Topological and Geometric Deep Learning

Research Project

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Subject Area

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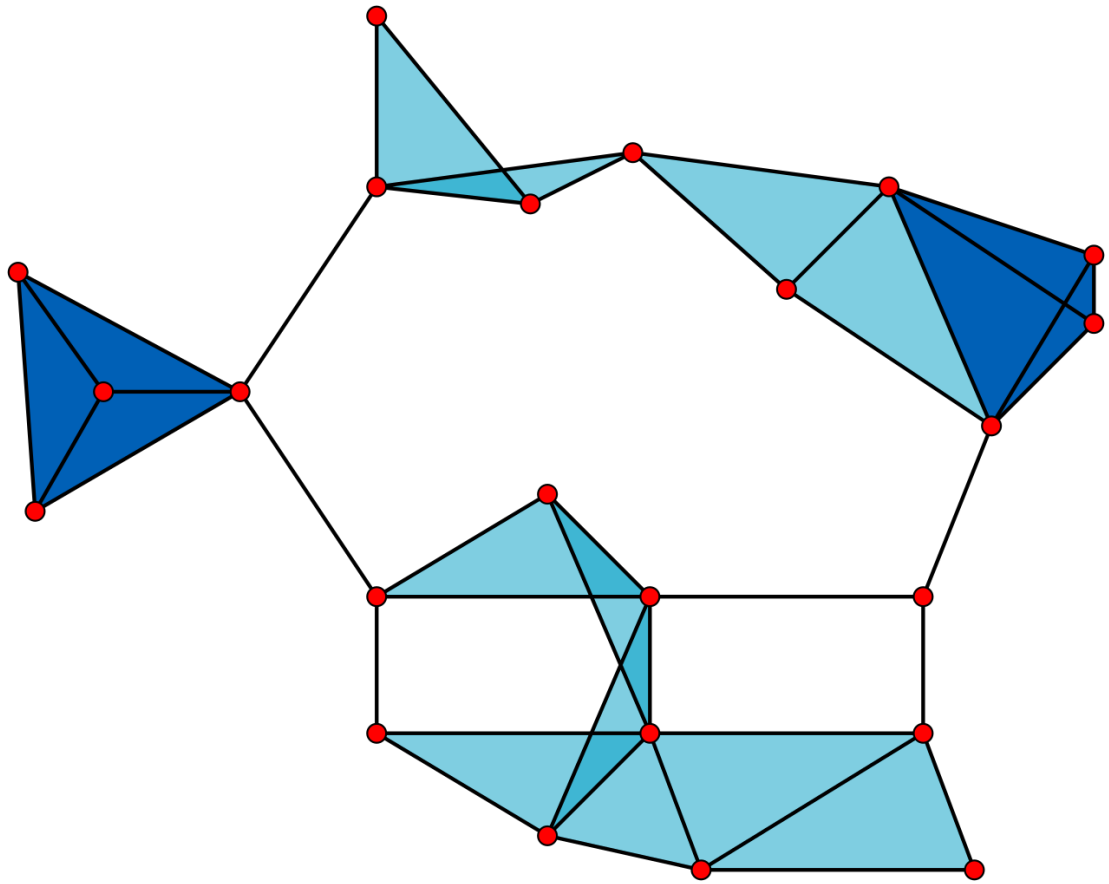
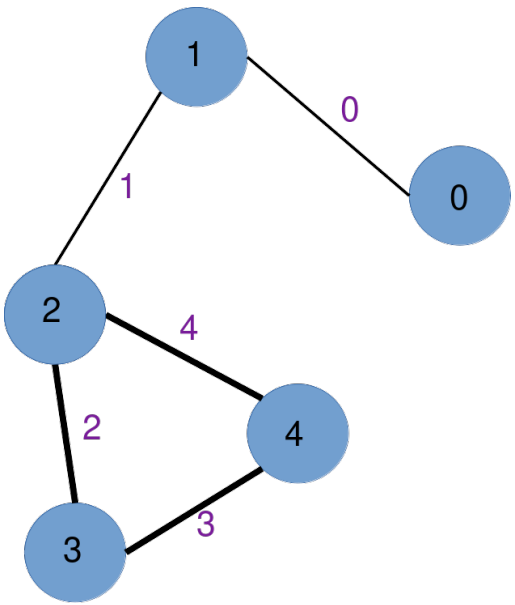
Clique

A graph clique is a subset of its nodes such that it is fully connected. We will work mainly with 3-cliques, and often will refer to them as triangles.



Incidence Matrix

If we have an undirected graph (V, E), its incidence matrix ∇ of size $|V| \times |E|$ such that $A_{i,j} = 1$ if i-th vertex is a vertex of j-th edge. It shows relations between nodes and edges.



$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

Laplacian matrix

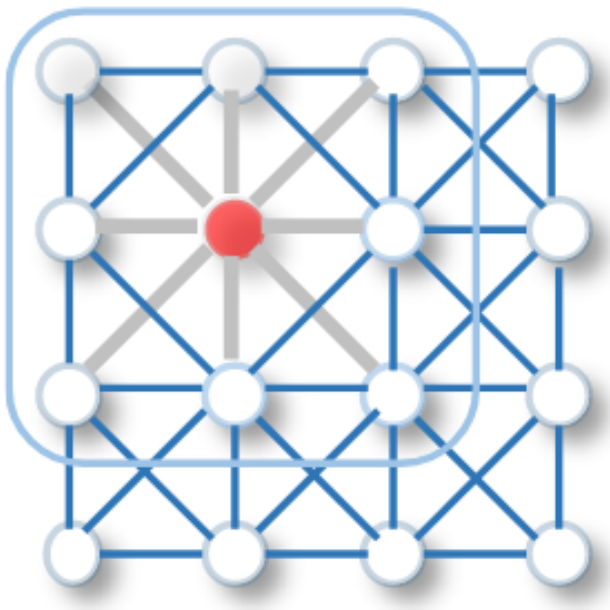
Another matrix representation of a graph. Usually is calculated using the following formula:

$$L_{i,j} = \begin{cases} \deg(v_i) & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } v_i \text{ is adjacent to } v_j \\ 0 & \text{otherwise,} \end{cases}$$

However, other definitions also take place: $L = D - A$, where D is a degree matrix and A is an adjacency matrix. Another way to calculate a Laplacian is $L = \nabla\nabla^T$, where ∇ is an incidence matrix.

Convolutional Graph Network I

A type of GNN which generalizes the convolution operation to graphs.



Convolution on image

Convolution on graph

Convolutional Graph Network II

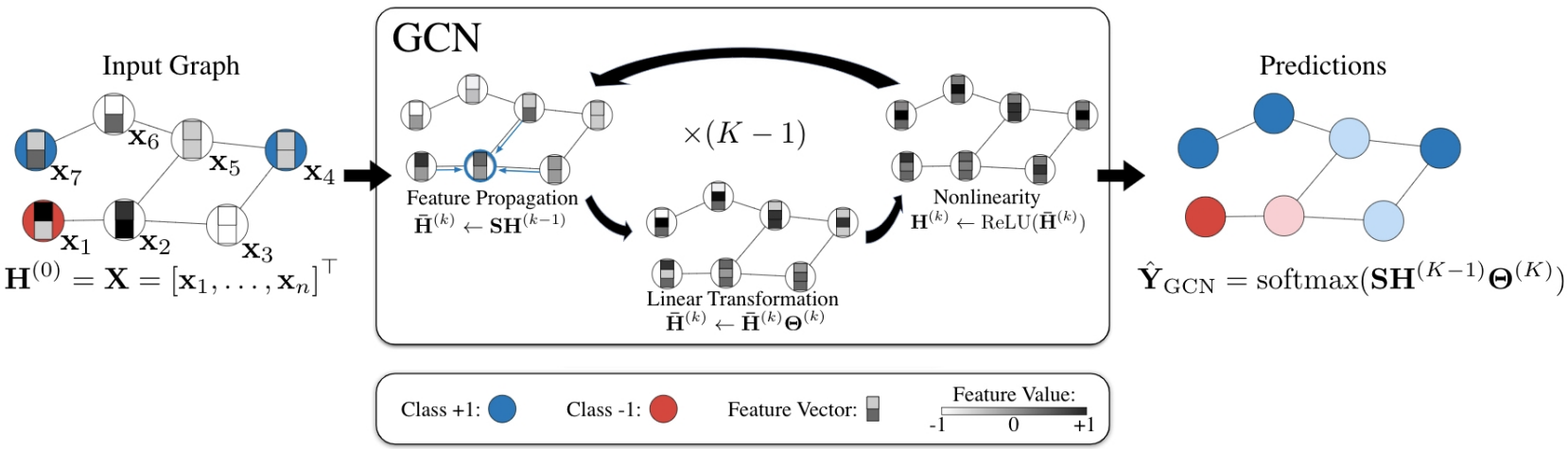
Assume we have a graph of N nodes, where each node has F features. We can construct an $N \times F$ matrix called feature matrix. The first layer takes the feature matrix, and performs the following operation: $Z = D^{-\frac{1}{2}} A D^{-\frac{1}{2}} X W$, where:

- Z is resulting $N \times C$ signal
- D is $N \times N$ degree matrix
- A is $N \times N$ adjacency matrix with self-loops
- X is $N \times F$ feature matrix (input signal)
- W is $F \times C$ learnable weight matrix

The last (output) layer usually applies *softmax* function to each row resulting in a new matrix S. Then, in order to classify a node v_i we simply take the index of maximum of S_i.

Convolutional Graph Network III

The architecture of a graph convolutional network is presented on the figure below.



Graph Attention Network I

A type of GNN which uses attention mechanism (also borrowed from 'casual' neural networks) which allows us to work with inputs of variable sizes and to focus on the most important features. The attention mechanism is a function $a : \mathbb{R}^C \times \mathbb{R}^C \to \mathbb{R}$ which takes two feature vectors X_i, X_j and returns a scalar representing how tight the connection between v_i and v_j is.

Graph Attention Network II

We introduce an $N \times N$ matrix e storing the attention between the nodes: $e_{i,j} = a\left(W \cdot X_i,\ W \cdot X_j\right)$.

Don't calculate all pairwise attentions! One suggested solution is to use a neighborhood $\mathcal{N}_i$ of a vertex v_i and then compute the attentions between v_i and its' neighbors. Existing models uses neighborhood of size 1, and perform great.

One might also want to normalize the coefficients. In order to do that, we can apply softmax function: $c_{i,j} = \text{softmax}_j\left(e_{i,j}\right)$.

Graph Attention Network III

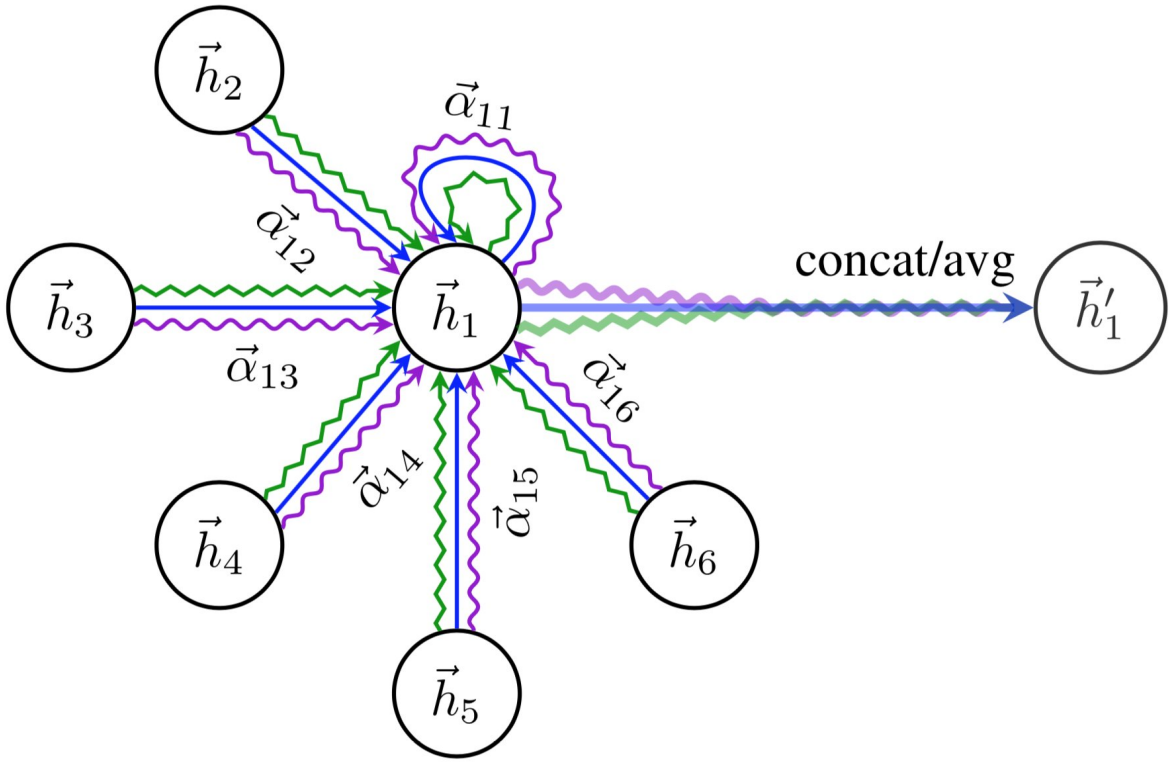


Figure: An example of multi-head attention in a neighborhood of size 1

Tasks solved by GNNs

- Node classification
- Graph classification
- Link prediction

Relevance

- The field is new, therefore, there is a lot of space for improvement
- GNNs allow us to analyze complex relations with great precision
- We can improve the performance by preprocessing the data
- We can improve models by tweaking them

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Any questions?