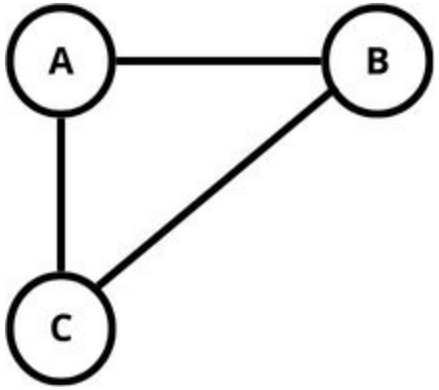
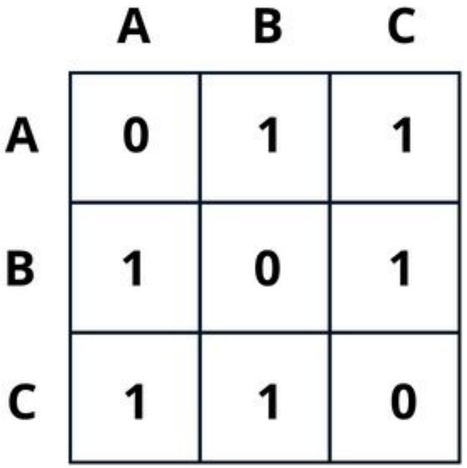
Hands on PyTorch-geometric; an introduction to Graph Neural Networks (GNNs)

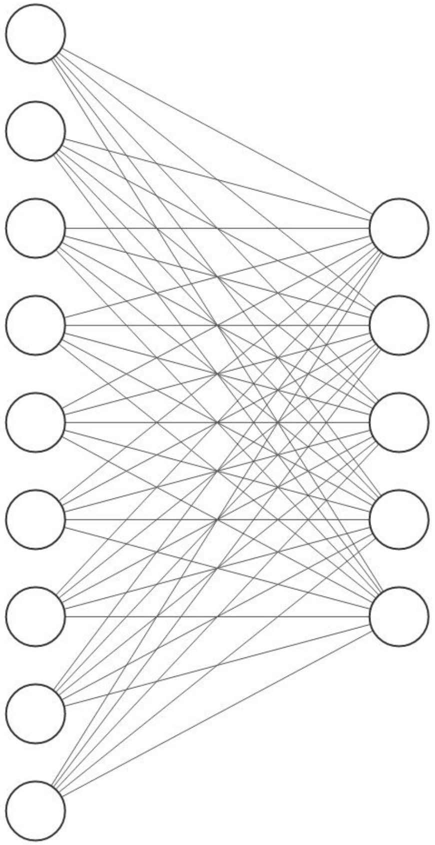
Mohamed Kherraz

Why Graph Neural Networks (GNN) ?





	A	B	C
A	0	1	1
B	1	0	1
C	1	1	0



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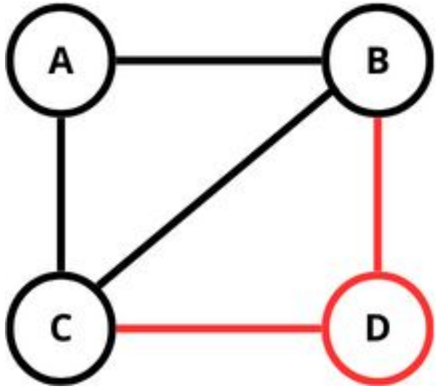
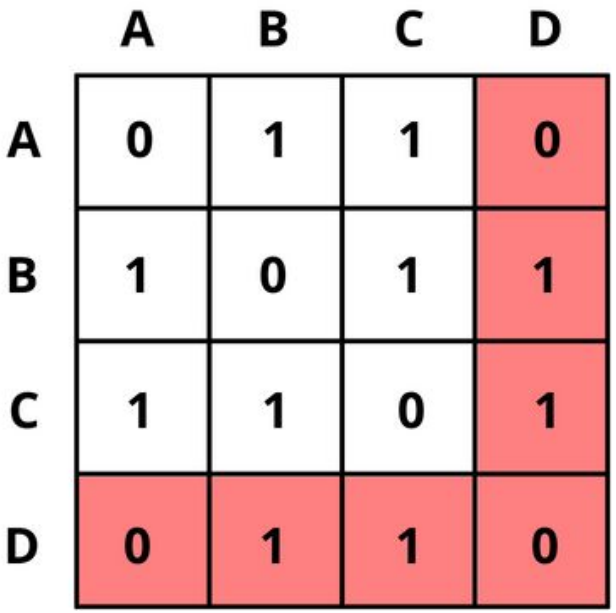
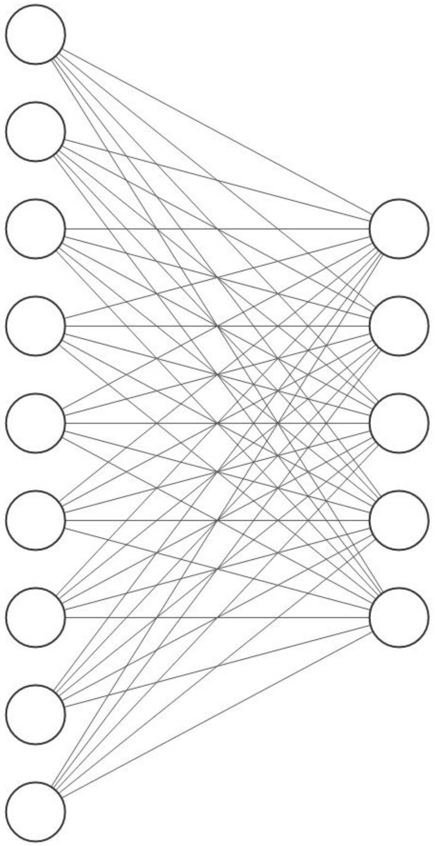




	A	B	C	D
A	0	1	1	0
B	1	0	1	1
C	1	1	0	1
D	0	1	1	0



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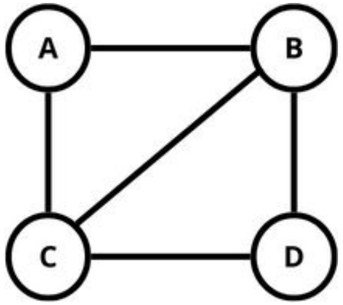
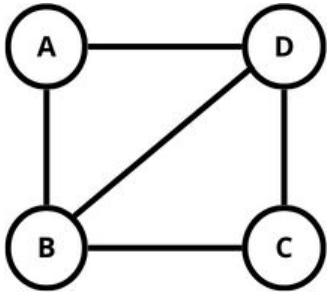
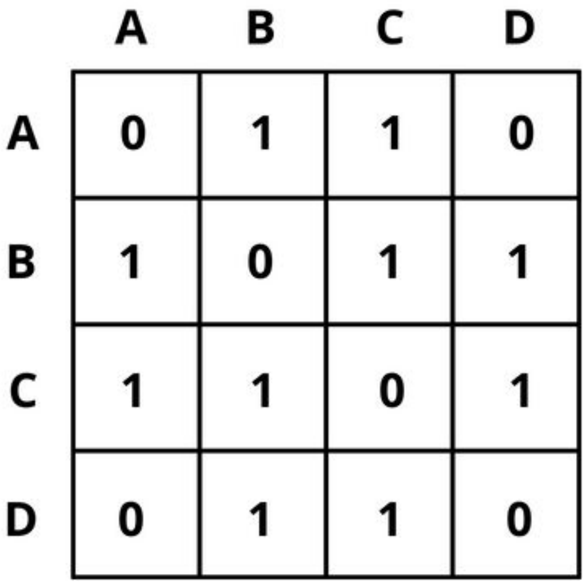
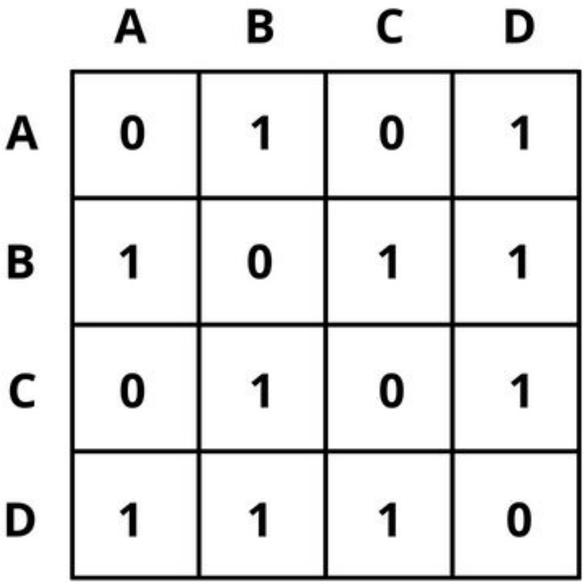






	A	B	C	D
A	0	1	1	0
B	1	0	1	1
C	1	1	0	1
D	0	1	1	0



	A	B	C	D
A	0	1	0	1
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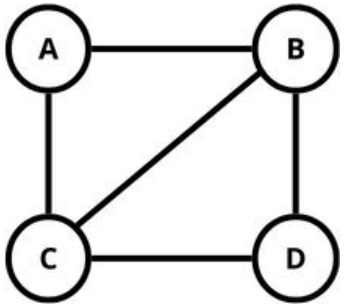
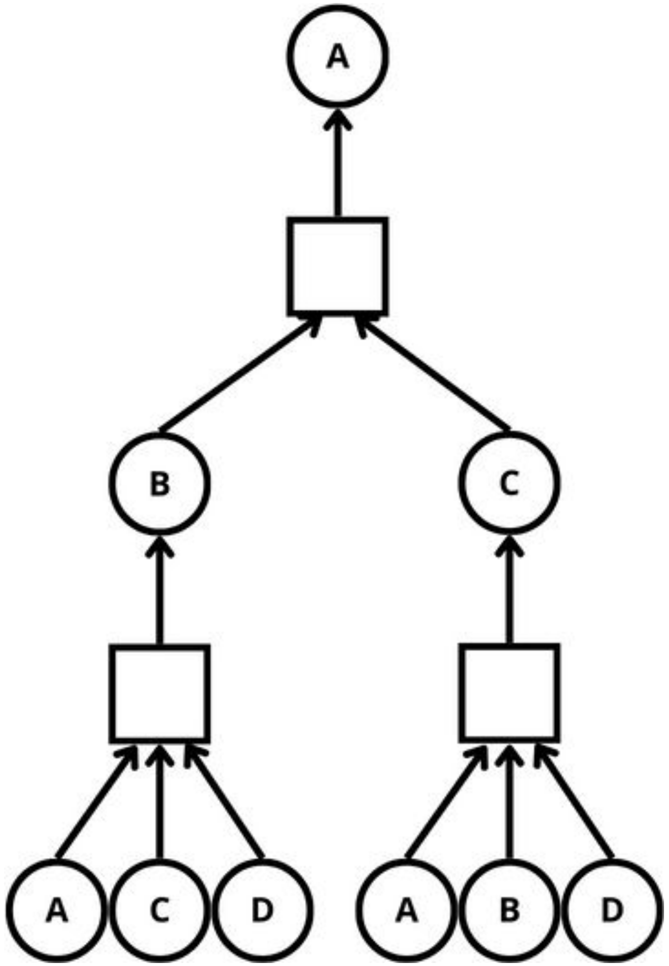
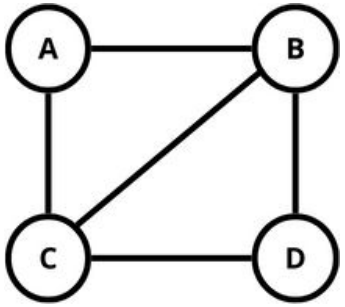
C	0	1	0	1
D	1	1	1	0

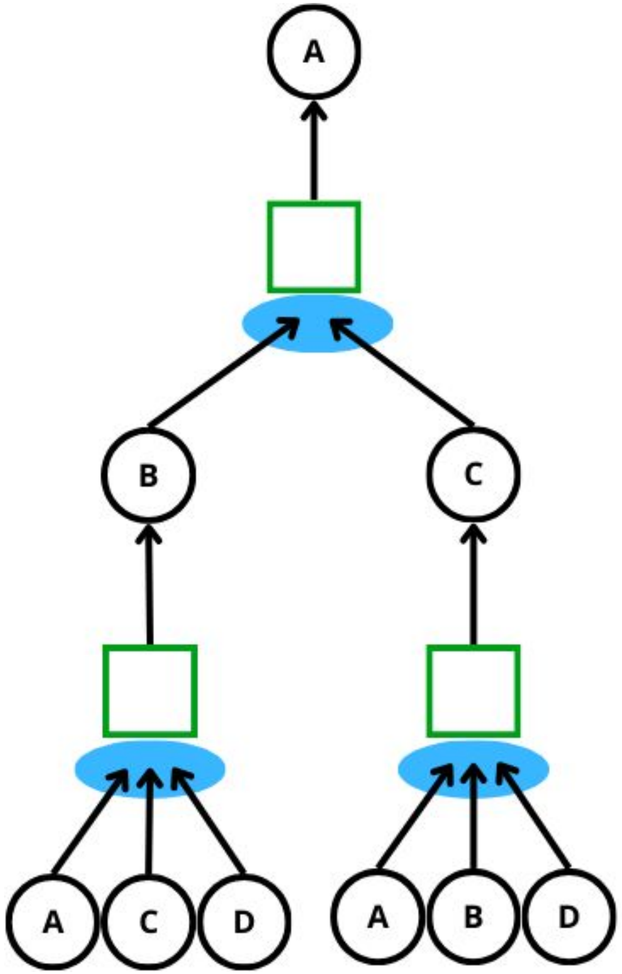
Graph Neural Networks (GNN)





Graph Neural Networks (GNN)

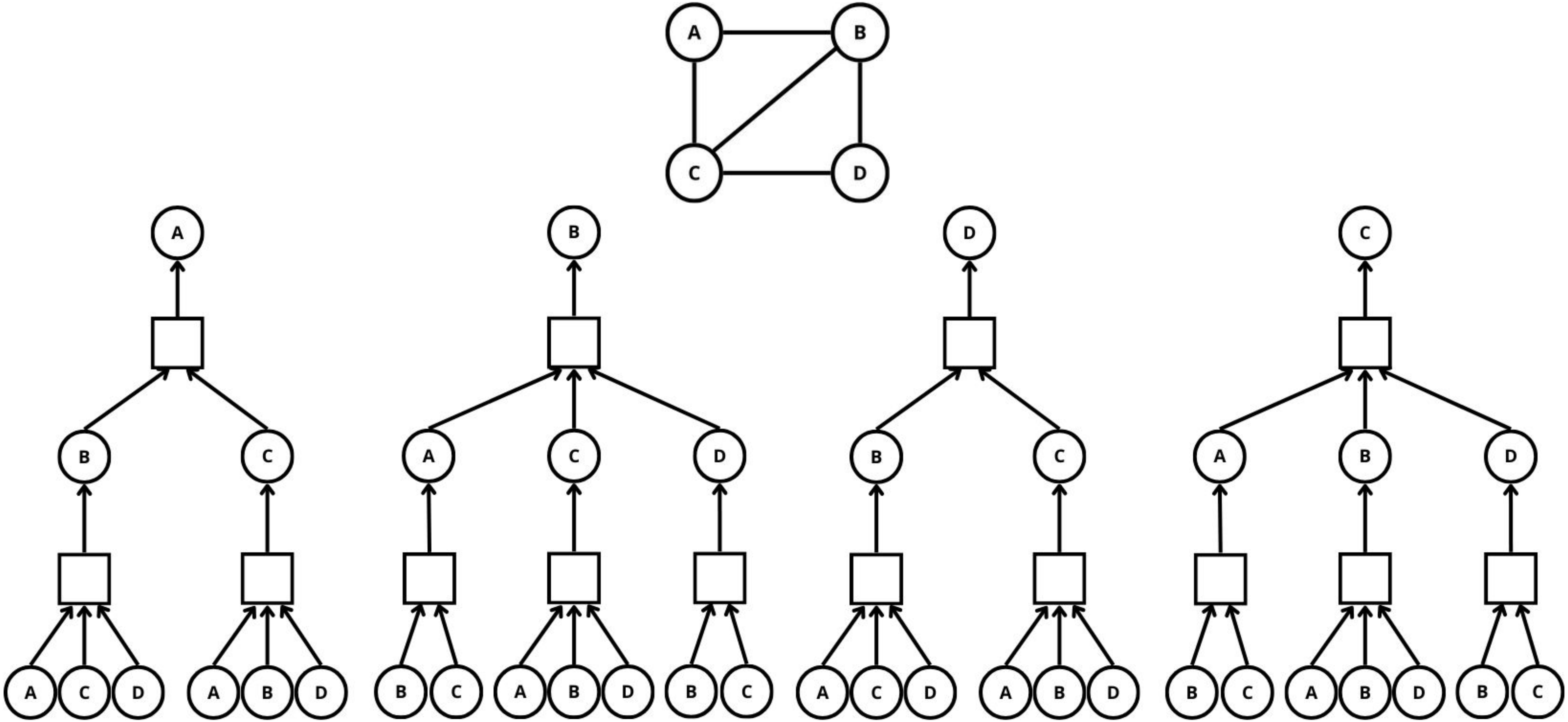




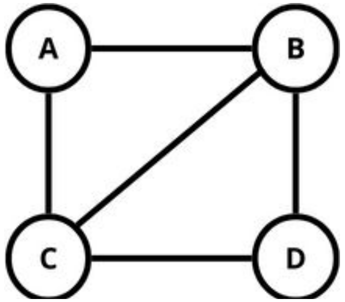
🟦 : *Ordering invariant* agrregation
(Ex : Mean, Sum, ...)

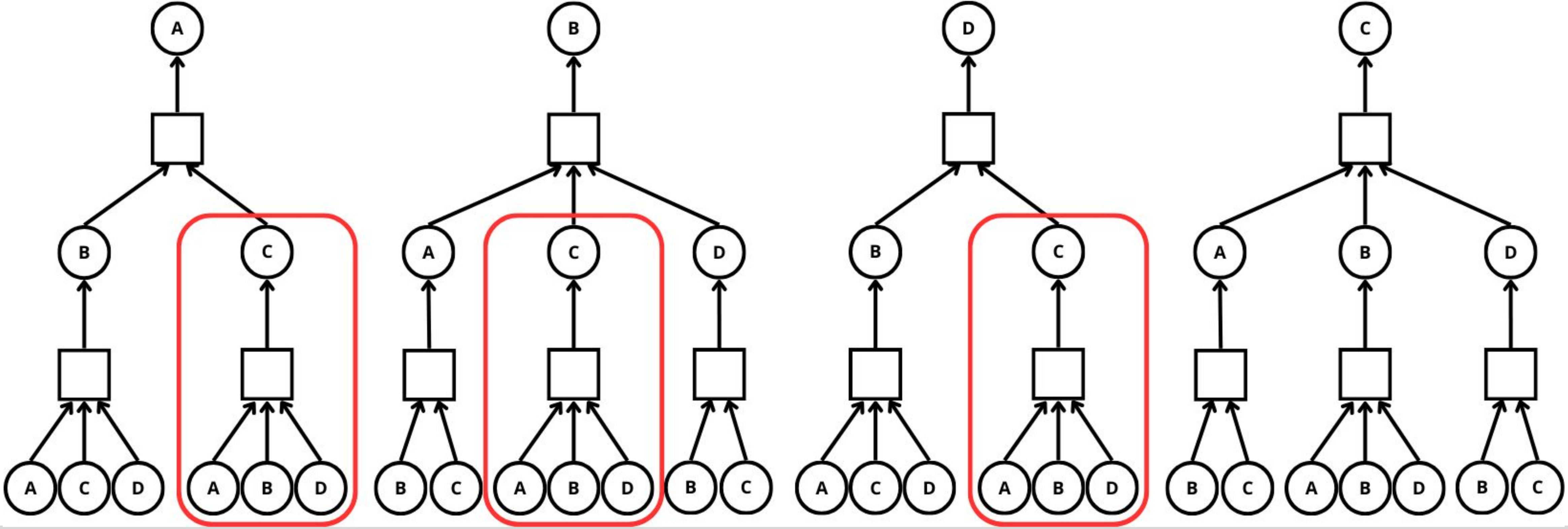
🟩 : Neural Network

Graph Neural Networks (GNN)

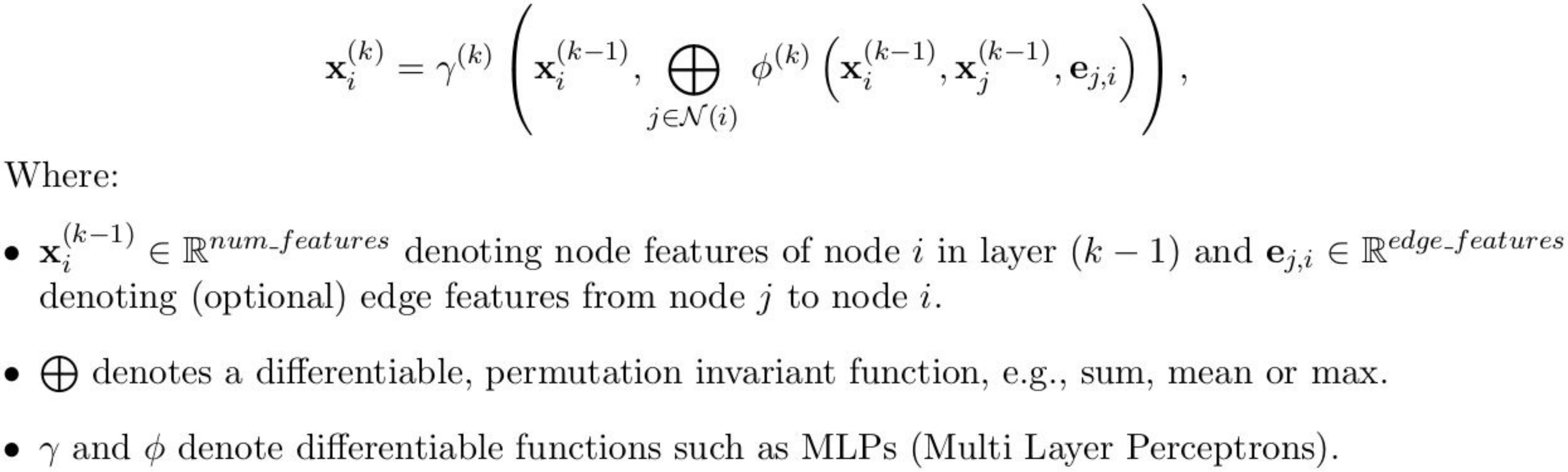


Graph Neural Networks (GNN)





Graph Neural Networks (GNN) - Message passing.



$$\mathbf{x}_i^{(k)} = \gamma^{(k)} \left(\mathbf{x}_i^{(k-1)}, \bigoplus_{j \in \mathcal{N}(i)} \phi^{(k)} \left(\mathbf{x}_i^{(k-1)}, \mathbf{x}_j^{(k-1)}, \mathbf{e}_{j,i} \right) \right),$$

Where:

- $\mathbf{x}_i^{(k-1)} \in \mathbb{R}^{num\_features}$ denoting node features of node i in layer $(k-1)$ and $\mathbf{e}_{j,i} \in \mathbb{R}^{edge\_features}$ denoting (optional) edge features from node j to node i.
- $\bigoplus$ denotes a differentiable, permutation invariant function, e.g., sum, mean or max.
- γ and ϕ denote differentiable functions such as MLPs (Multi Layer Perceptrons).

Graph Neural Networks (GNN) - GCNConv

$$\mathbf{x}_i^{(k)} = \gamma^{(k)} \left(\mathbf{x}_i^{(k-1)}, \bigoplus_{j \in \mathcal{N}(i)} \phi^{(k)} \left(\mathbf{x}_i^{(k-1)}, \mathbf{x}_j^{(k-1)}, \mathbf{e}_{j,i} \right) \right)$$

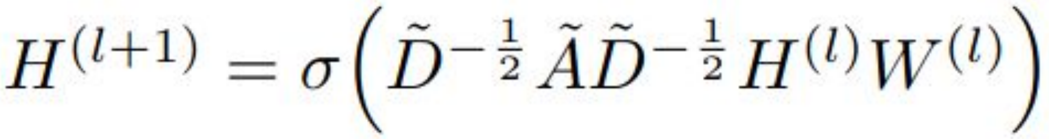
$$\tilde{A} = A + I_N$$

$$\tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$$

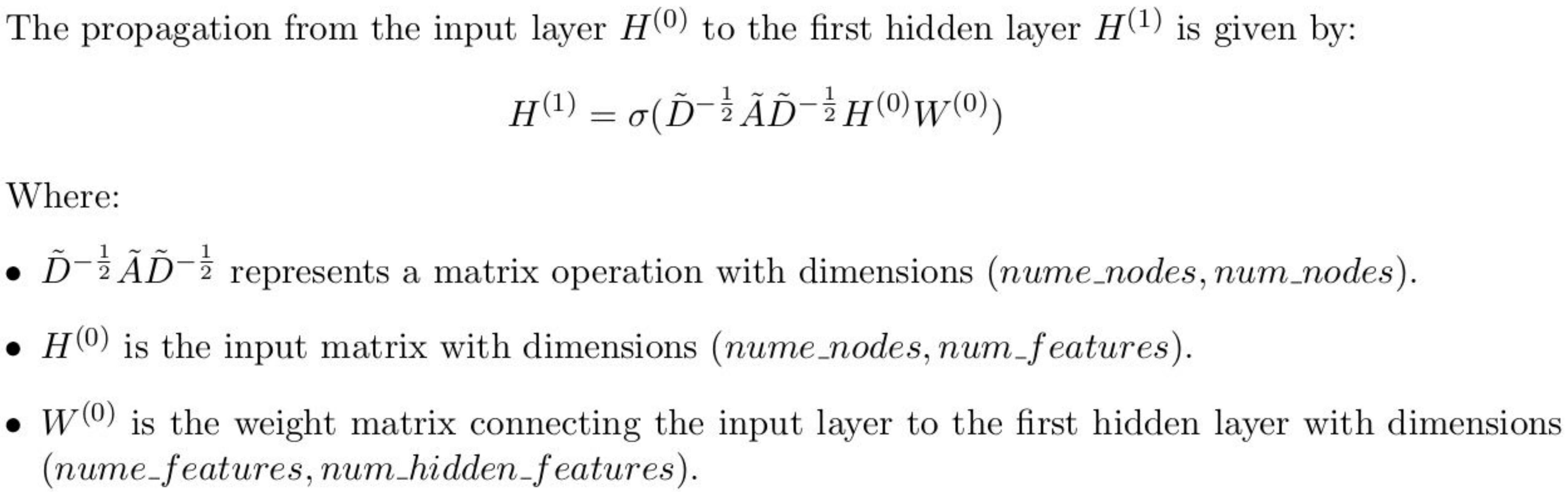
$$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right)$$

$$ReLU(.) = max(0, .)$$

Graph Neural Networks (GNN) - GCNConv



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



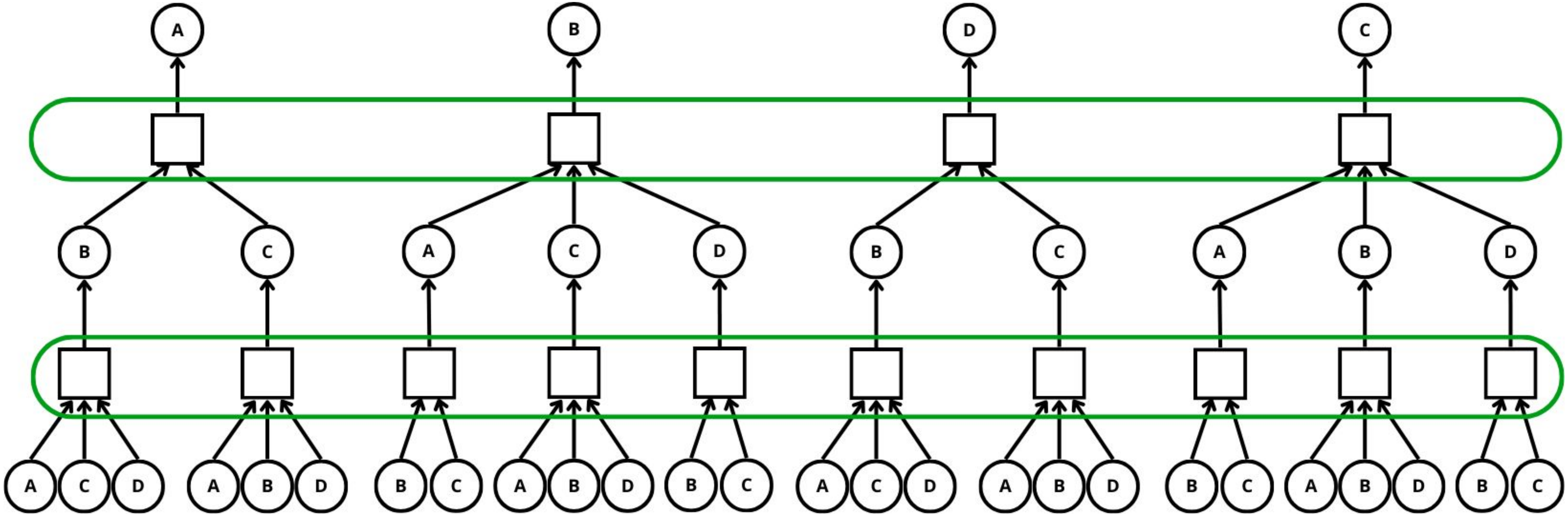
The propagation from the input layer $H^{(0)}$ to the first hidden layer $H^{(1)}$ is given by:

$$H^{(1)} = \sigma(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(0)}W^{(0)})$$

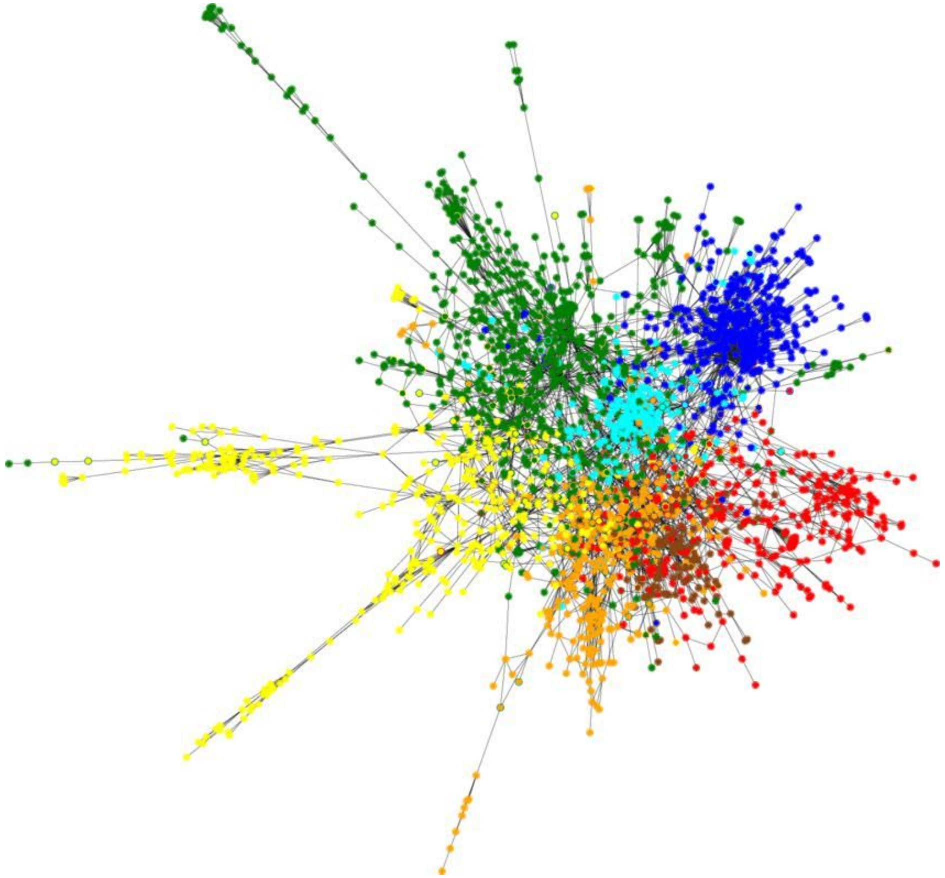
Where:

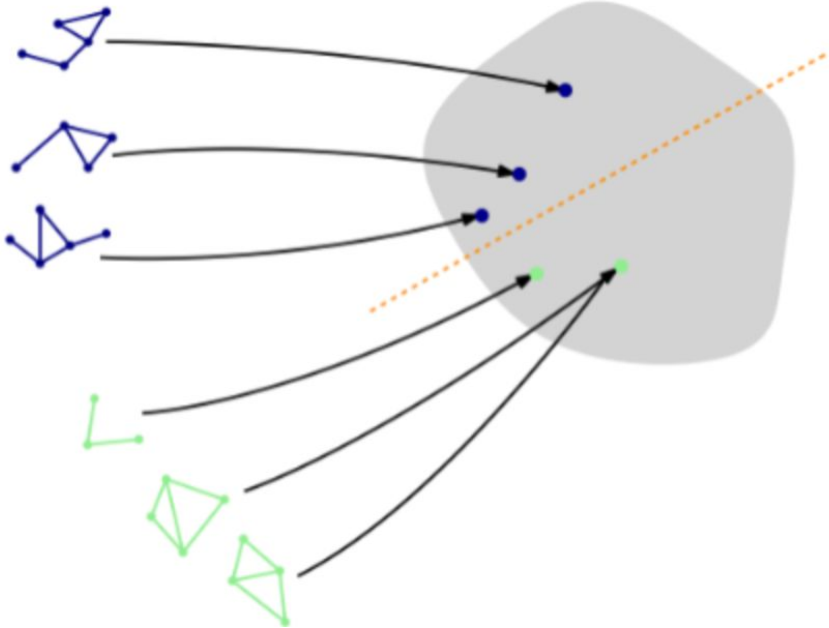
- $\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}$ represents a matrix operation with dimensions $(nume\_nodes, num\_nodes)$.
- $H^{(0)}$ is the input matrix with dimensions $(nume\_nodes, num\_features)$.
- $W^{(0)}$ is the weight matrix connecting the input layer to the first hidden layer with dimensions $(nume\_features, num\_hidden\_features)$.

Graph Neural Networks (GNN) – shared weights

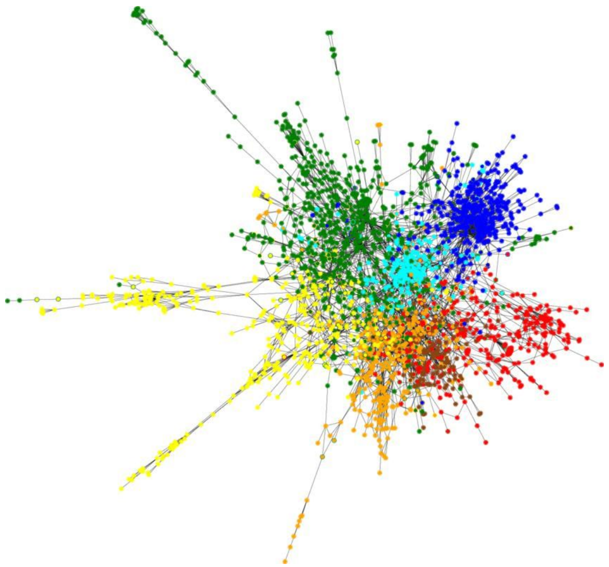


Application of GNNs.

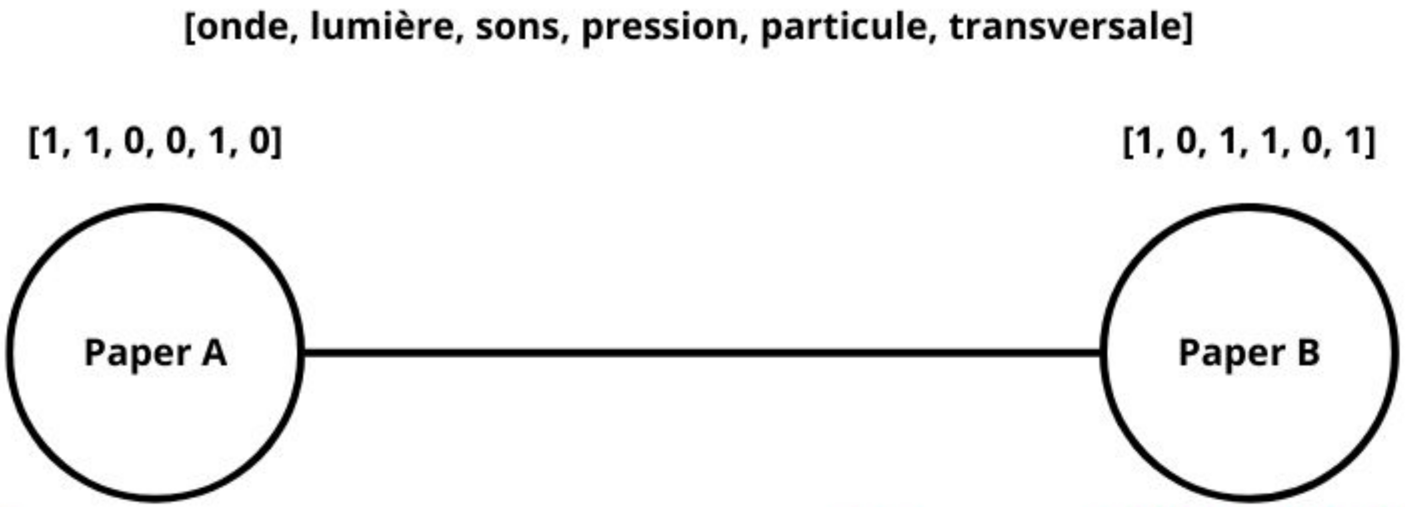




Node classification with GNNs. - Cora Dataset



Train on 5% only



[onde, lumière, sons, pression, particule, transversale]

[1, 1, 0, 0, 1, 0]

[1, 0, 1, 1, 0, 1]

Paper A

Paper B

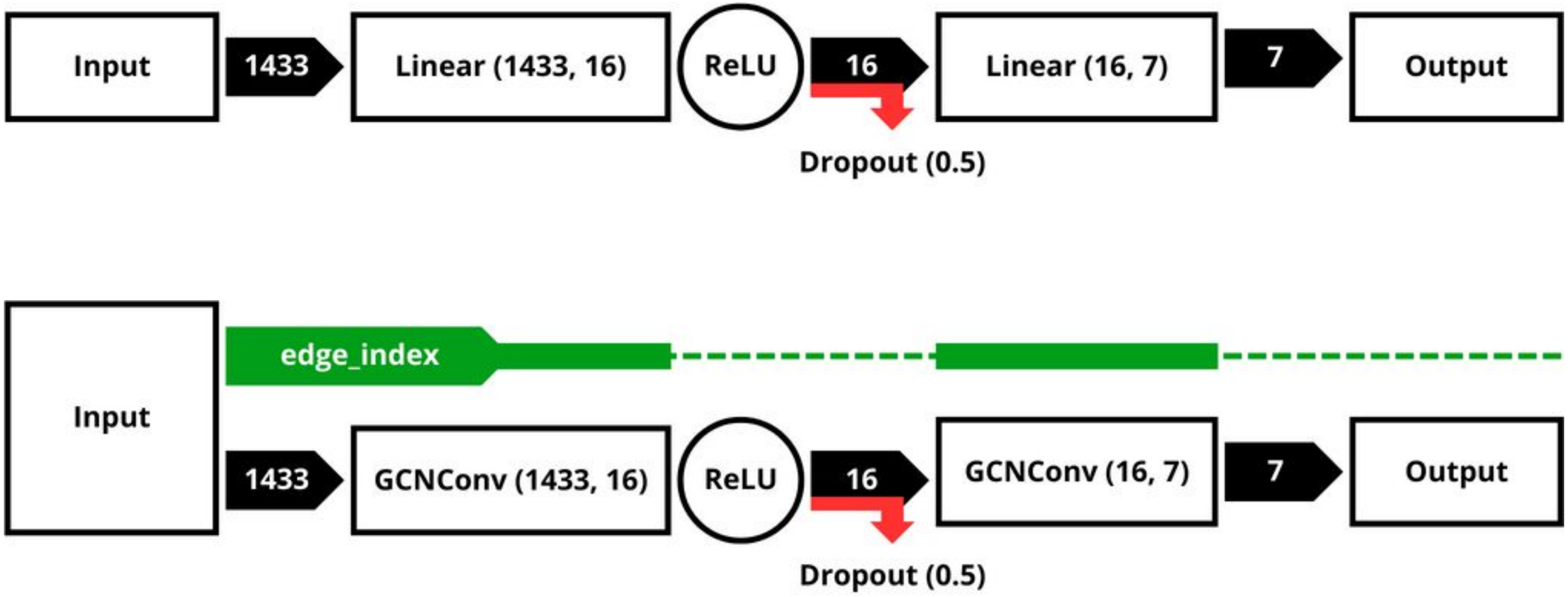
La lumière prends le comportement d'onde et particule en même temps.

Le sons est une onde transversale qui se propage dans l'air sous forme de différence de pression.

Time for practice !

https://colab.research.google.com/drive/1_fB3-rOURz0LldskC2TTd87U5Uu0aYzf?usp=sharing

Node classification with GNNs.



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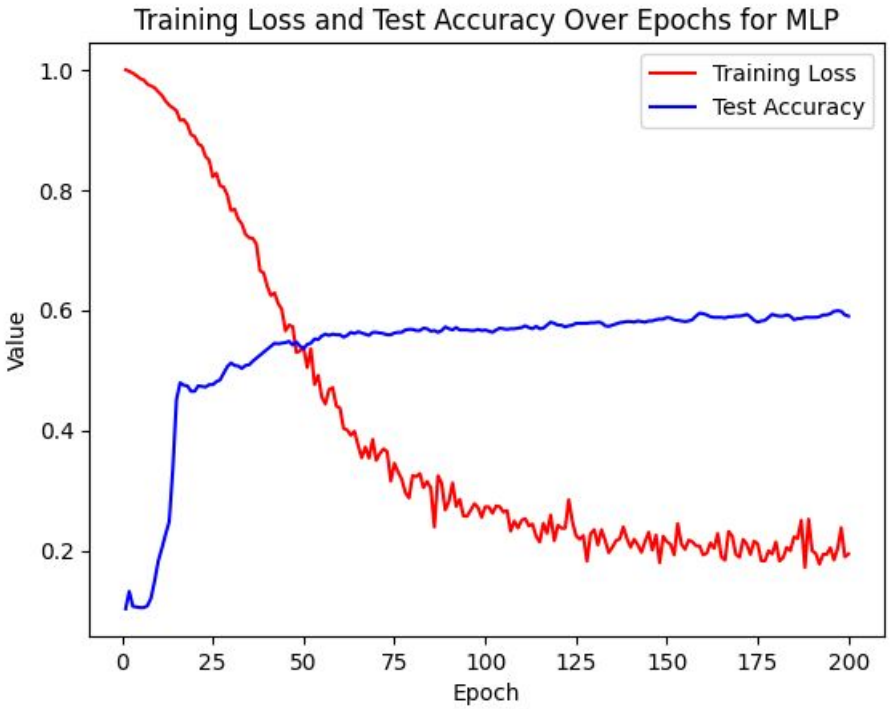
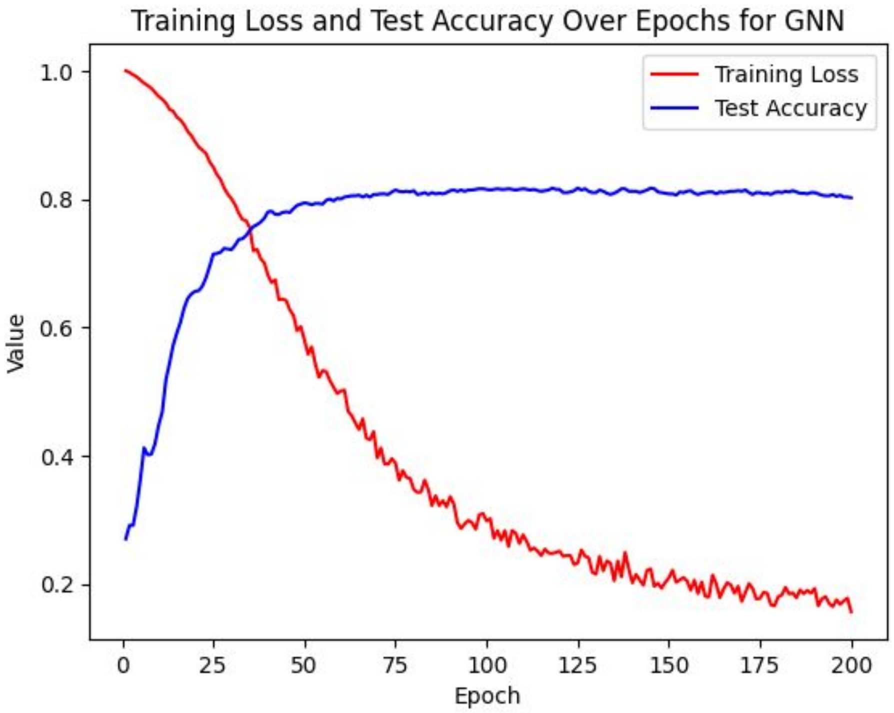
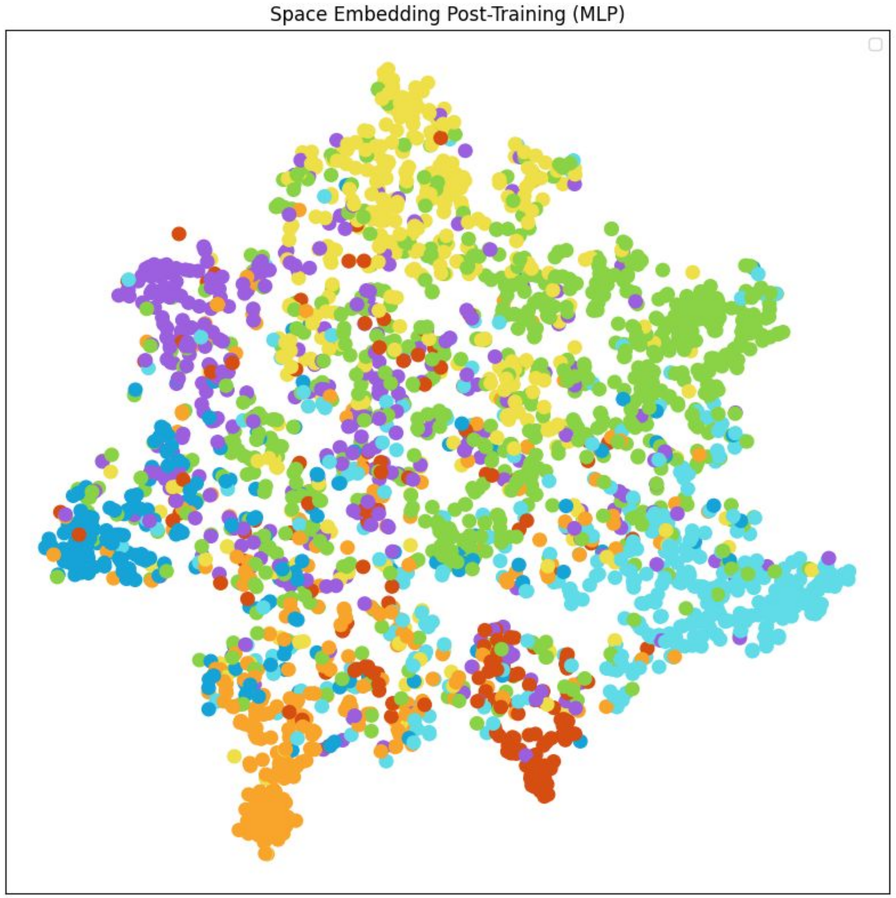


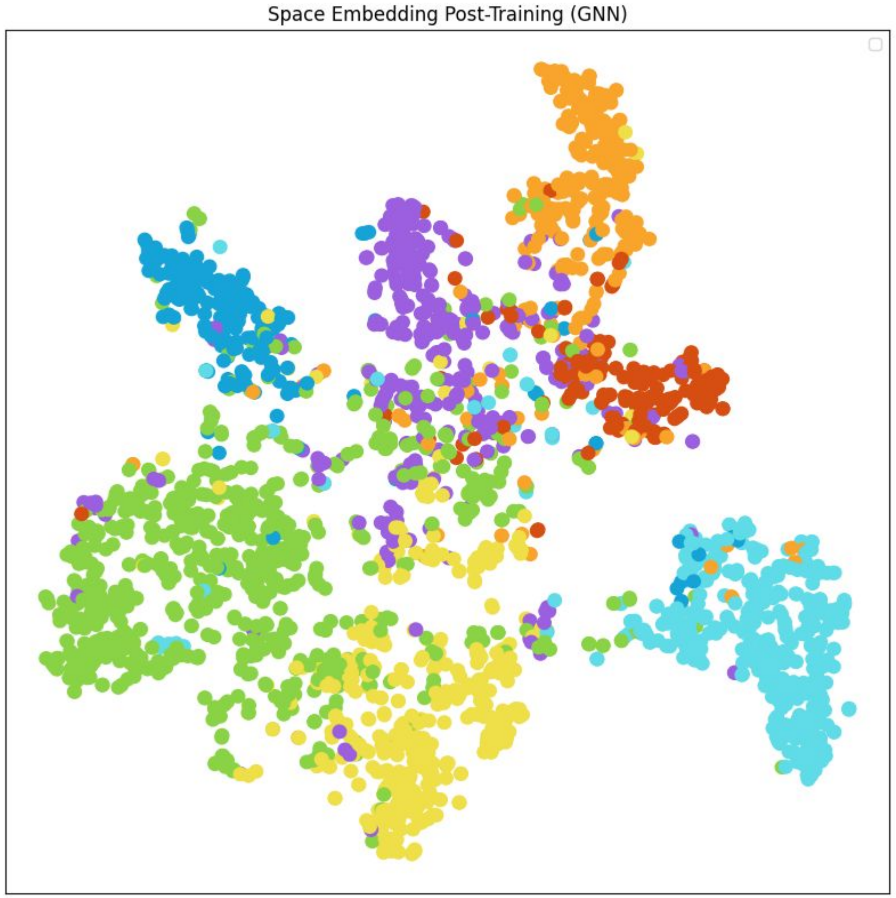
Training Loss and Test Accuracy Over Epochs for MLP



Training Loss and Test Accuracy Over Epochs for GNN

Node classification with GNNs.





Thank you!