Outline of Today's Lecture

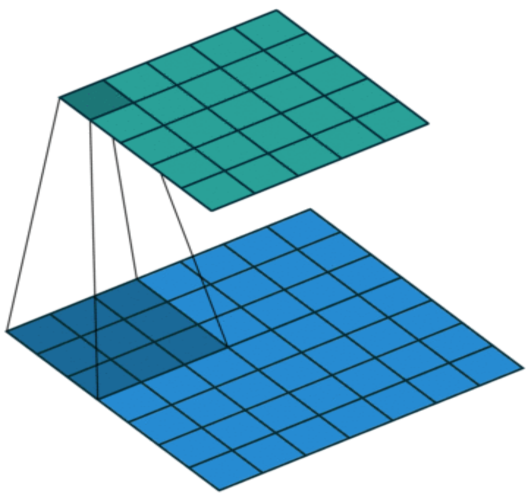
1. Basics of deep learning ✓
2. Deep learning for graphs ✓
3. Graph Convolutional Networks ✓
4. **GNNs subsume CNNs and Transformers**

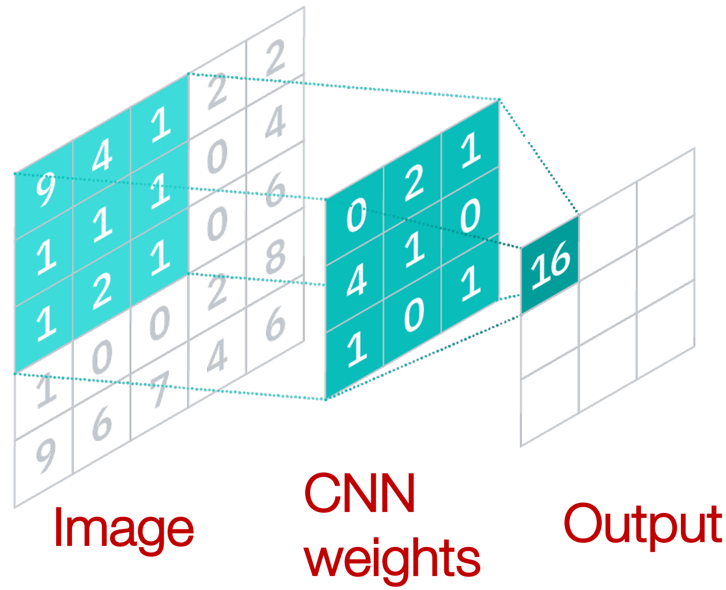
Architecture Comparison

- **How does GNNs compare to prominent architectures such as Convolutional Neural Nets, and Transformers?**

Convolutional Neural Network

Convolutional neural network (CNN) layer with 3x3 filter:



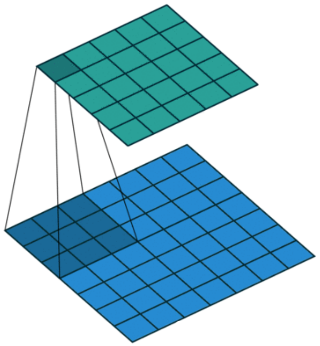


CNN formulation: $\mathrm{h}_v^{(l+1)} = \sigma(\sum_{u \in \mathrm{N}(v) \cup \{v\}} \mathrm{W}_l^u \mathrm{h}_u^{(l)}), \quad \forall l \in \{0, \ldots, L-1\}$

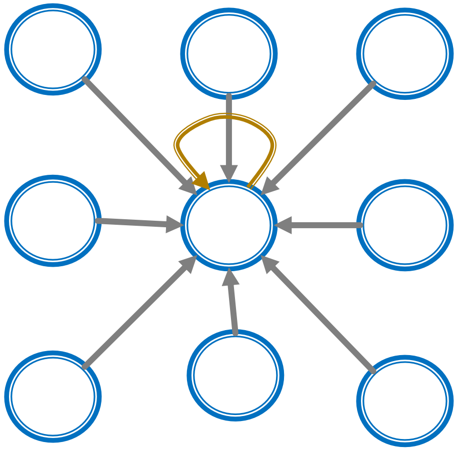
$\boldsymbol{N(v)}$ **represents the 8 neighbor pixels of** $\boldsymbol{v}$**.**

GNN vs. CNN

Convolutional neural network (CNN) layer with 3x3 filter:



Image



Graph

- GNN formulation (previous slide): $\mathrm{h}_v^{(l+1)} = \sigma(\mathbf{W}_l \sum_{u \in \mathrm{N}(v)} \frac{\mathrm{h}_u^{(l)}}{|\mathrm{N}(v)|} + \mathrm{B}_l \mathrm{h}_v^{(l)}), \forall l \in \{0, \dots, L-1\}$
- CNN formulation: $\mathrm{h}_v^{(l+1)} = \sigma(\sum_{u \in \mathrm{N}(v) \cup \{v\}} \mathrm{W}_l^u \mathrm{h}_u^{(l)}), \forall l \in \{0, \dots, L-1\}$

  if we rewrite: $\mathrm{h}_v^{(l+1)} = \sigma(\sum_{u \in \mathrm{N}(v)} \mathbf{W}_l^u \mathrm{h}_u^{(l)} + \mathrm{B}_l \mathrm{h}_v^{(l)}), \forall l \in \{0, \dots, L-1\}$

GNN vs. CNN

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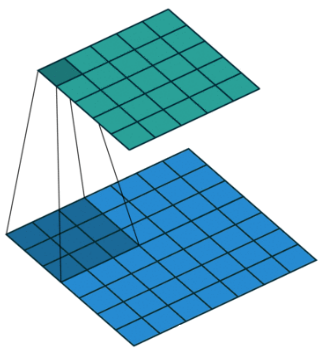
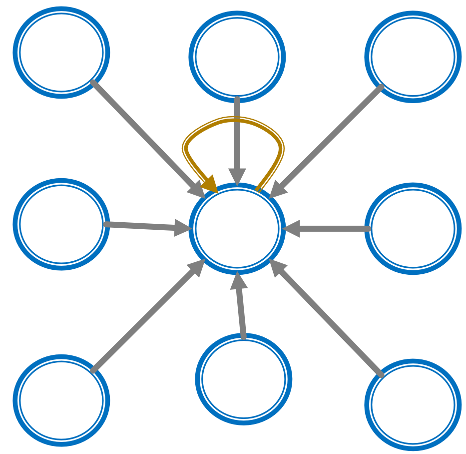


Image



Graph

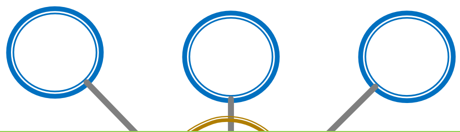
GNN formulation: $\mathrm{h}_v^{(l+1)} = \sigma(\mathbf{W}_l \sum_{u \in \mathrm{N}(v)} \frac{\mathrm{h}_u^{(l)}}{|\mathrm{N}(v)|} + \mathrm{B}_l \mathrm{h}_v^{(l)}), \forall l \in \{0, \dots, L-1\}$

CNN formulation: $\mathrm{h}_v^{(l+1)} = \sigma(\sum_{u \in \mathrm{N}(v)} \mathbf{W}_l^u \mathrm{h}_u^{(l)} + \mathrm{B}_l \mathrm{h}_v^{(l)}), \forall l \in \{0, \dots, L-1\}$

Key difference: We can learn different W_l^u for different "neighbor" u for pixel v on the image. The reason is we can pick an order for the 9 neighbors using **relative position** to the center pixel: {(-1,-1). (-1,0), (-1, 1), …, (1, 1)}

GNN vs. CNN

Convolutional neural network (CNN) layer with 3x3 filter:



- CNN can be seen as a special GNN with fixed neighbor size and ordering:
  - The size of the filter is pre-defined for a CNN.
  - The advantage of GNN is it processes arbitrary graphs with different degrees for each node.

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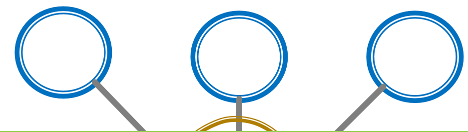
GNN vs. CNN

Convolutional neural network (CNN) layer with 3x3 filter:

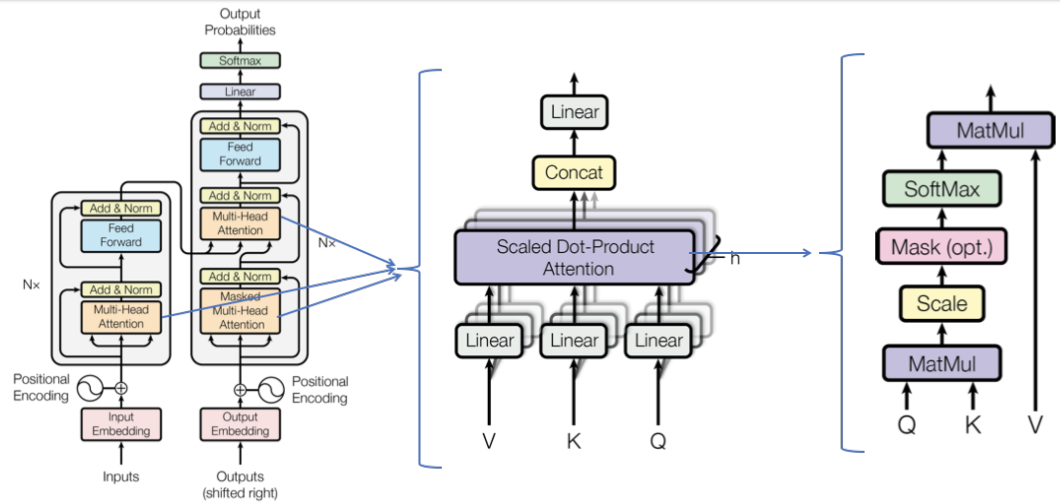


- **CNN can be seen as a special GNN with fixed neighbor size and ordering.**
- **CNN is not permutation equivariant.**
  - **Switching the order of pixels will leads to different outputs.**

Key difference: We can learn different W_l^u for different "neighbor" u for pixel v on the image. The reason is we can pick an order for the 9 neighbors using **relative position** to the center pixel: {(-1,-1). (-1,0), (-1, 1), …, (1, 1)}

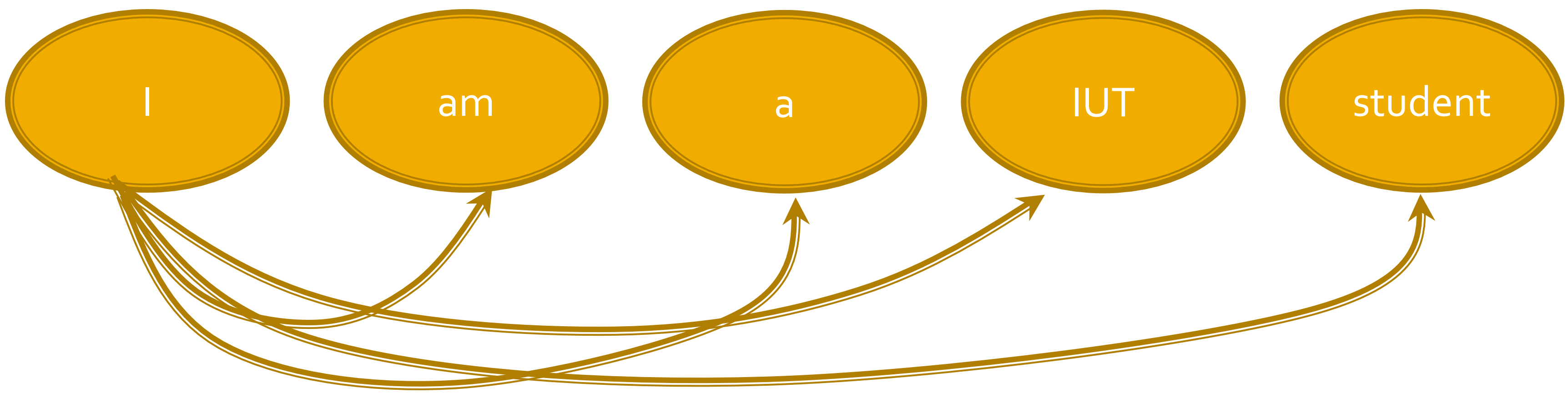
Transformer

Transformer is one of the most popular architectures that achieves great performance in many sequence modeling tasks.



Key component: self-attention

- Every token/word attends to all the other tokens/words via matrix calculation.

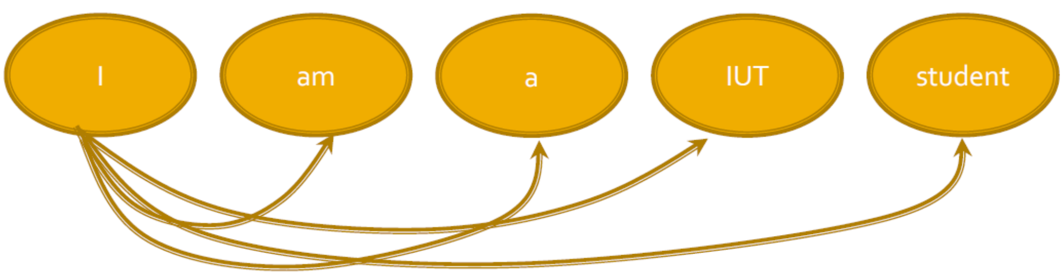


GNN vs. Transformer

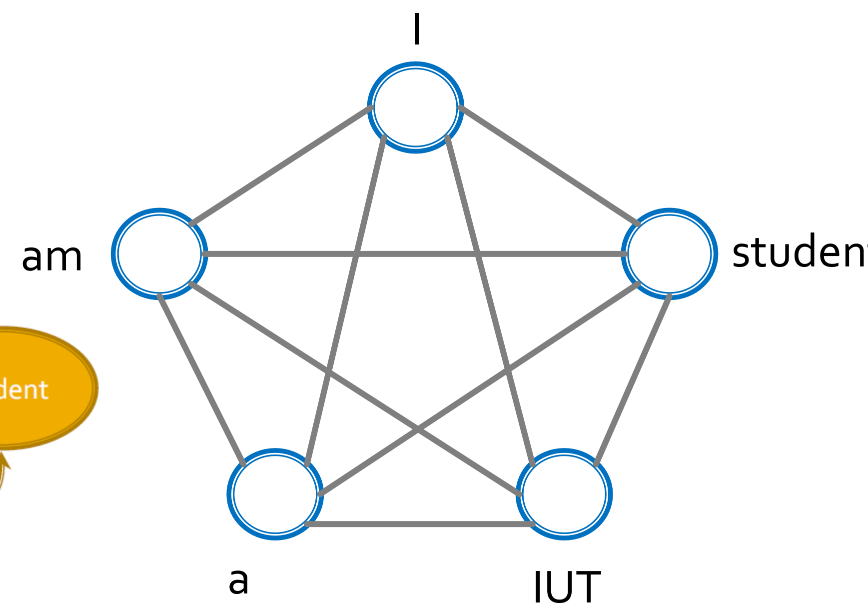
A nice blog plot for this: https://towardsdatascience.com/transformers-are-graph-neural-networks-bca9f75412aa

Transformer layer can be seen as a special GNN that runs on a fully-connected “word” graph!

Since each word attends to **all the other words**, the computation graph of a transformer layer is identical to that of a GNN on the **fully-connected “word” graph**.



Text



(Complete) Graph

Summary

- **In this lecture, we introduced**
  - Basics of neural networks
    - Loss, Optimization, Gradient, SGD, non-linearity, MLP
  - Idea for Deep Learning for Graphs
    - Multiple layers of embedding transformation
    - At every layer, use the embedding at previous layer as the input
    - Aggregation of neighbors and self-embeddings
  - Graph Convolutional Network
    - Mean aggregation; can be expressed in matrix form
  - GNN is a general architecture
    - CNN and Transformer can be viewed as a special GNN