Tutorial 8:
Graph Neural Network for Solving PDEs

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Data Format in our life

Sequence

Stock, Voice -> 1d sequence

Recurrent Neural Network

Image

Image -> 2D matrix

Convolutional Neural Network

Graph

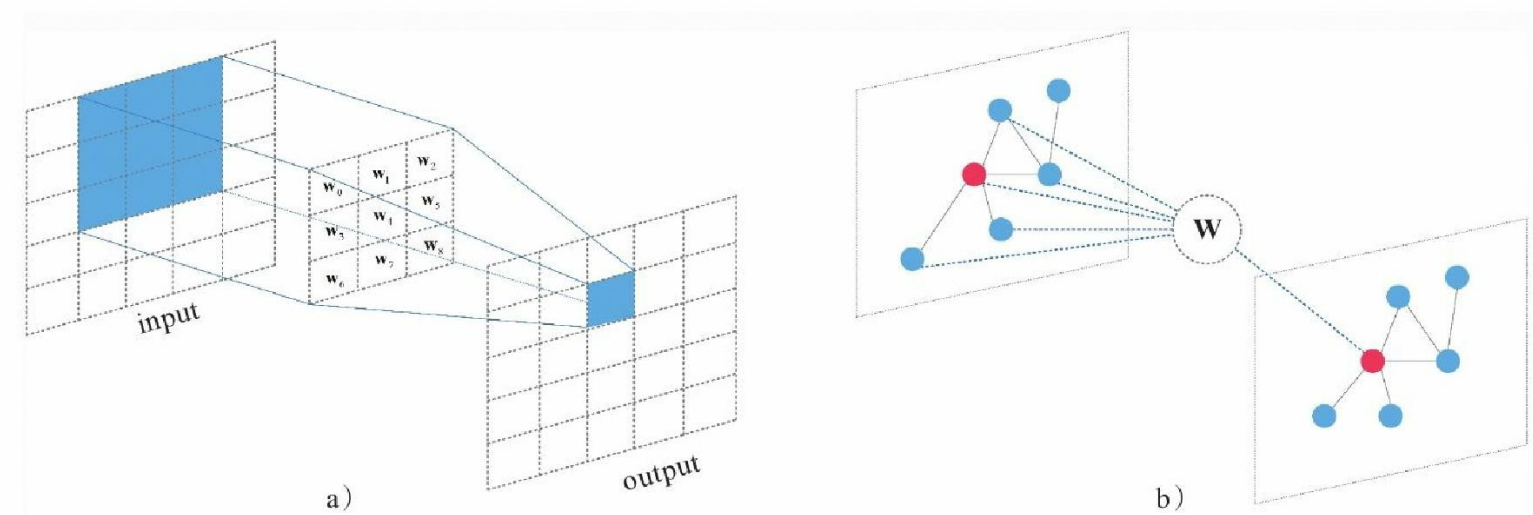
Social Network, Molecular, citation -> Graph connectivity

Graph Neural Network

Graph Convolutional Network

CNN

GCN



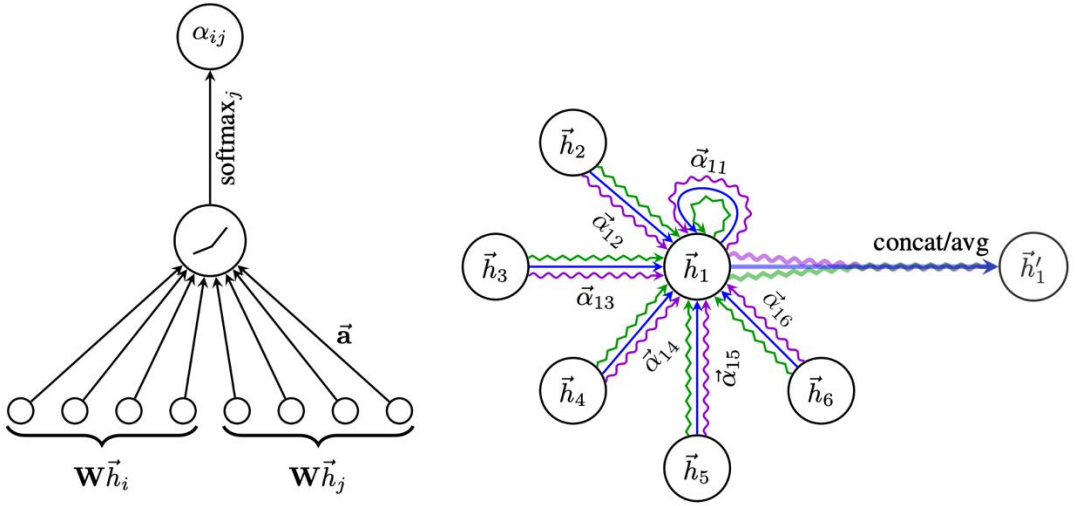
Convolution = weighted sum of neighbor pixels.

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

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)



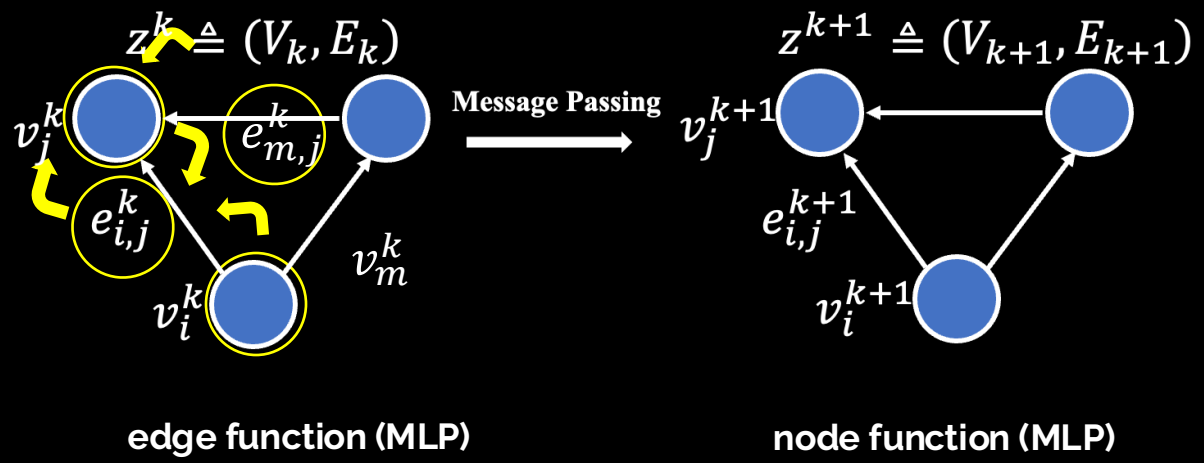
$$e_{ij} = a\left(W\boldsymbol{h}_i, W\boldsymbol{h}_j\right) \qquad \alpha_{ij} = \operatorname*{soft\,max}_j\left(e_{ij}\right) = \frac{\exp\left(e_{ij}\right)}{\sum_{v_k \in \tilde{N}(v_i)} \exp\left(e_{ik}\right)}$$

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

- Aggregated the neighboring information based on attentions.

Message Passing Neural Network

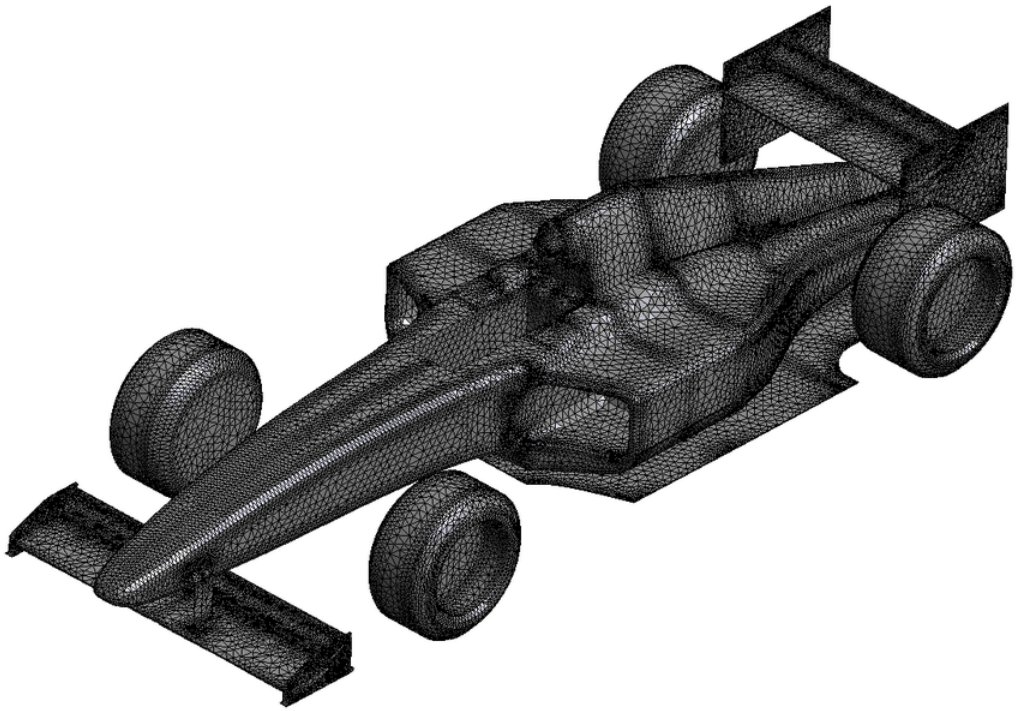
- Unified the Graph Neural Network
- For a very long time, the studies of graph neural network is to study these better node and edge update function



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

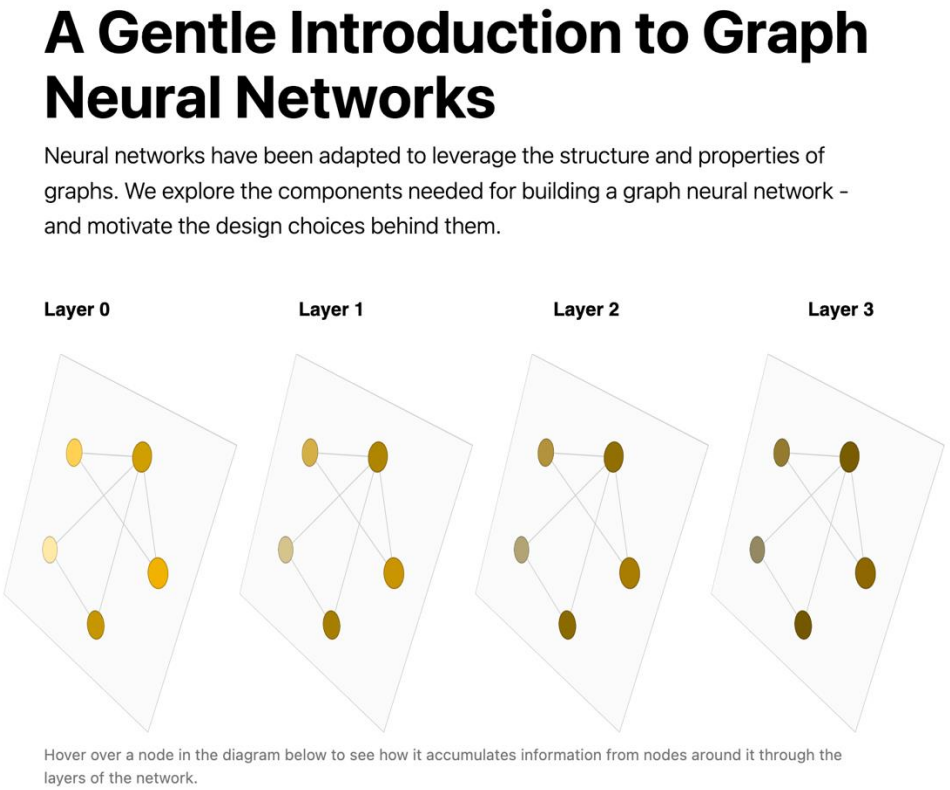
$$v_j^{k+1} = f_{Node}(v_j^k, \sum_{k \in \mathcal{N}(v_j^k)} e^k)$$

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



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

DL learning library for graph

1. Pytorch Geometric (PyG)

2. Deep Graph Library