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Project: Decomposing Graph Neural Networks

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Motivation

Many types of unstructured data can be effectively represented using graphs, for instance, social networks, molecular structures, or recommendation systems. These graphs consist of nodes (representing entities), which are connected by edges (depicting relationships between entities). Graph neural networks (GNNs) [2, 5] are machine learning techniques that are efficient in processing and analyzing such data. GNNs operate by iteratively passing information through the nodes and edges of a graph, allowing them to aggregate and update information based on their surroundings, i.e., neighboring nodes and edges. This enables the GNNs to capture complex relationships and patterns within the data.

However, despite their effectiveness in many practical applications, GNNs suffer from tedious and time-consuming training phases, especially in the case of large and complex graph data.

Figure 1: Social network described by a graph (background) and a shallow neural network (foreground).

Problem description

The aim of this project is to enhance the training process of GNNs by leveraging domain decomposition methods (DDMs) [6]. DDMs are classical numerical methods for solving boundary value problems based on partial differential equations (PDEs). Their effectiveness lies in exploiting the strength of local interaction of the PDEs and in reducing the global exchange of information. This project aims to extend the capabilities of traditional DDMs beyond PDEs, in particular, to training of GNNs by utilizing the local connectivity in graphs.

Since the training of a GNN involves solving a (non-convex) optimization problem, nonlinear domain decomposition techniques have to be considered; cf. [1]. In particular, we aim to extend the approach from [3], which employs a layer-based nonlinear domain decomposition to enhance the training of feedforward networks to GNNs. The proposed adaptation leverages the connectivity information, specifically the underlying graph structure. Given that not all nodes are connected and that the strength of these connections varies with the weights of the graphs, we seek to identify a partitioning of the graph. This partitioning will give rise to a decomposition, which ensures that nodes within the same partition exhibit particularly strong connections, while connections between nodes belonging to different subgraphs are comparatively weaker.

Tasks

1. Implement a GNN using a state-of-the-art deep learning software library[1] and train it on benchmark data; see, e.g., [4].
2. Get familiar with the `DistTraiNN` code and methodology of nonlinear domain decomposition for neural networks from [3]; The code will be provided.
3. Extend the `DistTraiNN` code from [3] to the GNNs from task #1, or implement the extension to GNNs from scratch.
4. Test the algorithm on benchmark data sets [4] and, if time allows, on some real-world application data sets.

[1]For example: PyTorch, TensorFlow, or Jax.

Prerequisites

A suitable candidate has:

- Experience in machine learning, in particular, with neural networks, and their implementation using a state-of-the-art deep learning software library[2].
- Basic knowledge in numerical methods and optimization.

Contact

If you are interested in this project and/or have further questions, please contact Alexander Heinlein, a.heinlein@tudelft.nl, or Alena Kopaničáková, alena_kopanicakova@brown.edu.

References

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[2]See footnote 1