Message Passing In Graph Neural Networks

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Today I present work that was done in collaboration with

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Graph Neural Networks

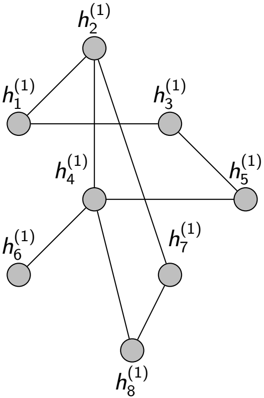
Graph Neural Networks (GNNs) are neural networks that take graph-structured data as input.

In this talk we will only see a specific type of GNN, the Message Passing Neural Networks.

$$
\begin{aligned}
m_v^{(k)} &= M^{(k)}\left(\left\{h_w^{(k-1)} : w \in \mathcal{N}(v)\right\}\right), \\
h_v^{(k)} &= U^{(k)}\left(h_v^{(k-1)}, m_v^{(k)}\right).
\end{aligned}
$$

E.g., the Graph Convolutional Network (GCN, Kipf and Welling, 2017)

$$
H^{(1)} = \mathrm{ReLU}\left(D^{-\frac{1}{2}} A D^{-\frac{1}{2}} X W^{(1)}\right).
$$



Iteratively performing the message-passing and update computations allows us to build 'deep' learning models, e.g., a 3-layer GCN

$$
\hat{y} = \sigma\left(D^{-\frac{1}{2}} A D^{-\frac{1}{2}} \; \mathrm{ReLU}\left(D^{-\frac{1}{2}} A D^{-\frac{1}{2}} \; \mathrm{ReLU}\left(D^{-\frac{1}{2}} A D^{-\frac{1}{2}} X W^{(1)}\right) W^{(2)}\right) W^{(3)}\right).
$$

Motivation & Outline

The message passing step is a defining component of GNNs.

> *"any function of interest we want to compute over graphs can, in all likelihood, be expressed using pairwise message passing – just over a potentially modified graph [...]"*

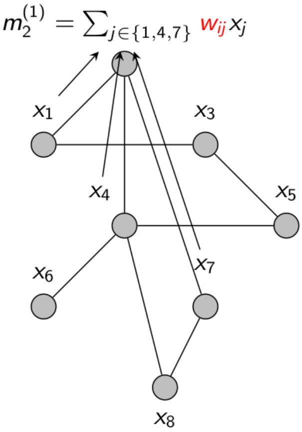
Petar Veličković (2022)

Topic of Today's Talk

Categorise several existing GNNs by their message passing step and place our recent work into that context.

Different Approaches to Message Passing

- Fixed Graph



Different Approaches to Message Passing

- Fixed Graph
  - GCN (Kipf and Welling, 2017)

    Message-Passing Operation: $D^{-\frac{1}{2}} A D^{-\frac{1}{2}} X.$

  - GIN (Xu et al., 2019)

    Message-Passing Operation: $(A + \epsilon I)\, X.$

  - PGSO-GNN (Dasoulas et al., 2021, ICLR)

    Message-Passing Operation: $(m_1 D_a^{e_1} + m_2 D_a^{e_2} A_a D_a^{e_3} + m_3 I_n)\, X,$

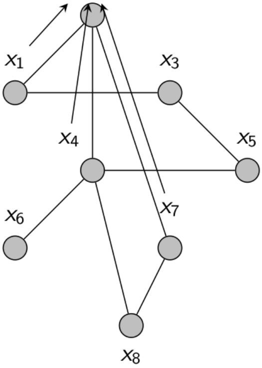
    where $A_a = A + aI_n$, $D_a = \mathrm{Diag}(A_a \mathbf{1}_n)$ and $(m_1, m_2, m_3, e_1, e_2, e_3, a)$ are scalar, *trainable* parameters.

$\mathcal{S} = (m_1,\ m_2,\ m_3,\ e_1,\ e_2,\ e_3,\ a)$	**Operator**	**Description**
$(0,\ 1,\ 0,\ 0,\ 0,\ 0,\ 0)$	A	Adjacency matrix and Summation Aggregation Operator of GNNs
$(1,\ -1,\ 0,\ 1,\ 0,\ 0,\ 0)$	$D - A$	Unnormalised Laplacian matrix L
$(1,\ 1,\ 0,\ 1,\ 0,\ 0,\ 0)$	$D + A$	Signless Laplacian matrix Q (Cvetkovic et al., 1997)
$(0,\ -1,\ 1,\ 0,\ -1,\ 0,\ 0)$	$I_n - D^{-1}A$	Random-walk Normalised Laplacian L_{rw}
$(0,\ -1,\ 1,\ 0,\ -\frac{1}{2},\ -\frac{1}{2},\ 0)$	$I_n - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$	Symmetric Normalised Laplacian L_{sym}
$(0,\ 1,\ 0,\ 0,\ -\frac{1}{2},\ -\frac{1}{2},\ 1)$	$D_1^{-\frac{1}{2}} A_1 D_1^{-\frac{1}{2}}$	Normalised Adjacency matrix of GCNs (Kipf and Welling, 2017)
$(0,\ 1,\ 0,\ 0,\ -1,\ 0,\ 0)$	$D^{-1}A$	Mean Aggregation Operator of GNNs (Xu et al., 2019)

Different Approaches to Message Passing

- Fixed Graph
- Feature-Dependent Reweighting of Edges

$$m_2^{(1)} = \sum_{j \in \{1,4,7\}} w_{ij}(X) x_j$$



Different Approaches to Message Passing

- Fixed Graph
- Feature-Dependent Reweighting of Edges
  - GAT (Veličković et al., 2018)
    Message-Passing Operation: $A_{att}X$,

$$\text{where } (A_{att})_{ij} = \begin{cases} 0, & \text{for } A_{ij} = 0; \\ \dfrac{\exp\left(\mathrm{LeakyReLU}\left(w_2^T \begin{bmatrix} W_1 h_i \\ W_1 h_j \end{bmatrix}\right)\right)}{\sum_{j \in \mathcal{N}(v_i)} \exp\left(\mathrm{LeakyReLU}\left(w_2^T \begin{bmatrix} W_1 h_i \\ W_1 h_j \end{bmatrix}\right)\right)}, & \text{for } A_{ij} \neq 0. \end{cases}$$

  - GATv2 (Brody et al., 2022)
    Message-Passing Operation: $A_{attv2}X$,

$$\text{where } (A_{attv2})_{ij} = \begin{cases} 0, & \text{for } A_{ij} = 0; \\ \dfrac{\exp\left(w_2^T \mathrm{LeakyReLU}\left(W_1 \begin{bmatrix} h_i \\ h_j \end{bmatrix}\right)\right)}{\sum_{j \in \mathcal{N}(v_i)} \exp\left(w_2^T \mathrm{LeakyReLU}\left(W_1 \begin{bmatrix} h_i \\ h_j \end{bmatrix}\right)\right)}, & \text{for } A_{ij} \neq 0. \end{cases}$$

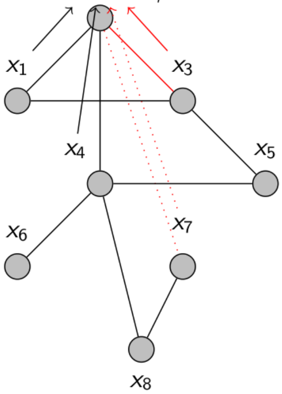
  - GCN-k (Seddik et al., 2022, AISTATS)
    Message-Passing Operation: $\left(\epsilon D^{-\frac{1}{2}} A D^{-\frac{1}{2}} + (1-\epsilon) D_K^{-\frac{1}{2}} K D_K^{-\frac{1}{2}}\right) X$,

$$\text{where } (K)_{ij} = \begin{cases} 0, & \text{for } A_{ij} = 0; \\ x_i^T x_j, & \text{for } A_{ij} \neq 0. \end{cases}$$

Different Approaches to Message Passing

- Fixed Graph
- Feature-Dependent Reweighting of Edges
- Adding and or Removing Edges

$$m_2^{(1)} = \sum_{j \in \{1,3,4,\cancel{7}\}} w_{ij} x_j$$

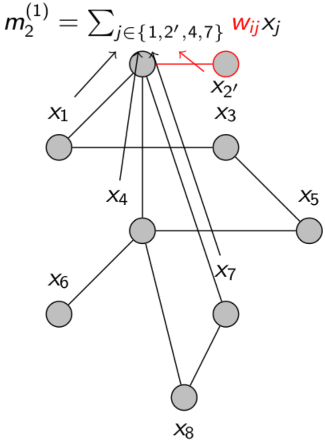


Different Approaches to Message Passing

- Fixed Graph
- Feature-Dependent Reweighting of Edges
- Adding and or Removing Edges
  - SDRF (Topping, Di Giovanni et al., 2022)
    Rewiring according to curvature metrics on graphs
  - PPRGo (Bojchevski et al., 2020)
    Rewiring according to thresholded Personalised PageRank Scores
  - CorePPR Ramos Vela et al. (2022, NeurIPS Workshop)
    Rewiring according to thresholded Personalised PageRank and CoreRank Scores
  - Modularity-Aware (V)GAE (Salha-Galvan et al., 2022, Neural Networks)
    Add edges based on Louvain Clustering

Different Approaches to Message Passing

- Fixed Graph
- Feature-Dependent Reweighting of Edges
- Adding and or Removing Edges
- Explicitly Representing Substructures of Graphs



Different Approaches to Message Passing

- Fixed Graph
- Feature-Dependent Reweighting of Edges
- Adding and or Removing Edges
- Explicitly Representing Substructures of Graphs
    - Subgraph GNNs (Frasca et al., 2022)
    - PathNNs (Michel et al., 2023, ICML)
        1) At layer k, a PathNN uses an LSTM to learn path representations of all paths emanating from a node of length k.
        2) Path Representations are subsequently aggregated.

Different Approaches to Message Passing

- Fixed Graph
- Feature-Dependent Reweighting of Edges
- Adding and or Removing Edges
- Explicitly Representing Substructures of Graphs
- Some GNNs are difficult categorise
  - GOAT (Chatzianastasis et al., 2023, AAAI)
    1) A self-attention mechanism is used to obtain a ranking of nodes in neighbourhoods.
    2) An LSTM processed the ordered neighbourhoods to produce updated node representation.

Conclusions

- If the original graph is sufficient for the performed learning task, then we should simply aggregate over the fixed graph.
- If the node features contain complementary information to the graph on the relevance of neighbours to a given node, then we should use a feature-dependent reweighting scheme on the edges.
- If the graph structure is insufficient for the learning task, e.g., necessary information presents itself as a long-range effect on the original graph, then we should pick a criterion to limit the search space of n^2 node pairs and rewire accordingly.
- If we are aware of certain substructures of particular relevance to our learning task or require a highly expressive model, then we should explicitly represent these substructures in the message passing scheme.

We are currently looking for Postdocs & Research Engineers!

More detailed job postings are on Twitter and our group's website.

Thank you for your attention!

@JLutzeyer

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