LIFAT Internship ANR CodeGNN

During 2022 - Tours France

Internship position in France - Structural attention mechanism for Graph Transformers

Master Subject

Context Most of the objects of interest of our today's life are based on discrete objects with sequential (strings) or more complex (graph) relationships. We can evoke the relationships between people in social graphs, the bounds between atoms in a molecule or the topographic distance between speed sensors in traffic analysis, to name a few. The prediction of the properties of such objects falls in the scope of structural pattern recognition.

Graph Neural Networks A first breakthrough in this field has been provided by the introduction of Graph Neural Networks (GNNs) [4]. As graph kernels, these networks provide a strong connection between graphs and machine leaning techniques. Moreover, as other deep learning techniques, GNNs avoid handcrafting the design of a similarity measure between graphs. GNNs are based on two operations, namely, Graph convolution and Graph decimation/pooling.

Graph Transformers A second breakthrough in this field has been provided by Transformer that were adapted to graph [1]. The main adaptations of the transformers to the graph domains are : 1°) The attention mechanism is a function of the neighborhood connectivity for each node in the graph. 2°) Second, the positional encoding that provides a structural context for each node in the graph. 3°) The architecture is extended to edge feature representation.

Internship objectives and tasks : Including structural information in the attention mechanism In previous works [2, 3], a first GNN architecture working directly into graph space was proposed. Convolution and pooling operators are defined in graph domain while allowing the use a back-propagation algorithm during the learning step. Especially, the convolution is replaced by a graph matching solver [5] applied on a subgraph rooted around each node of the

graph. The idea to be developed in the master thesis is to investigate the use of a graph matching solver in the objective to a structural attention mechanism.

The aim of this master thesis is to :

1. Study alternative computation of attention mechanism to take into structural information.
2. Propose a graph transformer model based on structural attention mechanism.
3. Program these models (in Python), and compare them to the state-of-the-art on standard datasets for different applications.

Suggested code : Interested readers could see the following code as a baseline: `https://github.com/graphdeeplearning/graphtransformer`

The Project

This internship is proposed in the context of a French National Project (ANR) called CodeGNN.

Supervisors

Jean-Yves Ramel (University of Tours, France) `ramel@univ-tours.fr`
Romain Raveaux (University of Tours, France) `romain.raveaux@univ-tours.fr`

Skills

Bachelor degree in Computer Science, Applied Mathematics, Data Science, or similar. Skills (with experiences): neural networks, deep learning, Python programming, numerical analysis.

When, where and how much

The internship will start from xx to xx. The internship will be granted with xx euros. This position is limited to 6 months but it could be continued by a PhD position. Funding for a PhD have been already obtained.

The internship will take place at the Computer science laboratory of Tours / Laboratoire d'Informatique Fondamentale et Appliquées de Tours (LIFAT, `http://lifat.univ-tours.fr`), Tours, France

How to apply

Please submit pdf files of your CV to: `ramel@univ-tours.fr` and `romain.raveaux@univ-tours.fr`. If your application is selected, you will then be contacted for further information and interview details.

References

[1] Vijay Prakash Dwivedi and Xavier Bresson. A generalization of transformer networks to graphs. *CoRR*, abs/2012.09699, 2020.

[2] Maxime Martineau, Romain Raveaux, Donatello Conte, and Gilles Venturini. A convolutional neural network into graph space. *CoRR*, abs/2002.09285, 2020.

[3] Maxime Martineau, Romain Raveaux, Donatello Conte, and Gilles Venturini. Graph matching as a graph convolution operator for graph neural networks. *Pattern Recognit. Lett.*, 149:59–66, 2021.

[4] Lilapati Waikhom and Ripon Patgiri. Graph neural networks: Methods, applications, and opportunities. *CoRR*, abs/2108.10733, 2021.

[5] Zhoubo Xu, Puqing Chen, Romain Raveaux, Xin Yang, and Huadong Liu. Deep graph matching meets mixed-integer linear programming: Relax at your own risk ? *CoRR*, abs/2108.00394, 2021.