

ASSIGNMENTS

January 12, 2022

1 Subgraph matching

Let $K = (V, A)$ be a connected graph and consider another graph G that can be disconnected. We can think of G either as a collection of graphs or as a big network.

Write a GNN-based algorithm for solving the graph matching of K in G . You are expected to begin from the solution proposed during the lecture given then 11th of February 2021 and carry out an experimental session according to the following items:

- *Prepare yourself a learning task* by constructing the learning and the test set. You can start from the Python scripts discussed during the lecture for the generation of random and scale-free graphs as well as from the script for the construction of graphs by specifically defining the nodes and edges;
- Propose the GNN architecture and carry out the experiments by using the *GNN with relaxation*;
- Propose the GNN architecture and carry out the experiments by using the *convolutional graph* approach;
- Discuss the two experimented solutions.

2 Graph isomorphism

Let $G = (V, A)$ be a collection of graphs. Write a GNN-based algorithm for solving the graph isomorphism problem.

- *Prepare yourself a learning task* by constructing the learning and the test set. You can start from the Python scripts discussed during the lecture for the generation of random and scale-free graphs as well as from the script for the construction of graphs by specifically defining the nodes and edges;
- Propose the GNN architecture and carry out the experiments by using the *GNN with relaxation*;
- Propose the GNN architecture and carry out the experiments by using the *convolutional graph* approach;
- Write an algorithm for graph isomorphism that uses PageRank;
- Discuss the two experimented solutions and compare with the solution determined by PageRank. Special attention must be given to the case of graphs with symmetries.

3 Clique detection and communities

Let $K = (V, A)$ be a connected graph and consider another graph G that can be disconnected. We can think of G either as a collection of graphs or as a big network.

Write a GNN-based algorithm for determining the cliques of K in G . You are expected to begin from the solution proposed during the lecture given then 11th of February 2021 and carry out an experimental session according to the following items:

- *Prepare yourself a learning task* by constructing the learning and the test set. You can start from the Python scripts discussed during the lecture for the generation of random and scale-free graphs as well as from the script for the construction of graphs by specifically defining the nodes and edges;
- Propose the GNN architecture and carry out the experiments by using the *GNN with relaxation*;
- Propose the GNN architecture and carry out the experiments by using the *convolutional graph* approach;
- Discuss the two experimented solutions.

4 Classification of generated graphs

Let G be a collection of graphs disconnected. Write a GNN-based algorithm for classifying the single graphs. You are expected carry out an experimental session according to the following items:

- *Prepare yourself a learning task* by constructing the learning and the test set. You can start from the discussed Python scripts for the generation of random and scale-free graphs as well as from the script for the construction of graphs by specifically defining the nodes and edges;
- Propose the GNN architecture and carry out the experiments by using the *GNN with relaxation*;
- Propose the GNN architecture and carry out the experiments by using the *convolutional graph* approach;
- Discuss the two experimented solutions with special emphasis to the joint role of information in the nodes and in the vertexes.

Hints: Examples of learning tasks can easily be obtained from the previous discussion on graphs with cliques and with a special sub-graph. The classification would become the task of detecting whether a given graph contains the sub-graph which defines the category. Another remarkable example is that of classifying graphs depending on their underlying generation mechanism. For example, an interesting learning task is one whose purpose is to classify between Erdos' random graphs and scale-free graphs.

5 MNIST handwritten character recognition by graphs

Based on the material available at <https://www.kaggle.com/kmader/mnist-based-graphs> set up an experimental environment based on GNN for the recognition of handwritten chars. The assignment is supposed to undergo the following steps:

- Construct a graph-based representation of the MNIST database

- Propose the GNN architecture and carry out the experiments by using the *GNN with relaxation*;
- Propose the GNN architecture and carry out the experiments by using the *convolutional graph* approach;
- Discuss the performance.

6 Learning PageRank

Write a program for computing PageRank on a given graph. Then construct a collection of random graphs and compute the corresponding PageRank on each node of the graphs. Use this collection of graphs along with the corresponding value of PageRank as a training set and use GNN for learning. The assignment is supposed to undergo the following steps:

- Construct a graph-based using the Erdos' random graph and scale-free generation;
- Propose the GNN architecture and carry out the experiments by using the *GNN with relaxation*;
- Propose the GNN architecture and carry out the experiments by using the *convolutional graph* approach;
- Discuss the performance.

7 Karate network