Curvature-GAT : Improve graph attention with local structural information

Hugo Attali *, Adrien Guille *
Stephane Chretien *

* Université de Lyon, Lyon 2, ERIC UR 3083
{hugo.attali,adrien.guille,stephane.chretien}@univ-lyon2.fr,

Résumé. The success of deep learning in the Euclidean domain prompted a great interest to generalize neural networks to non-Euclidean domains e.g. graph. The main idea of GNNs is to find a good way to aggregate the features of neighboring nodes. The majority of Graph Neural Network (*GNN*) are based on message passing, where by information between neighboring nodes is propagated through the graph. GNNs update their representations in different ways. The GCN Kipf et Welling (2017) updates the nodes embeddings based on the neighbors using the degrees of the nodes while the graph architecture GAT Veličković et al. (2018) weighs the importance of the features of the neighboring vertices with an attention mechanism. GNNs can be confronted with a certain number of problems in particular of less good performance in heterophilic environment Zhu et al. (2020), when the neighboring nodes are not similar or at least give very different information. The phenomenon of over-smoothing which arrives when the message passing is carried out in an excessive way, in this case all the representations of the vertices of the graph are going to be similar Oono et Suzuki (2020) Cai et Wang (2020). In this case results of node classification task will be rapidly degraded Kipf et Welling (2017) Qimai Li (2018). Another problem is the botleneck phenomenon in a graph which happens when two parts of a graph are connected by very few edges Alon et Yahav (2020). So when passing a message the information will have to be condensed inevitably causing a loss of information. Recently, it has been shown that the bottleneck phenomenon comes from certain areas of the graphs, which can be identified by a measure of edge curvature. More specifically Topping et al. (2022) show that the negatively curved edges are characteristic of the bottleneck phenomenon and therefore disrupts message passing. So they propose to modify the structure of the graph by adding and removing edges to address this issue. This method it's a way to break the bottleneck and improves results in node classification task. In this paper we propose to modify the GAT attention mechanism to modulate the attention weights according to the curvature of the edges, much richer measure compared to previously ones that focus only on the degree. Giving a higher importance to the negative edges seems to mitigate the bottleneck problem and experiments conducted on different datasets show that our method is more efficient and improves the original GAT method in the classification of nodes.

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