$ $\mathbf{h}^{tu}_{\mathcal{N}_v} = \sum_{l=1}^{K} \mathbf{U}^u_l\mathbf{h}^{t-1}_{vl}$	
Graph LSTM in (Peng et al., 2017)	$\mathbf{h}^{ti}_{\mathcal{N}_v} = \sum_{k\in\mathcal{N}_v} \mathbf{U}^i_{m(v,k)}\mathbf{h}^{t-1}_k$ $\mathbf{h}^{tf}_{\mathcal{N}_v k} = \mathbf{U}^f_{m(v,k)}\mathbf{h}^{t-1}_k$ $\mathbf{h}^{to}_{\mathcal{N}_v} = \sum_{k\in\mathcal{N}_v} \mathbf{U}^o_{m(v,k)}\mathbf{h}^{t-1}_k$ $\mathbf{h}^{tu}_{\mathcal{N}_v} = \sum_{k\in\mathcal{N}_v} \mathbf{U}^u_{m(v,k)}\mathbf{h}^{t-1}_k$	

Graph neural networks: A review of methods and applications

Jie Zhou [a,1], Ganqu Cui [a,1], Shengding Hu [a], Zhengyan Zhang [a], Cheng Yang [b], Zhiyuan Liu [a,*], Lifeng Wang [c], Changcheng Li [c], Maosong Sun [a]

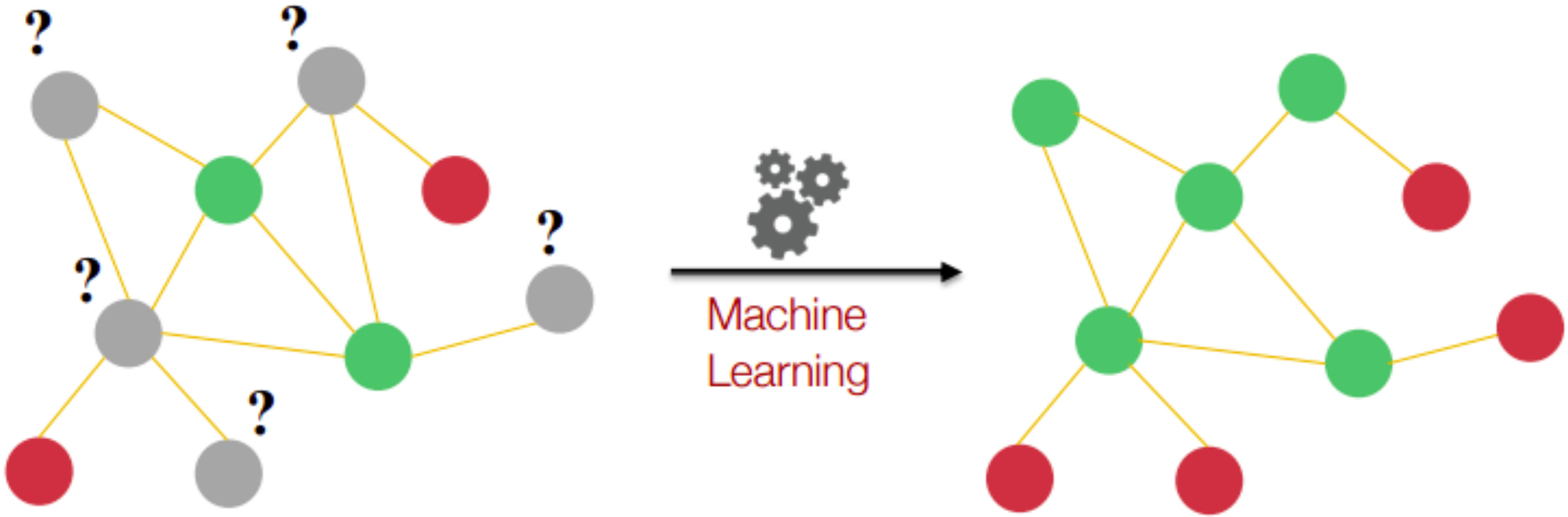
[a] Department of Computer Science and Technology, Tsinghua University, Beijing, China
[b] School of Computer Science, Beijing University of Posts and Telecommunications, China
[c] Tencent Incorporation, Shenzhen, China


QUIZ TIME

Outline

- Objective
- Introduction to Graph Data
- Graph Data with Neural Network
- Node Classification Problem: Cora Citation Dataset
- Summary

Node Classification Problem



GNN: Node Classification

Knowledge Graphs and Node Classification

We have one large graph and not many individual graphs (like molecules)
We infere on unlabeled nodes in this large graph and hence perform node-level predictions
--> We have to use different nodes of the graph depending on what we want to do

Dataset Introduction: Cora Citation Dataset in PyTorch Geometric

The Cora dataset consists of 2708 scientific publications classified into one of seven classes.
Each publication in the dataset is described by a 0/1-valued word vector indicating the absence/presence of the corresponding word from the dictionary.

- The dictionary consists of 1433 unique words.
- Nodes = Publications (Papers, Books ...)
- Edges = Citations Node Features = word vectors
- 7 Labels = Pubilcation
- type e.g. Neural_Networks, Rule_Learning, Reinforcement_Learning, Probabilistic_Methods...

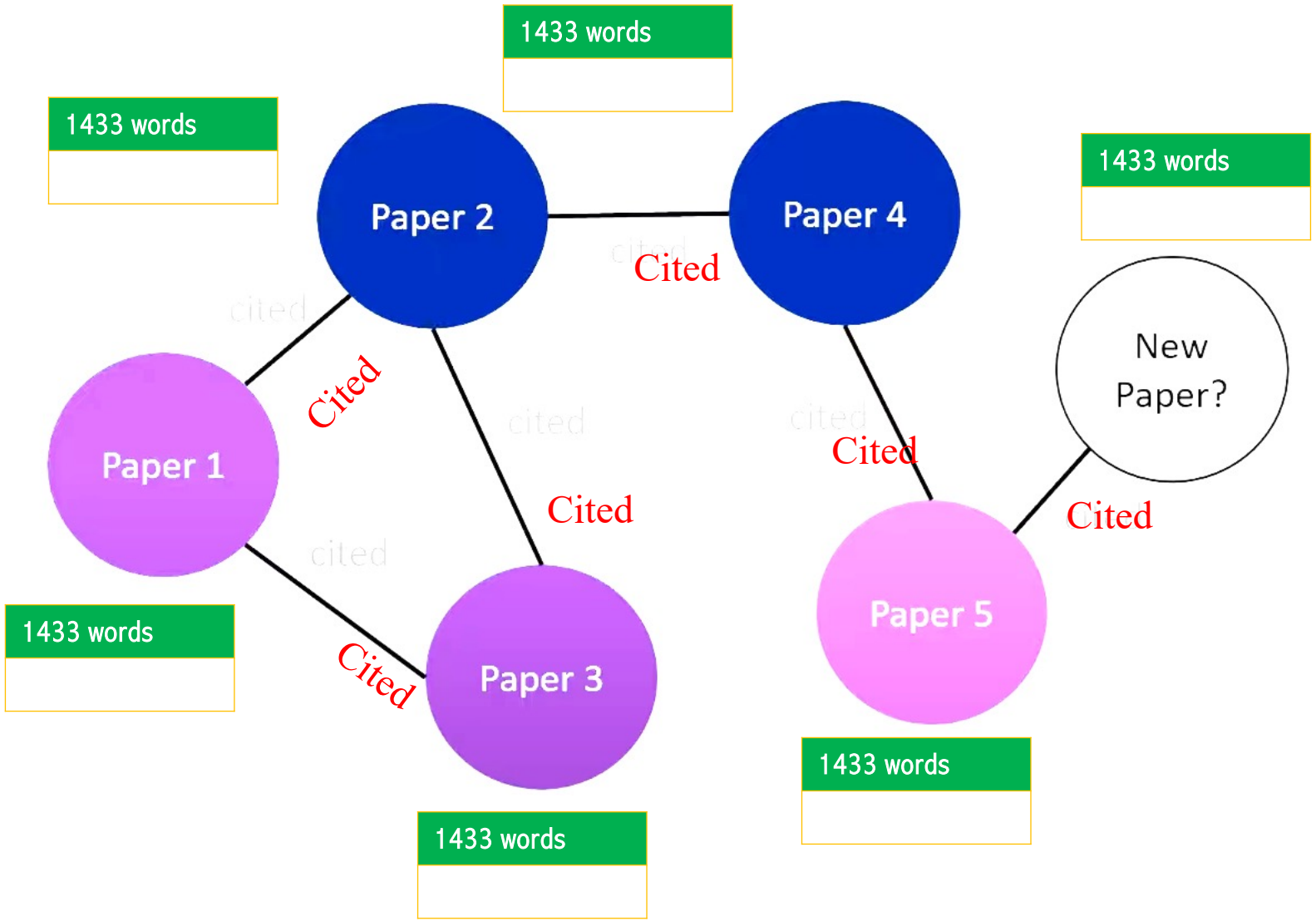
BoW Representation

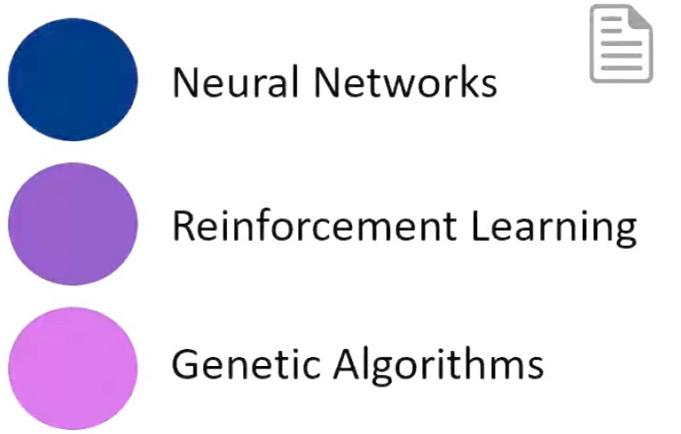
Dictionary

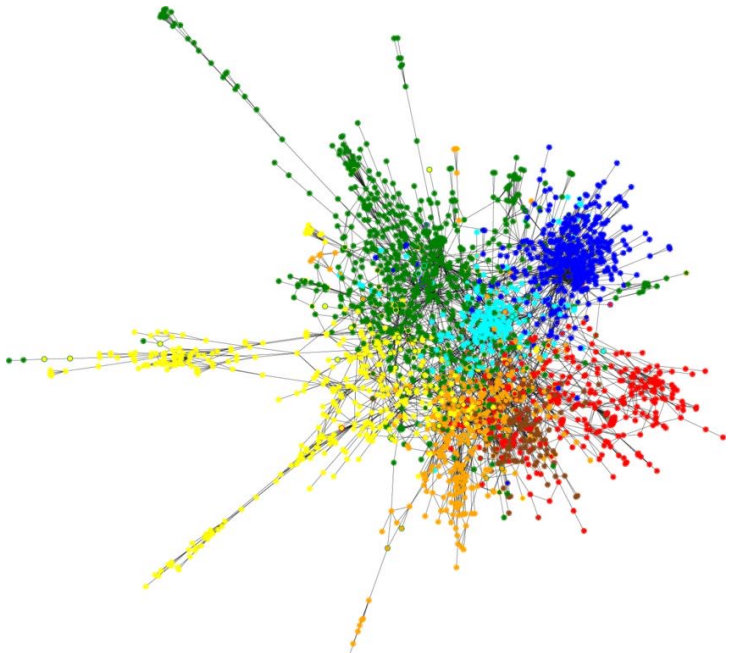
Neural	Network	ReLU	Reinforcement	... 1433 words
2	7	1	0	

Neural	Network	ReLU	Reinforcement	... 1433 words
0.43	0.88	0.03	0.00	

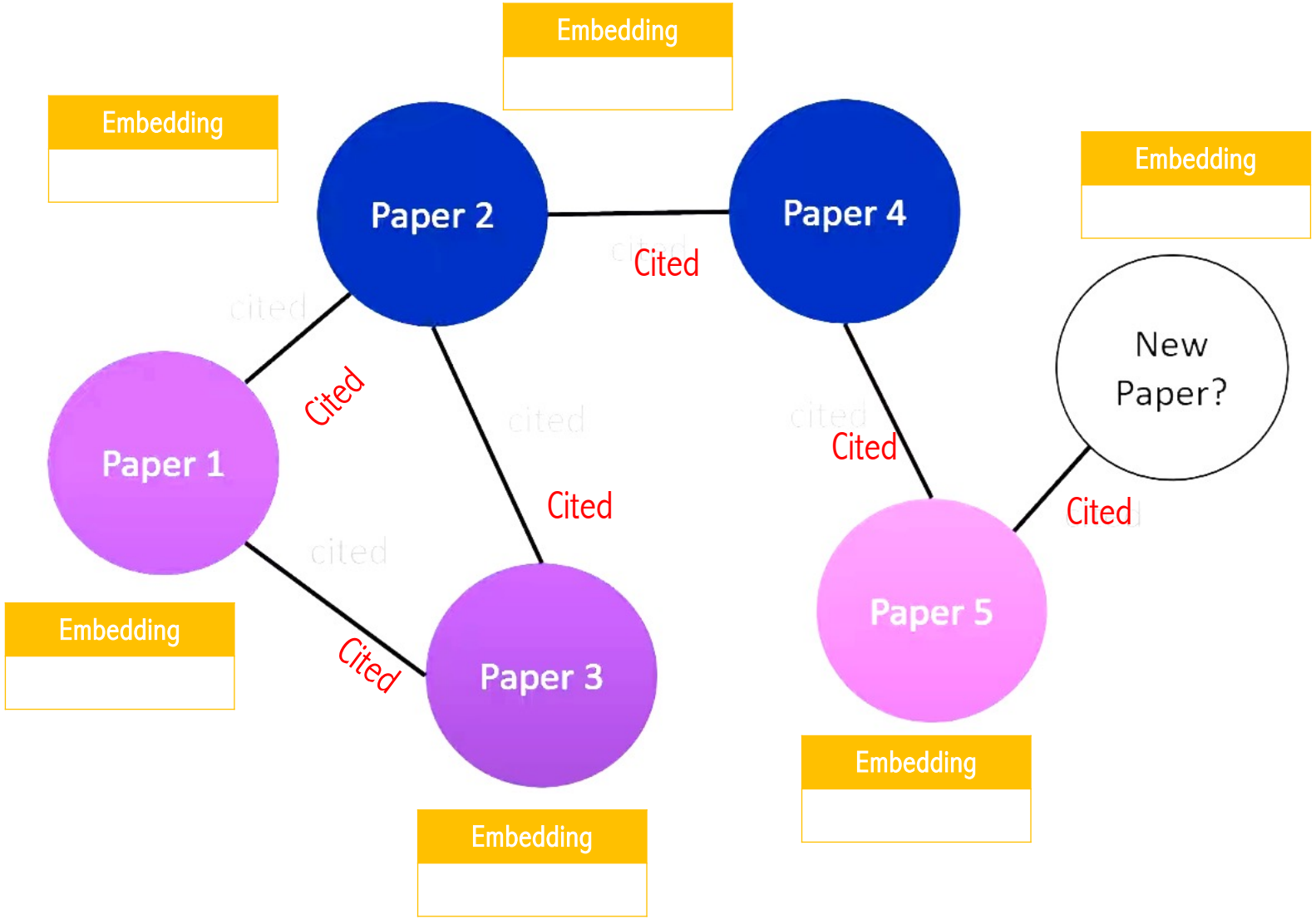
Cora Citation Dataset

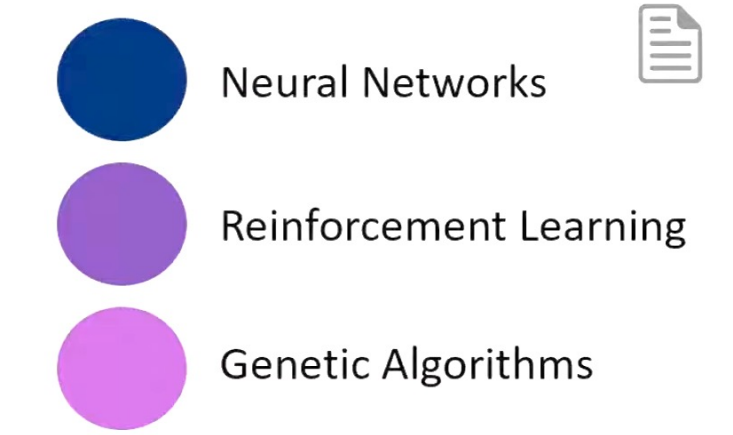


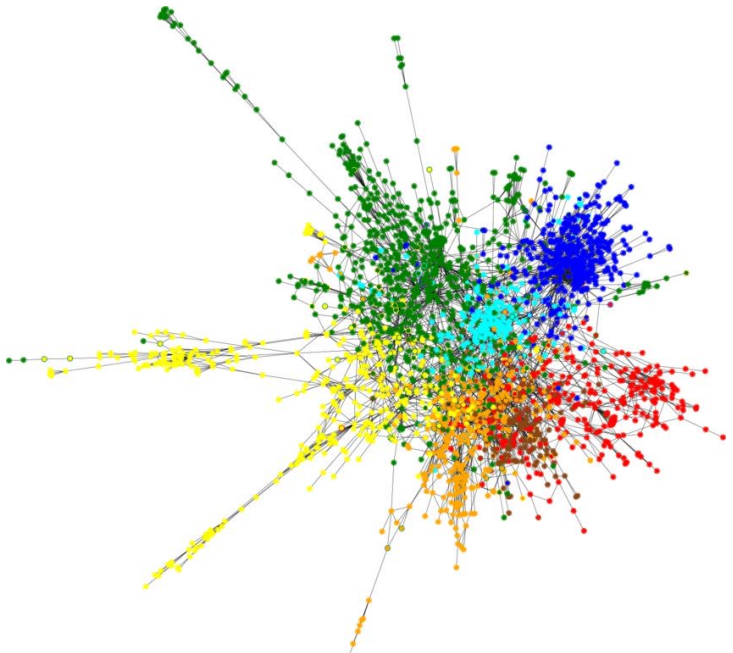




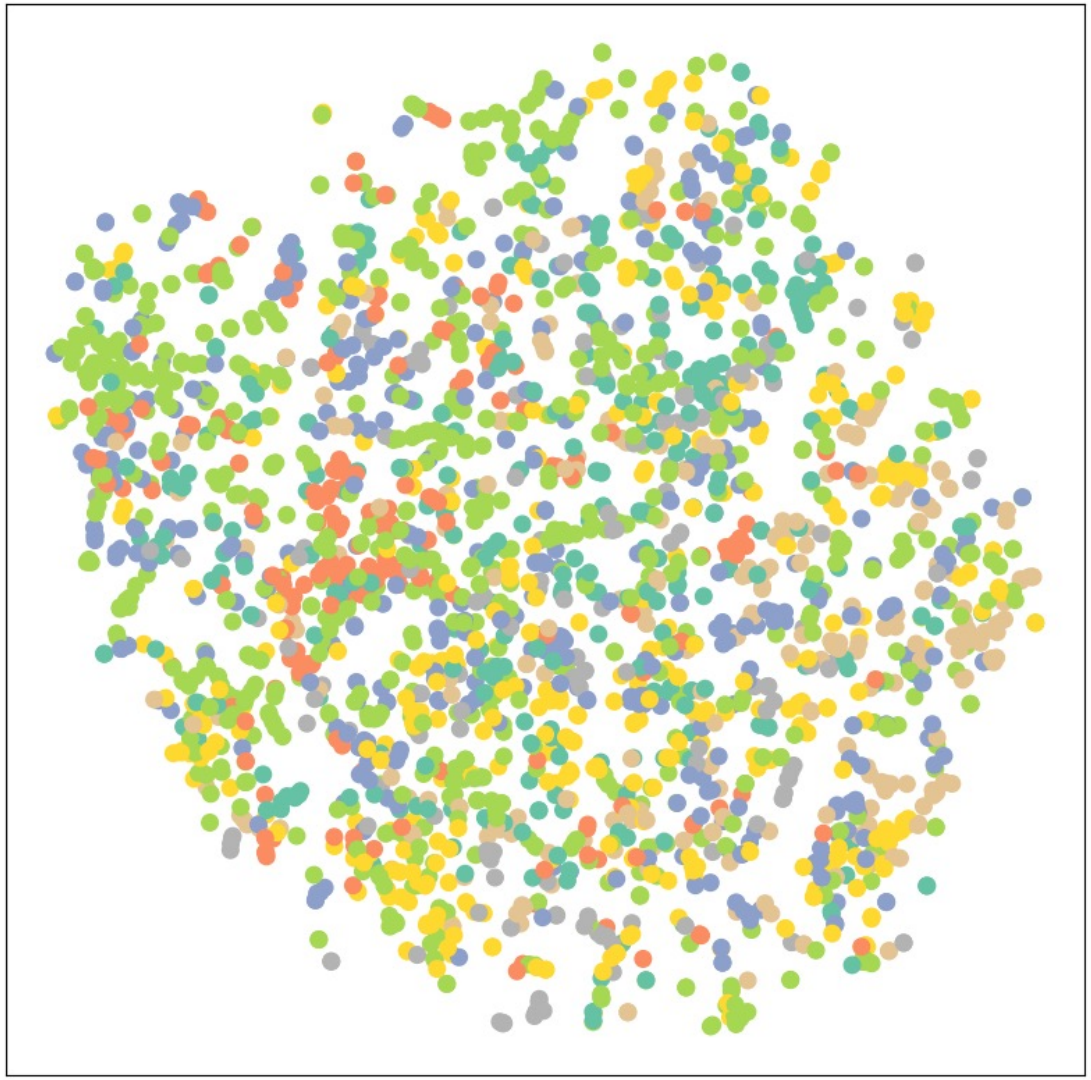
Cora Citation Dataset







Visualize the node embeddings of the untrained GCN network



```
model = GCN(hidden_channels=16)
model.eval()

out = model(data.x, data.edge_index)
visualize(out, color=data.y)
```

GNN: Node Classification

Install Pytorch Geometric

```
# Check CUDA Version
!python -c "import torch; print(torch.version.cuda)"

# Add this in a Google Colab cell to install the correct version of Pytorch Geometric.
import torch

def format_pytorch_version(version):
  return version.split('+')[0]

TORCH_version = torch.__version__
TORCH = format_pytorch_version(TORCH_version)

def format_cuda_version(version):
  return 'cu' + version.replace('.', '')

CUDA_version = torch.version.cuda
CUDA = format_cuda_version(CUDA_version)

!pip install torch-scatter     -f https://pytorch-geometric.com/whl/torch-{TORCH}+{CUDA}.html
!pip install torch-sparse      -f https://pytorch-geometric.com/whl/torch-{TORCH}+{CUDA}.html
!pip install torch-cluster     -f https://pytorch-geometric.com/whl/torch-{TORCH}+{CUDA}.html
!pip install torch-spline-conv -f https://pytorch-geometric.com/whl/torch-{TORCH}+{CUDA}.html
!pip install torch-geometric
```

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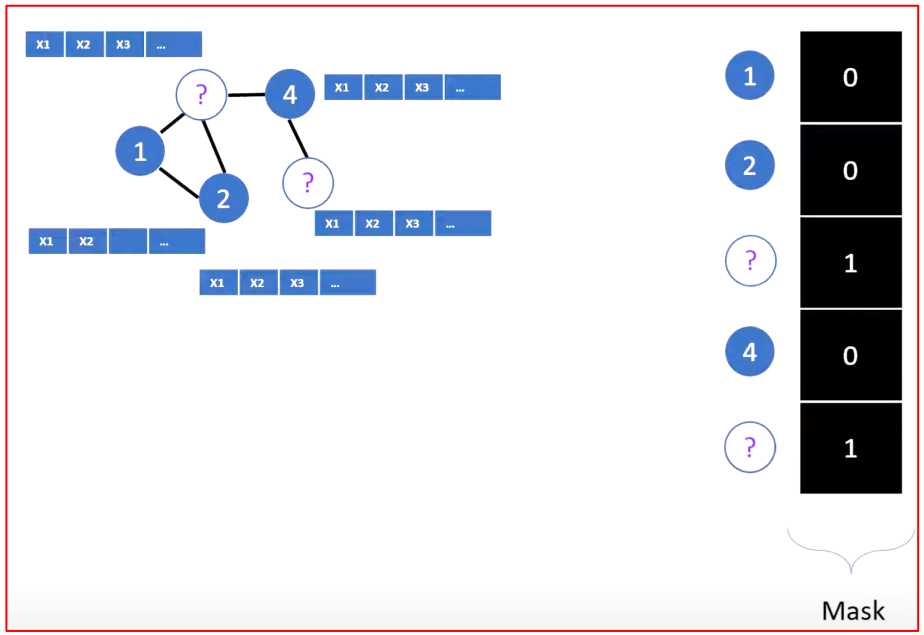
GNN: Node Classification

Load Cora Dataset

```python
from torch_geometric.datasets import Planetoid
from torch_geometric.transforms import NormalizeFeatures

dataset = Planetoid(root='data/Planetoid', name='Cora', transform=NormalizeFeatures())

# Get some basic info about the dataset
print(f'Number of graphs: {len(dataset)}')
print(f'Number of features: {dataset.num_features}')
print(f'Number of classes: {dataset.num_classes}')
print(50*'=')

# There is only one graph in the dataset, use it as new data object
data = dataset[0]

# Gather some statistics about the graph.
print(data)
print(f'Number of nodes: {data.num_nodes}')
print(f'Number of edges: {data.num_edges}')
print(f'Number of training nodes: {data.train_mask.sum()}')
print(f'Training node label rate: {int(data.train_mask.sum()) / data.num_nodes:.2f}')
print(f'Is undirected: {data.is_undirected()}')
```




```
Number of graphs: 1
Number of features: 1433
Number of classes: 7
==================================================
Data(x=[2708, 1433], edge_index=[2, 10556], y=[2708], train_mask=[2708], val_mask=[2708], test_mask=[2708])
Number of nodes: 2708
Number of edges: 10556
Number of training nodes: 140
Training node label rate: 0.05
Is undirected: True
```

GNN: Node Classification MLP

Define MLP

Here, we first reduce the 1433-dimensional feature vector to a low-dimensional embedding (hidden_channels=16), while the second linear layer acts as a classifier that should map each low-dimensional node embedding to one of the 7 classes.

```python
import torch
from torch.nn import Linear
import torch.nn.functional as F


class MLP(torch.nn.Module):
    def __init__(self, hidden_channels):
        super().__init__()
        torch.manual_seed(12345)
        self.lin1 = Linear(dataset.num_features, hidden_channels)
        self.lin2 = Linear(hidden_channels, dataset.num_classes)

    def forward(self, x):
        x = self.lin1(x)
        x = x.relu()
        x = F.dropout(x, p=0.5, training=self.training)
        x = self.lin2(x)
        return x

model = MLP(hidden_channels=16)
print(model)
```

```
test_acc = test()
print(f'Test Accuracy: {test_acc:.4f}')

Test Accuracy: 0.5900
```

GNN: Node Classification MLP

How to Train

Here, we first reduce the 1433-dimensional feature vector to a low-dimensional embedding (hidden_channels=16), while the second linear layer acts as a classifier that should map each low-dimensional node embedding to one of the 7 classes.

```
test_acc = test()
print(f'Test Accuracy: {test_acc:.4f}')
```

```
Test Accuracy: 0.5900
```

```
from IPython.display import Javascript  # Restrict height of output cell.
display(Javascript('''google.colab.output.setIframeHeight(0, true, {maxHeight: 300})'''))

model = MLP(hidden_channels=16)
criterion = torch.nn.CrossEntropyLoss()  # Define loss criterion.
optimizer = torch.optim.Adam(model.parameters(), lr=0.01, weight_decay=5e-4)  # Define optimizer.

def train():
      model.train()
      optimizer.zero_grad()  # Clear gradients.
      out = model(data.x)  # Perform a single forward pass.
      loss = criterion(out[data.train_mask], data.y[data.train_mask])  # Compute the loss solely based on the
      loss.backward()  # Derive gradients.
      optimizer.step()  # Update parameters based on gradients.
      return loss

def test():
      model.eval()
      out = model(data.x)
      pred = out.argmax(dim=1)  # Use the class with highest probability.
      test_correct = pred[data.test_mask] == data.y[data.test_mask]  # Check against ground-truth labels.
      test_acc = int(test_correct.sum()) / int(data.test_mask.sum())  # Derive ratio of correct predictions.
      return test_acc
```

GNN: Node Classification GCN

Define GCN

```
class GCN(torch.nn.Module):
    def __init__(self, hidden_channels):
        super().__init__()
        torch.manual_seed(1234567)
        self.conv1 = GCNConv(dataset.num_features, hidden_channels)
        self.conv2 = GCNConv(hidden_channels, dataset.num_classes)

    def forward(self, x, edge_index):
        x = self.conv1(x, edge_index)
        x = x.relu()
        x = F.dropout(x, p=0.5, training=self.training)
        x = self.conv2(x, edge_index)
        return x

model = GCN(hidden_channels=16)
print(model)
```

```
GCN(
  (conv1): GCNConv(1433, 16)
  (conv2): GCNConv(16, 7)
)
```

we will use on of the most simple GNN operators, the **GCN layer** (Kipf et al. (2017)), which is defined as

$$\mathbf{x}_v^{(\ell+1)} = \mathbf{W}^{(\ell+1)} \sum_{w \in \mathcal{N}(v) \cup \{v\}} \frac{1}{c_{w,v}} \cdot \mathbf{x}_w^{(\ell)}$$

GNN: Node Classification GCN

Define GCN

```
class GCN(torch.nn.Module):
    def __init__(self, hidden_channels):
        super(GCN, self).__init__()
        torch.manual_seed(42)

        # Initialize the layers
        self.conv1 = GCNConv(dataset.num_features, hidden_channels)
        self.conv2 = GCNConv(hidden_channels, hidden_channels)
        self.out = Linear(hidden_channels, dataset.num_classes)

    def forward(self, x, edge_index):
        # First Message Passing Layer (Transformation)
        x = self.conv1(x, edge_index)
        x = x.relu()
        x = F.dropout(x, p=0.5, training=self.training)

        # Second Message Passing Layer
        x = self.conv2(x, edge_index)
        x = x.relu()
        x = F.dropout(x, p=0.5, training=self.training)

        # Output layer
        x = F.softmax(self.out(x), dim=1)
        return x
```

Dropout is only applied in the training step, but not for predictions

We have 2 Message Passing Layers and one Linear output layer

We use the softmax function for the classification problem

The output of the model are 7 probabilities, one for each class

we will use on of the most simple GNN operators, the **GCN layer** (Kipf et al. (2017)), which is defined as

$$\mathbf{x}_v^{(\ell+1)} = \mathbf{W}^{(\ell+1)} \sum_{w \in \mathcal{N}(v) \cup \{v\}} \frac{1}{c_{w,v}} \cdot \mathbf{x}_w^{(\ell)}$$

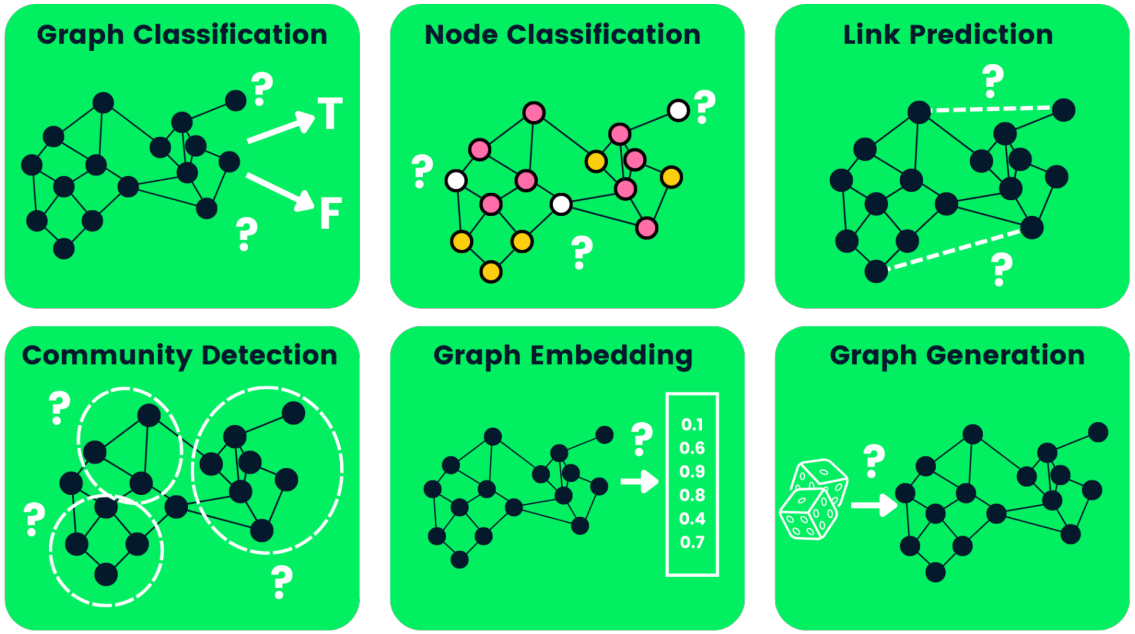
GNN: Node Classification GCN

```python
from IPython.display import Javascript  # Restrict height of output cell.
display(Javascript('''google.colab.output.setIframeHeight(0, true, {maxHeight: 300})'''))

model = GCN(hidden_channels=16)
optimizer = torch.optim.Adam(model.parameters(), lr=0.01, weight_decay=5e-4)
criterion = torch.nn.CrossEntropyLoss()

def train():
      model.train()
      optimizer.zero_grad()  # Clear gradients.
      out = model(data.x, data.edge_index)  # Perform a single forward pass.
      loss = criterion(out[data.train_mask], data.y[data.train_mask])  # Compute the loss solely based on the
      loss.backward()  # Derive gradients.
      optimizer.step()  # Update parameters based on gradients.
      return loss

def test():
      model.eval()
      out = model(data.x, data.edge_index)
      pred = out.argmax(dim=1)  # Use the class with highest probability.
      test_correct = pred[data.test_mask] == data.y[data.test_mask]  # Check against ground-truth labels.
      test_acc = int(test_correct.sum()) / int(data.test_mask.sum())  # Derive ratio of correct predictions.
      return test_acc


for epoch in range(1, 101):
    loss = train()
    print(f'Epoch: {epoch:03d}, Loss: {loss:.4f}')
```

```python
test_acc = test()
print(f'Test Accuracy: {test_acc:.4f}')
```

```
Test Accuracy: 0.8150
```

Summary



1. What is Graph Data Around Us
2. Understand Graph Neural Network
3. Understand Graph Convolutional Neural Network
4. Node Classification with Cora Citation Dataset


Thank you