



## Tutorial 8: Graph Neural Network for Solving PDEs

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# Data Format in our life



Sequence

Stock, Voice -> 1d sequence



Image

Image -> 2D matrix

Recurrent Neural Network



Graph

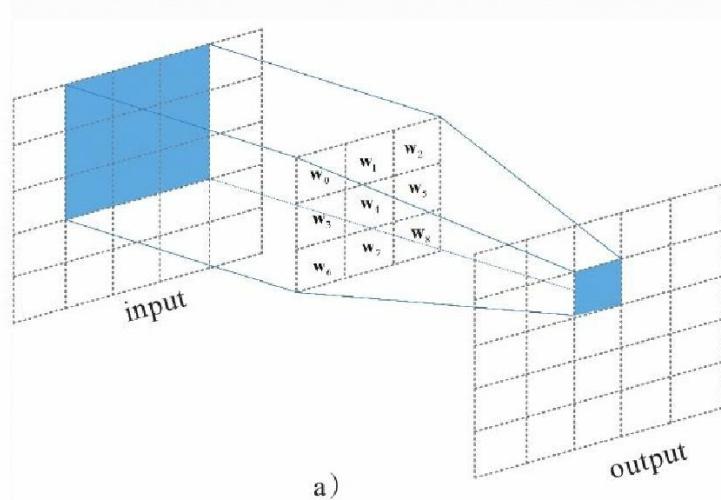
Social Network, Molecular, citation -  
> Graph connectivity

Convolutional Neural Network

Graph Neural Network

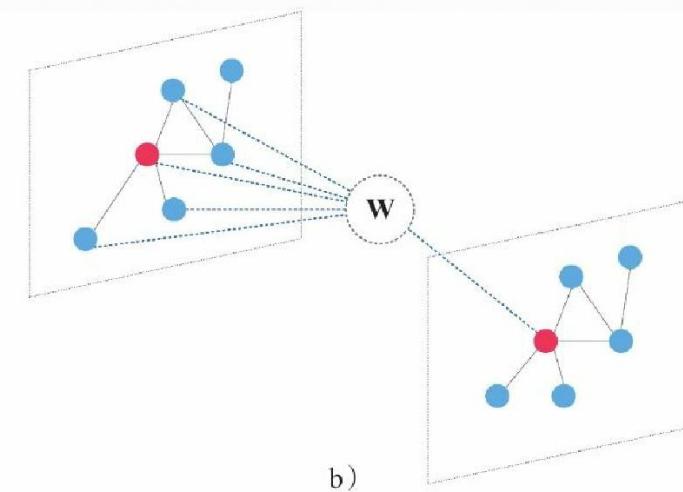
# Graph Convolutional Network

CNN



a)

GCN



b)

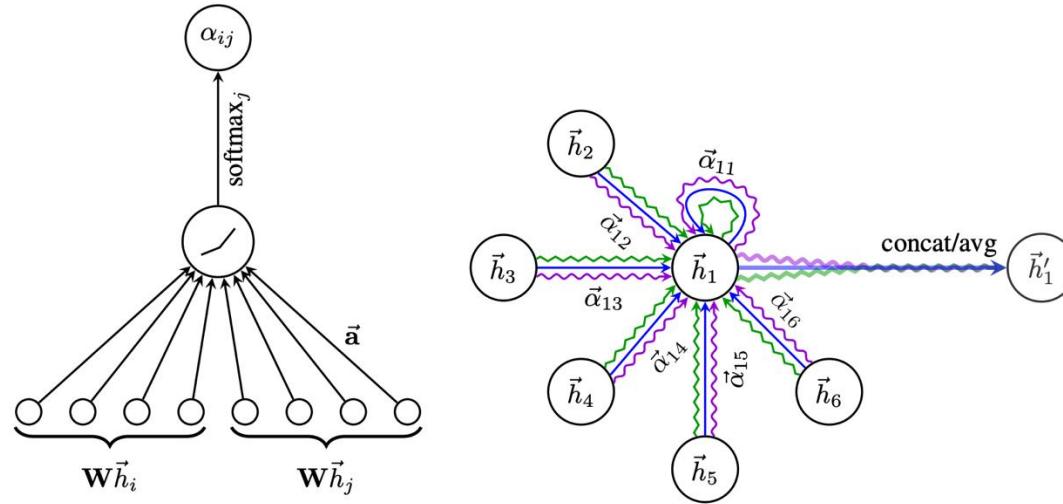
Convolution = weighted sum of neighbor pixels.

GCN Layer:  $X' = \sigma(\tilde{L}_{\text{sym}} X W)$        $\tilde{L}_{\text{sym}} = \tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2}, \quad \tilde{A} = A + I, \quad \tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$

Node Level:  $\mathbf{x}_i = \sigma\left(\sum_{v_j \in N(v_i)} \tilde{L}_{\text{sym}}[i, j] (W \mathbf{x}_j)\right)$

**Basic Design Logic in DL:**  
weight sharing + local computation -> Enjoy the advantages of depth by stacking simple layers.

# Graph Attention Network (GAT)



$$e_{ij} = a(\vec{W}\vec{h}_i, \vec{W}\vec{h}_j)$$

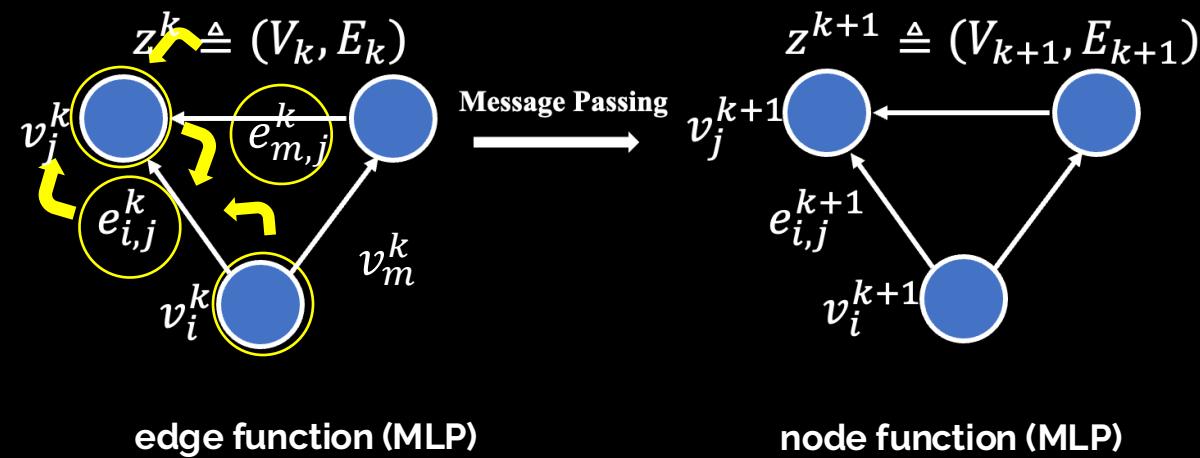
$$\alpha_{ij} = \text{soft max}_j(e_{ij}) = \frac{\exp(e_{ij})}{\sum_{v_k \in \tilde{N}(v_i)} \exp(e_{ik})}$$

$$\vec{h}'_i = \sigma \left( \sum_{v_j \in \tilde{N}(v_i)} \alpha_{ij} \vec{W}\vec{h}_j \right)$$

- Aggregated the neighboring information based on attentions.

# Message Passing Neural Network

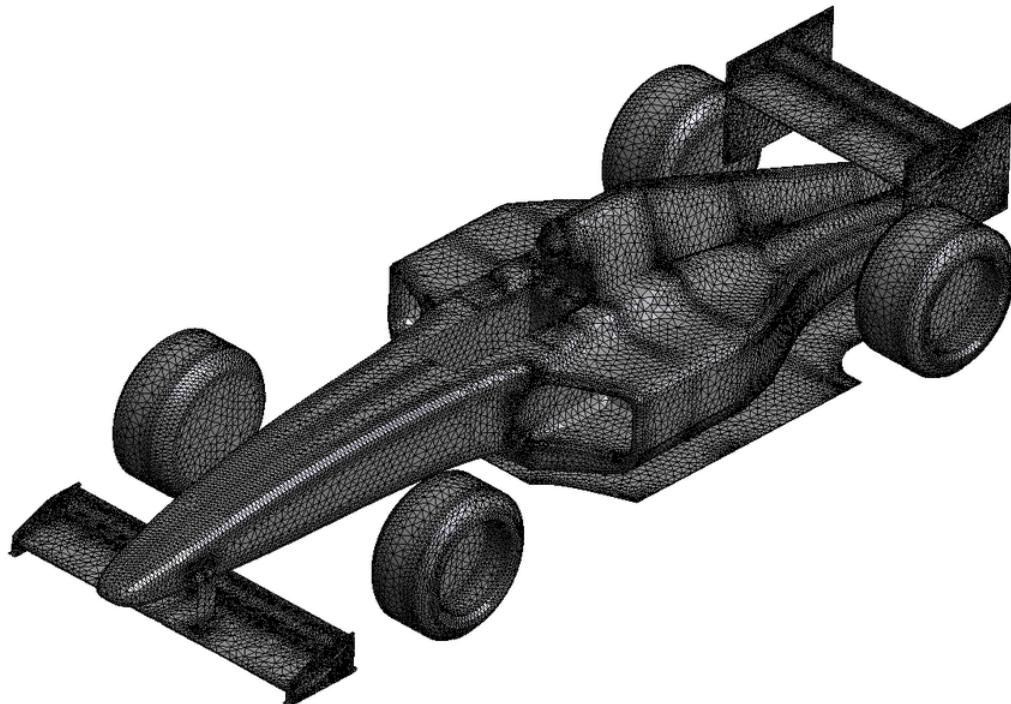
- Unified the Graph Neural Network
- For a very long time, the studies of graph neural network is to study these better node and edge update function



$$e_{ij}^k = f_{\text{Edge}}(v_j^k, v_i^k)$$

$$v_j^{k+1} = f_{\text{Node}}(v_j^k, \sum_{k \in \mathcal{N}(v_j^k)} e^k)$$

# PDE in real scenarios

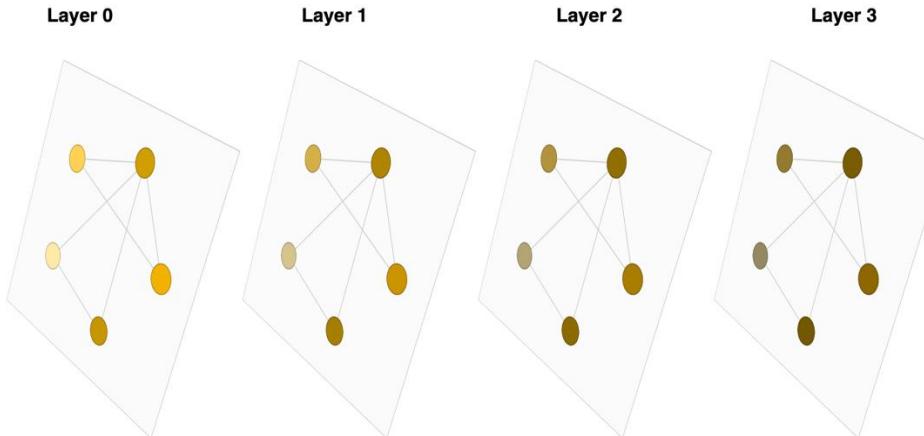


- In real scenarios, the information is unstructured.
- The neural operators (FNO, CNO, ViT, Unet) learnt so far is all structured.
- We need graph-based neural network to process this scenarios.

# Good reading materials

## A Gentle Introduction to Graph Neural Networks

Neural networks have been adapted to leverage the structure and properties of graphs. We explore the components needed for building a graph neural network – and motivate the design choices behind them.



Hover over a node in the diagram below to see how it accumulates information from nodes around it through the layers of the network.

<https://distill.pub/2021/gnn-intro/>

# DL learning library for graph

1. Pytorch Geometric (PyG)



2. Deep Graph Library

