Project Report

Graph Attention Networks

Justin Pauckert

Supervised by

Prof. Sebastian Pokutta

Christoph Graczyk

June 24, 2021

Seminar on Discrete Optimization and Machine Learning

Berlin Institute of Technology

Introduction

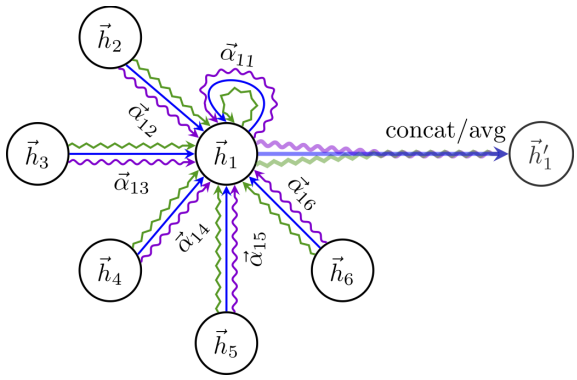
As machine learning models find their way in more and more fields of science, allowing them to work with graph data has been a research topic with increasing popularity in recent years. Graphs are commonly used across various fields such as social science (social networks), natural science (protein-protein interactions) and knowledge graphs [Zhou et al., 2021]. In order to allow for this unique data structure, special neural networks have been developed, called **graph neural networks (GNNs)**. With advancements in the field of deep learning, especially the invention and success of convolutional neural networks, the development of similar methods for graphs suggests itself. In both cases, extracting localized features and composing them to more complex and expressive representations is a major step towards high-performance models for classification and clustering tasks. One way of generalizing convolutions in the graph domain are so-called spatial methods ([Hamilton et al., 2018], [Monti et al., 2016]), where convolutions are defined directly on the graph, operating on groups of spatially close neighbors. Inspired by this idea, [Veličković et al., 2018] proposed a new architecture to compute node representations by attending over a node's neighbors and assessing their individual importance, called **graph attention networks (GATs)**. This report covers a short explanation of the proposed idea and discusses some of its benefits in specific applications. Finally, we will give an overview of related developments in the field, including concerns over prevalent data sets used for benchmarks and limitations of architectures like GATs.

GAT Architecture

Graph attention networks are build by stacking graph attentional layers, which we will briefly explain in this section, closely following [Veličković et al., 2018]. The input of a layer is a set of node features, $h = \{h_1, ..., h_N\}, h_i \in \mathbb{R}^F$, where N is the number of nodes and F the number of features in each node. The layer produces a new feature representation $h'_i \in \mathbb{R}^{F'}$ for each node h_i, possibly of different cardinality F'. To that end, a learnable weight matrix $\mathbf{W} \in \mathbb{R}^{F' \times F}$ and a shared attention mechanism $a : \mathbb{R}^{F'} \times \mathbb{R}^{F'} \to \mathbb{R}$ are introduced. The importance of a node's neighbor, called *attention coefficient*, is then computed as $a(\mathbf{W}h_i, \mathbf{W}h_j)$. Denoting the normalized coefficients as α_{ij}, the hidden state of a node h_i can then be obtained by

$$h'_i = \sigma(\sum_{j \in \mathcal{N}_i} \alpha_{ij} \mathbf{W} h_j)$$

where $\mathcal{N}_i$ is the set of indices for neighbors of h_i and σ a nonlinear function. This process can be initiated multiple times, resulting in multiple attention mechanism. This popular method is called *multi-head attention* and was adapted from [Vaswani et al., 2017]. The resulting features can then be concatenated or averaged to improve the models performance as illustrated in Figure 1.



Multi-head attention with three heads by node h_1. [Veličković et al., 2018]

An important observation is that.... properties of GATs

Applications

Examples for brain data and text models. As machine learning models find their way in more and more fields of science, allowing them to work with graph data has been a research topic with increasing popularity in recent years. Graphs are commonly used across various fields such as social science (social networks), natural science (protein-protein interactions) and knowledge graphs [Zhou et al., 2021]. In order to allow for this unique data structure, special neural networks have been developed, called **graph neural networks (GNNs)**. With advancements in the field of deep learning, especially the invention and success of convolutional neural networks, the development of similar methods for graphs suggests itself. In both cases, extracting localized features and composing them to more complex and expressive representations is a major step towards high-performance models for classification and clustering tasks. One way of generalizing convolutions in the graph domain are so-called spatial methods ([Hamilton et al., 2018], [Monti et al., 2016]), where convolutions are defined directly on the graph, operating on groups of spatially close neighbors. Inspired by this idea, [Veličković et al., 2018] proposed a new architecture to compute node representations by attending over a node's neighbors and assessing their individual importance, called **graph attention networks (GATs)**. This report covers a short explanation of the proposed idea and discusses some of its benefits in specific applications. Finally, we will give an overview of related developments in the field, including concerns

over prevalent data sets used for benchmarks and limitations of architectures like GATs.

Benchmarking GNNs

benchmarks in Question depth of GNNs the road ahead?

Going deep with GNNs

benchmarks in Question depth of GNNs the road ahead?

References

[Hamilton et al., 2018] Hamilton, W. L., Ying, R., and Leskovec, J. (2018). Inductive representation learning on large graphs.

[Monti et al., 2016] Monti, F., Boscaini, D., Masci, J., Rodolà, E., Svoboda, J., and Bronstein, M. M. (2016). Geometric deep learning on graphs and manifolds using mixture model cnns.

[Vaswani et al., 2017] Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., Kaiser, L., and Polosukhin, I. (2017). Attention is all you need.

[Veličković et al., 2018] Veličković, P., Cucurull, G., Casanova, A., Romero, A., Liò, P., and Bengio, Y. (2018). Graph attention networks.

[Zhou et al., 2021] Zhou, J., Cui, G., Hu, S., Zhang, Z., Yang, C., Liu, Z., Wang, L., Li, C., and Sun, M. (2021). Graph neural networks: A review of methods and applications.