NATIONAL RESEARCH UNIVERSITY
HIGHER SCHOOL OF ECONOMICS

Faculty of Computer Science
Bachelor's Programme 'Data Science and Business Analytics'

UDC _____

Research Project Report
On the topic 'Topological and Geometric Deep Learning'

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February 17, 2022
Grade: _____ Signature: _____

Moscow, 2022

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1 Introduction

1.1 Abstract

Nowadays, a need to analyze more complex data arises. Some objects and relations can not be represented as vectors in Euclidean space, and, therefore, we have to consider graphs — sets of nodes and connections between them — as a subject of analysis. This poses a huge problem: we have to invent new algorithms, adapt known techniques and constantly improve them in order to work with such a complex data. Our goal is to research the efficiency of several tweaks of existing models.

1.2 Relevance

The field of research (graph neural networks) might be considered relatively new, and, therefore, there is a huge number of possible improvements to be made to existing models and approaches. Our ultimate goal is to improve the accuracy of node and graph classification.

For example, one of the proposed changes is to modify a Laplacian in such a way that it does not break existing model and improves it. Our initial results have shown that our approach indeed works well on Karate club dataset, where we had to classify nodes:

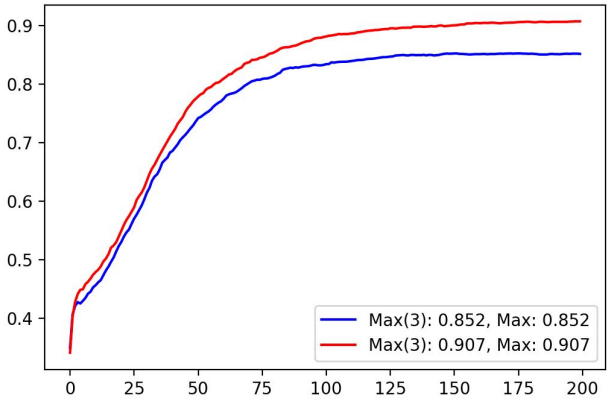


Figure 1: Default Laplacian (in blue) versus our Laplacian (in red). Y-axis is the accuracy, X-axis is the number of epochs

1.3 Subject of research

Let us explain the tasks we can solve using GNNs in more detail. There are three of them:

- *Node classification* — given a graph with several labeled nodes and several classes predict a class of an unlabeled node. For example, given a set of scientific papers and their citations, determine the type of new paper.
- *Graph classification* — determine type of graph. For instance, check if a molecule affects certain parameters of an organism.
- *Link prediction* — determine if two given nodes should have an edge between them. A simple example could be friends suggestions in a social network.

In our research we will only consider the first two problems.

As we established, we want to consider several changes in order to improve the accuracy. The tweaks we propose include but are not limited to:

- *Altering the way we compute Laplacian* — a characteristic matrix of a graph.
- *Edge embeddings*
- *Using connectivity over simplices of higher dimension*. This means that in some cases we might want to consider a group of nodes as a separate object, therefore, increasing the connectivity factor. We will only work with 3-simplices:

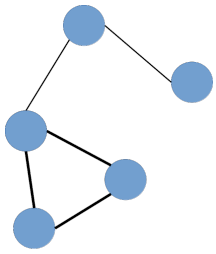


Figure 2: A part of some graph

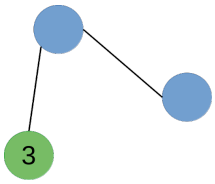


Figure 3: Three nodes from the left image united in 3-simplex having properties of the initial vertices

2 Definitions

Graph

Graph is a tuple (V, E), where V is the set of all nodes v, and E is the set of edges $e_i = (v_j, v_k)$.

Graphs can be undirected ($(v_j, v_k) \equiv (v_k, v_j)$) and directed, where presence of the edge (v_j, v_k) does not imply that edge (v_j, v_j) exists. Edges can also have weights which show some information about the tightness of connection of two nodes. In this case $e_i = (v_j, v_k, w_i)$.

For instance, a road map of a country is an undirected weighted graph, where cities are nodes, roads are edges, and distances are weights.

Clique

A graph clique is a subset of its nodes such that it is fully connected. So, n-clique is a set of n nodes and $\frac{n \cdot (n-1)}{2}$ edges [1].

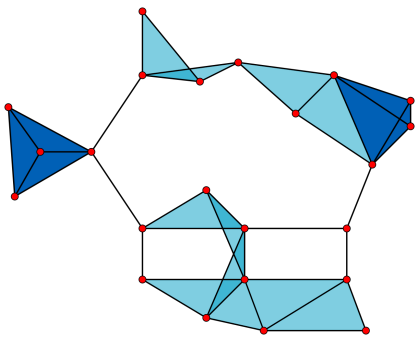


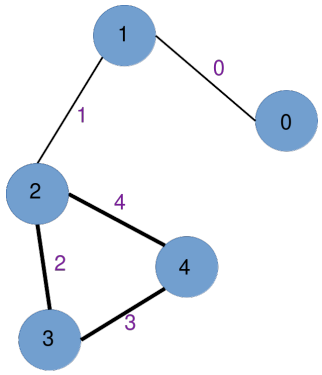
Figure 4: A graph with 23 1-vertex cliques (the vertices), 42 2-vertex cliques (the edges), 19 3-vertex cliques (light and dark blue triangles), and 2 4-vertex cliques (dark blue areas).

Adjacency Matrix

$|V| \times |V|$ adjacency matrix A is defined as follows: $A_{i,j} = 1$ if there is an edge from v_i to v_j. In our project we will consider undirected graphs with self-loops. This means that $\forall i, j \; A_{i,j} = A_{j,i}$ and $\forall i \; A_{i,i} = 1$.

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. In directed case, we mark the initial vertex as -1, and the terminal as 1.



The incidence matrix of the graph on the left would be as follows:

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

Degree Matrix

$|V| \times |V|$ diagonal degree matrix D is defined as follows: $D_{i,i} = \Sigma_j A_{i,j}$ (that is, $D_{i,i} = in\_degree(v_i) + out\_degree(v_i)$)

Laplacian matrix

Laplacian matrix — A matrix representation of a graph. Usually is calculated using the following formula [2]:

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

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

CGN *(Convolutional Graph Network)* — A type of GNN which generalizes the convolution operation to graphs. Often we encounter convolution while we work

with grid-structured data like images, but here we use same idea (aggregate features of the neighbors) on nodes instead of pixels [6].

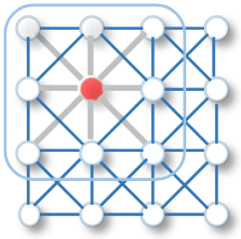


Figure 5: Convolution on image

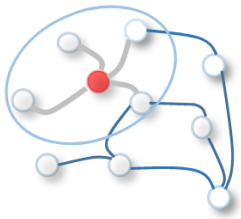


Figure 6: Convolution on graph

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: $Z = D^{-\frac{1}{2}}AD^{-\frac{1}{2}}XW$, 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

Then the output Z is directed into next layer, which does practically the same. There might be many convolutional layers, but usually models only have 2.

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.

Graph Attention Network

GAT *(Graph Attention Network)* — 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 [5]. 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.

We introduce an $N \times N$ matrix e storing the attention between the nodes: $e_{i,j} = a\left(W \cdot X_i,\ W \cdot X_j\right)$. Now we have to be careful about choice of i and j, since if we calculate the attention between all the nodes, we will completely drop structural information of the graph. One suggested solution is to use a neighborhood $\mathcal{N}_i$ of a vertex v_i and then compute $e_{i,j}$ for all $j \in \mathcal{N}_i$. Existing model [5] uses neighborhood of size 1 (that is, v_i itself and all of its neighbors v_j such that $\exists e = (v_i, v_j)$), and it seems to perform great.

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

3 Work schedule

3.1 Done

At this point, I have understood the subject area by thoroughly reading the papers mentioned in the reference section. Also, I started implementing my own implementation of a Graph Convolutional Network from scratch (that is, without any frameworks at all) [3].

We made this decision in order to be able to dig even deeper into the topic. Another benefit is the fact that improves the flexibility, since it is much easier to experiment with code written by yourself, rather than try to modify existing models.

3.2 Future plans

1. *Finish implementing the model*. It still lacks some crucial modules to work, however, we are almost at the finish line. The only part missing at the moment is the backpropagation logic. This should be done by the end of February 2022.

2. *Find additional datasets*. There are several datasets which are used for benchmarks [4] [7], however, it is always great to find new ones in order to see how existing models perform and how our tweaks influence the results. This is an ongoing task, so it does not have a particular deadline.

3. *Generalization of Laplacian*. Extraordinary simple to implement as soon as our model is done, but requires some time finding the generalizations.

4. *Work with simplices of higher dimensions*. This requires development of some kind of preprocessing mechanism, which takes graph as an input and provides the neural network with another graph. Efficiency is important, so the development might take significant time. I estimate the deadline to be in the middle of March 2022.

5. *Come up with new experiments*

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[5] Petar Veličković et al. "Graph Attention Networks". In: (2018). arXiv: 1710.10903 [stat.ML].

[6] Zonghan Wu et al. "A Comprehensive Survey on Graph Neural Networks". In: *IEEE Transactions on Neural Networks and Learning Systems* 32.1 (2021), pp. 4–24. DOI: 10.1109/TNNLS.2020.2978386.

[7] *Zachary's karate club dataset*. URL: http://www.konect.cc/networks/ucidata-zachary/.