Paper Review “Towards Sparse Hierarchical Graph Classifiers”

Cangea et al. [1]

Suresh Kumar Choudhary / 20.12.2021

Course: Geometric Data Analysis
Course Instructor: Professor Christoph von Tycowicz

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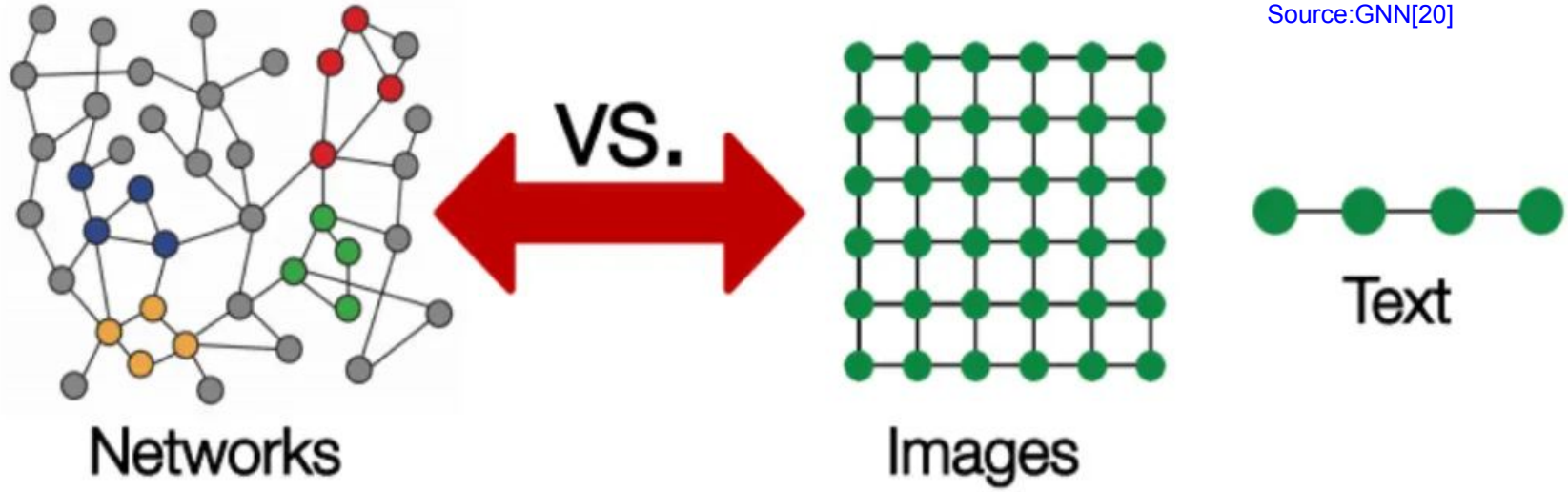
Goal of the study

- Sparse Hierarchical Graph Classification: Predicting a single label for the entire graph

Motivation

- The previous prominent approach to pooling has quadratic memory requirements during training, therefore not scalable to large graphs

Introduction: Graph vs Images



Source:GNN[20]

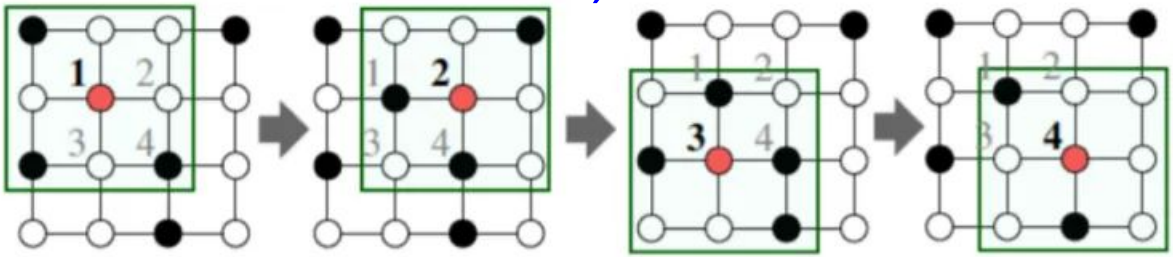
- Arbitrary in size
- Complex topology(no spatial locality)
- Non euclidean
- No fixed node ordering

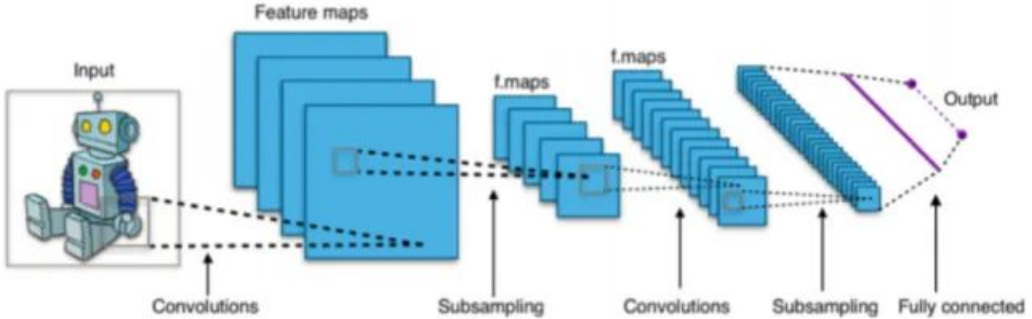
- Grid (Spatial locality)
- Structured data
- Deep learning designed for grid and sequences

Introduction: Why CNN fails on Graph?

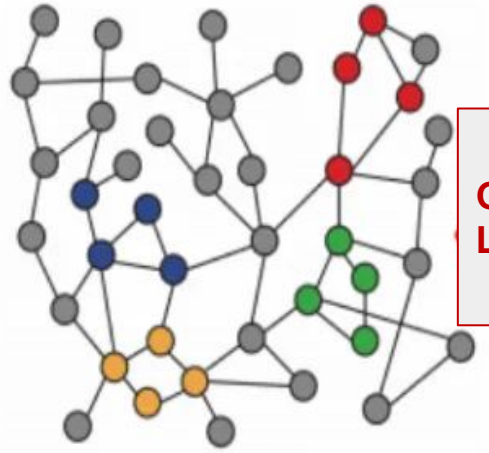
- Locality
- Aggregation
- Composition(function of a function)

Source:GNN[20]



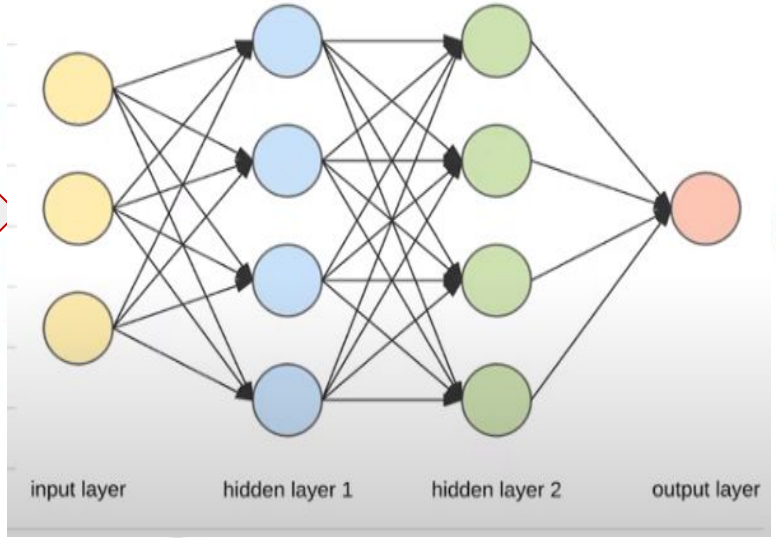


Introduction: Geometric deep learning



Networks

Geometric Deep Learning



How Train Graphs using Neural Networks?

- ?

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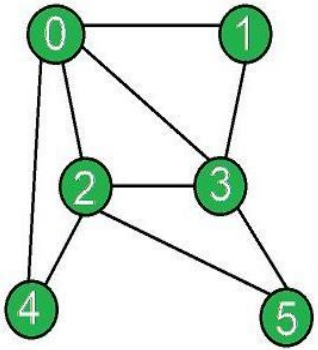
- Converting Graphs into Adjacency Matrix

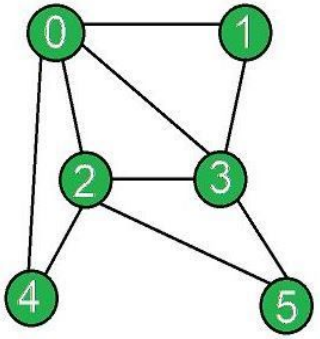


	0	1	2	3	4	5
0	0	1	1	1	1	0
1	1	0	0	1	0	0
2	1	0	0	1	1	1
3	1	1	1	0	0	1
4	1	0	1	0	0	0
5	0	0	1	1	0	0

How Train Graphs using Neural Networks?

- Converting Graphs into Adjacency Matrix

- Not invariant to
  Node ordering



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- Not applicable to different graph sizes

How Train Graphs using Neural Networks?

- 2nd approach: use same approach as in CNN
  - Locality
  - Aggregation
  - Stacking layers (composition)
- How?

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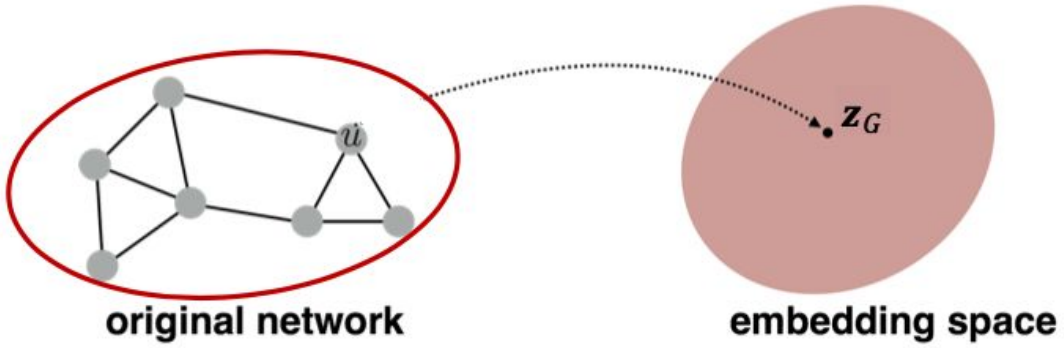

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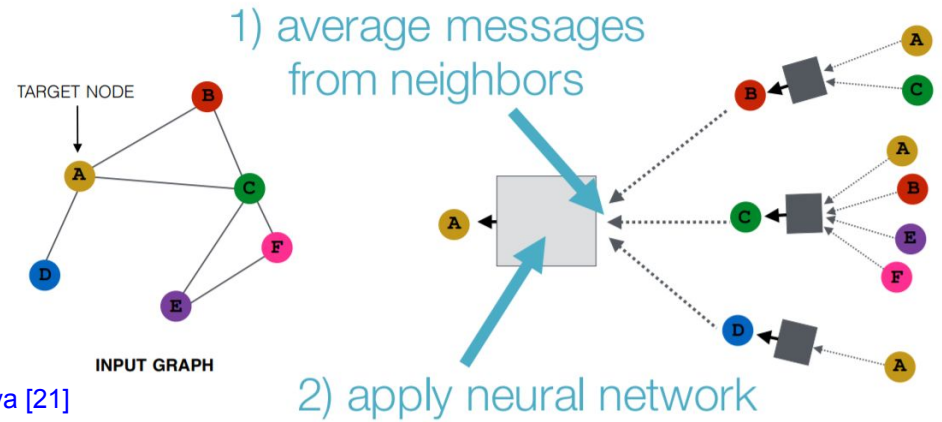


Source: AnalyticsVidya [21]

Related Work

Paper	Study Focus
Krizhevsky et al. [2]	ImageNet Classification with Deep Convolutional Neural Networks
[4,6,14, 16,17]	Graph convolutional layers
[12-15]	Aggregation of node representations: Global pooling layer
[3-11]	Clusters which coarsen the graph in a hierarchical manner through a fixed and pre-defined cluster assignment
Ying et al. [3]	Soft clustering assignments, learned in a differentiable way (DiffPool)

Model

- Input graphs
- Layers
- Architecture

Model: Input Graphs

- The input graph is represented by:
  - Matrix of node features:

$$X \in R^{N \times F}$$

  - Adjacency matrix:

$$A \in R^{N \times N}$$

  - where N is the number of nodes in the graph and F the number of features for each node.
- A is binary and symmetric.

Model Layers

- Convolutional layer
- Pooling layer
- Readout layer

Model: Convolutional Layer

- The architecture makes use of a mean-pooling propagation rule:

$$MP(X, A) = \sigma(\hat{D}^{-1}\hat{A}X\Theta + X\Theta')$$

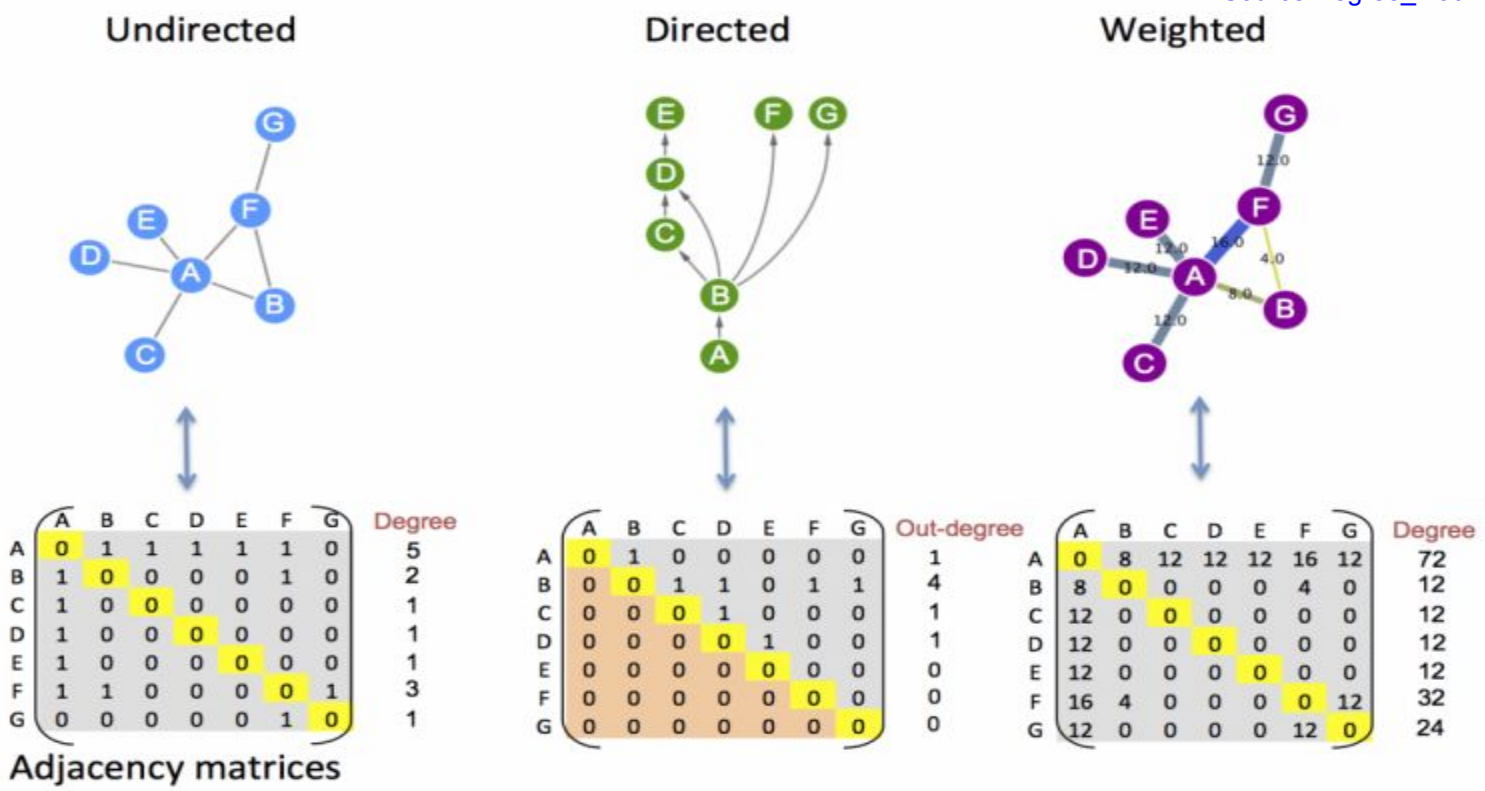
Skip - Connection

Where:

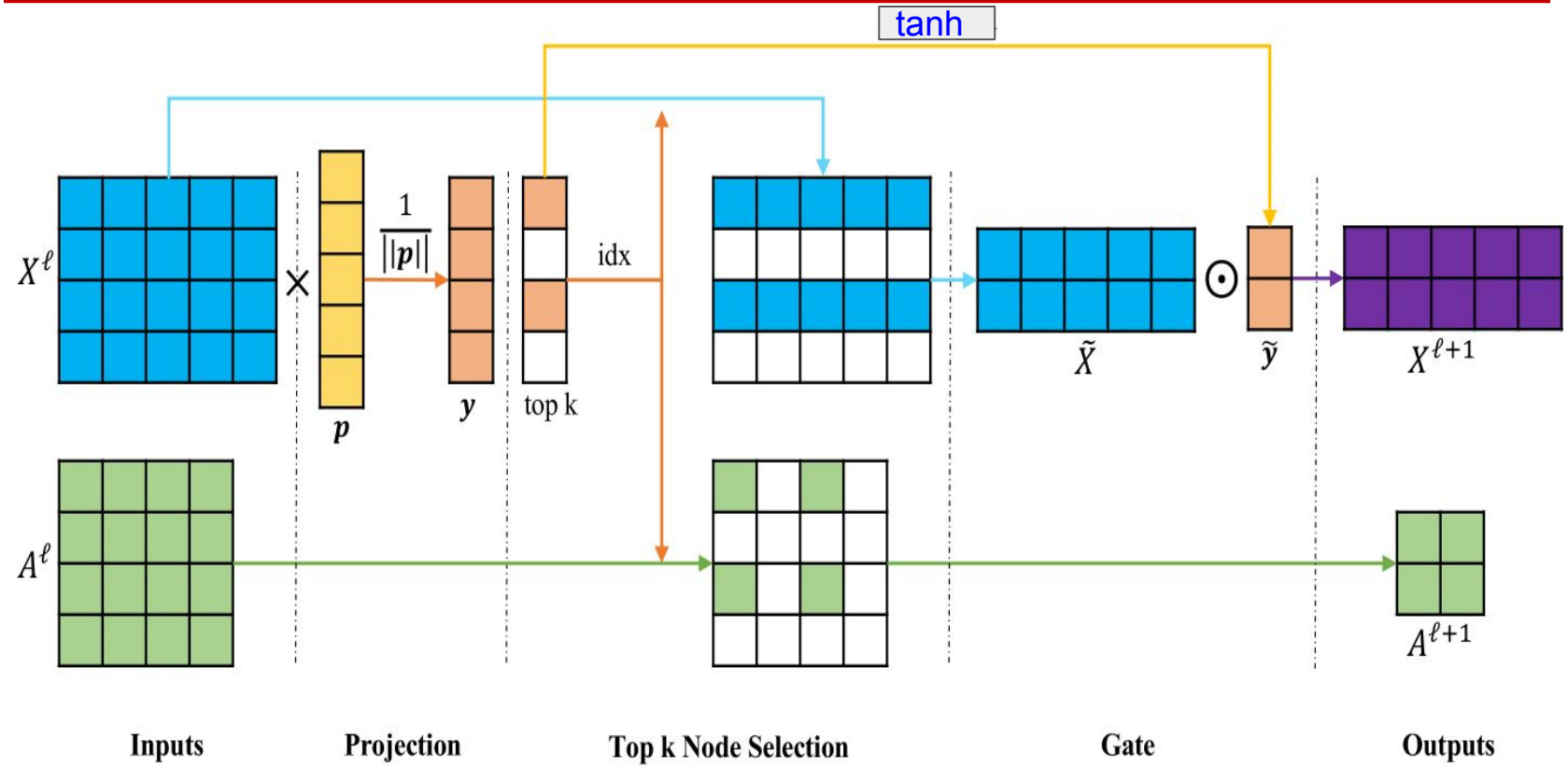
  - σ is rectified linear (ReLU) activation function
  - $\hat{A} = A + I_N$ Adjacency matrix with inserted self-loops
  - $\hat{D}$ is its corresponding degree matrix $\hat{D}_{ii} = \sum_j \hat{A}_{ij}$
  - $\Theta, \Theta' \in R^{F \times F'}$ are learnable linear transformations

Model: Convolution Layers

Source:Degree_matrix [22]



Model: Pooling Layer



Model: Pooling Layer

- computing a pooled graph, (X' , A'), from an input graph (X, A)) can be expressed as follows:

$$\vec{y} = \frac{X\vec{p}}{||\vec{p}||} \quad \vec{i} = top - k(\vec{y}, k) \quad X' = (X \odot tanh(\vec{y}))_{\vec{i}} \quad A' = A_{\vec{i},\vec{i}}$$

- Here, ||.|| is the L2 norm, top-k selects the top-k indices from a given input vector,
- broadcasted element wise multiplication
- Vector i is an indexing operation which takes slices at indices specified by vector i.

Model: Pooling Layer

- The hierarchical pooling layer reduces the graph with a pooling ratio, $k \in (0,1]$, decreasing the number of nodes in a graph from N to $\lceil kN \rceil$.
- The choice of the nodes to drop is done based on a projection score against a learnable vector , which is also used as gating value.

Model: Readout Layer

- The readout layer flatten the information about the input graph in a fixed-size representation.
- Concatenate the results of a global average pooling and a global max pooling at the end of each conv-pool block.
- Apply a global sum pooling before submitting the information to an MLP to obtain final predictions.

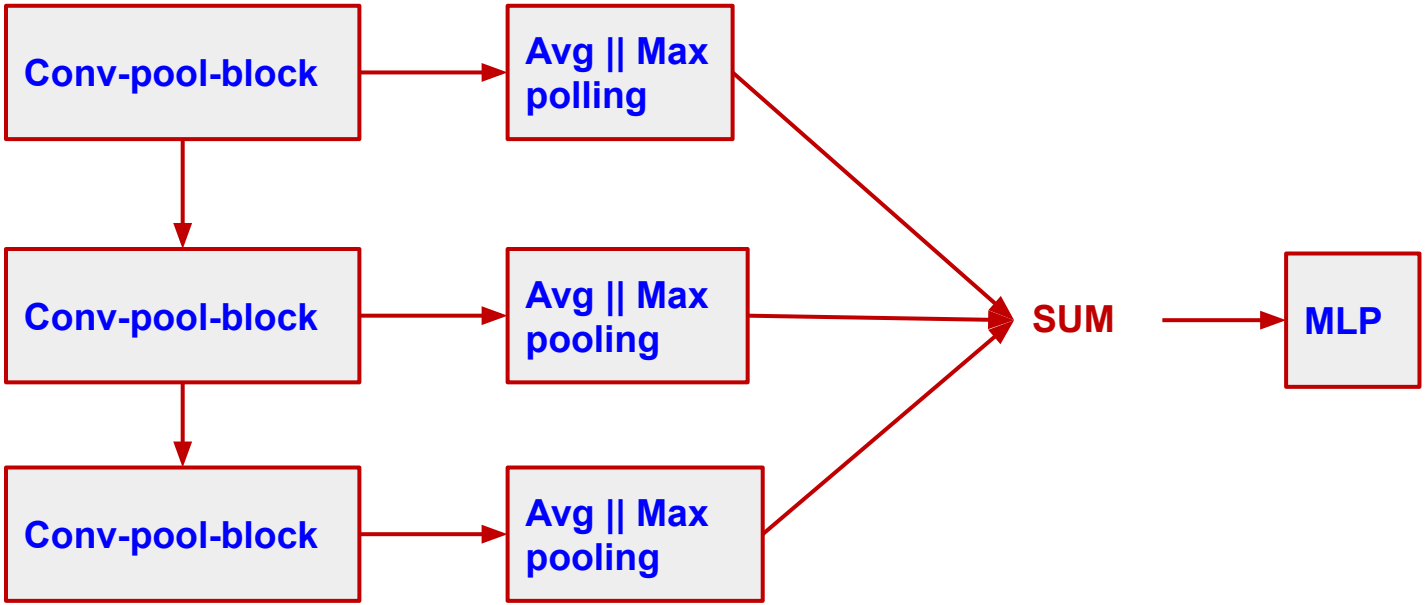
Model: Readout Layer

$$\vec{s}^{(l)} = \frac{1}{N^{(l)}} \sum_{i=1}^{N^{(l)}} \vec{x}_i^{(l)} \,\|\, \max_{i=1}^{N^{(l)}} \vec{x}_i^{(l)} \qquad \vec{s} = \sum_{l=1}^{L} \vec{s}^{(l)}$$

Predictions = MLP ($\vec{s}$)

- where N is the number of nodes of the graph at layer l
- Vector x_i are the i-th node's feature vector.
- || denotes concatenation

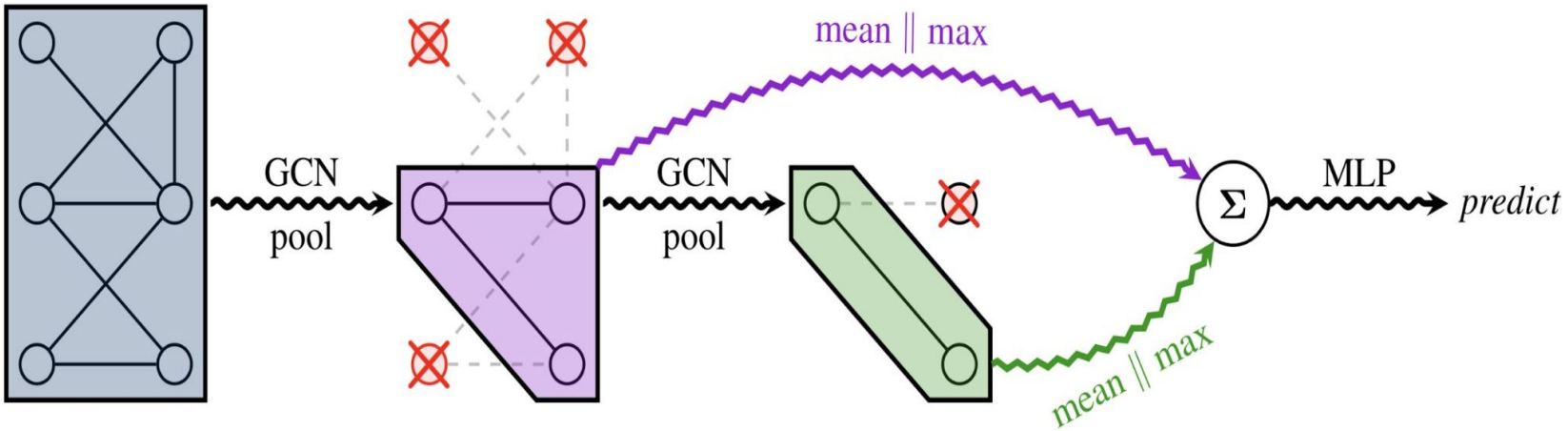
Model: Readout Layer



Model Architecture:

- The presented architecture comprises three conv-pool blocks (in the image they are only two)

Source: Cangea et al. [1]



Experiments: Datasets & Model Parameters

Type	Dataset	Size	No. of Classes	No. of Feature Layers	Learning Rate	Epochs
Biological	Enzymes	597	6	128	0.0005	100
	Proteins	1113	2	64	0.005	40
	D & D	1178	2	64	0.005	20
Scientific collaboration	Collab	5000	3	128	0.005	30

- Pooling ratio k = 0.8, and used Adam optimizer
- 10-fold cross validation approach is used for evaluation

My implementation:

- Used Pytorch and colab
- Implemented all the layers from scratch
- Replicated the same architecture
- Used the same parameters described in paper
- Tested on enzymes dataset only
- Code can be found at Github [23]

Result: Classification Accuracy in %

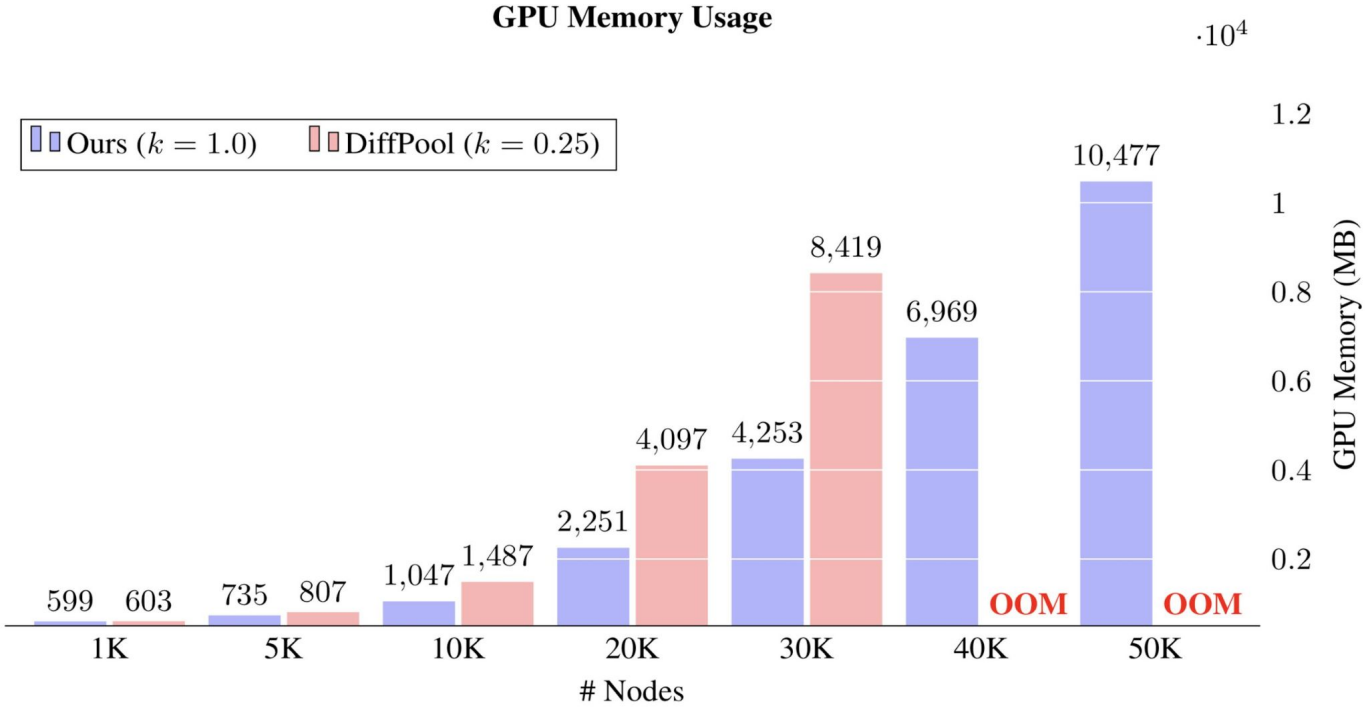
Source:Cangea et al.[1]

	Model	Datasets			
		Enzymes	*D&D*	*Collab*	*Proteins*
Kernel based	Graphlet	41.03	74.85	64.66	72.91
	Shortest-path	42.32	78.86	59.10	76.43
	1-WL	53.43	74.02	78.61	73.76
	WL-QA	60.13	79.04	80.74	75.26
GNN	PatchySAN	–	76.27	72.60	75.00
	GraphSAGE	54.25	75.42	68.25	70.48
	ECC	53.50	74.10	67.79	72.65
	Set2Set	60.15	78.12	71.75	74.29
	SortPool	57.12	79.37	73.76	75.54
	DiffPool-Det	58.33	75.47	**82.13**	75.62
	DiffPool-NoLP	62.67	79.98	75.63	77.42
	DiffPool	**64.23**	**81.15**	75.50	**78.10**
	Ours	64.17	78.59	74.54	75.46

Result: GPU Memory Usage

- Paper's method and DiffPool during training

Source:Cangea et al.[1]



Conclusion and Discussion

- Accuracy at most with in range of 1% as state of art algorithm (diffpool)
- State of art (diffpool) requires a quadratic $O(kV^2)$ storage complexity to be executed.
- Proposed approach requires only $O(V + E)$ storage complexity.

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- Proposed approach requires only $O(V + E)$ storage complexity.
- Hierarchical Graph Pooling with Structure Learning?
- Bridging the Gap Between Spectral and Spatial Domains in Graph Neural Networks?

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Questions?

Thank You