Master Thesis

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Master Thesis

Efficient Training of Graph Convolutional Networks for Dynamic Phenomena

Graph Neural Networks (GNNs) have shown great potential for use cases that can be described as graphs, e.g., predicting interactions in protein-protein networks or modeling fluid dynamics in physio-chemical processes. However, training GNNs presents unique challenges due to the characteristics of graph data. Several extensions of GNNs have been proposed, so that they can handle tasks that were so far only possible on non-graph data. For instance, [1] have proposed Spatial Graph Convolutional Networks (SGCNs) to take into account the ordering of node neighbors. They generalize 2D convolutions to leverage the structural information of the graph. Each layer in SGCN is modeled as a message-passing process, and each node aggregates the features of its neighbors.

Our use case for dynamic phenomena is the so-called "injection molding process" from materials science, which describes the injection of hot materials into a cavity to produce composite materials. This process can be modelled accurately with numerical simulations. However, these simulations are computationally expensive, and finding good parameter values for the process involves much trial-and-error, even for simple geometries.

We propose to represent the geometry of a part as a graph and to design a GCN surrogate model to approximate the simulation output, as in [2]. Our goal is to have a much faster model with similar accuracy as the numerical simulation. The following aspects are important:

Learning efficiency: There is a trade-off between the number of message passing layers and efficiency of the node embeddings capturing the relationship between adjacent nodes. Adding more layers lets the model capture long-distance interactions, but reduces the effectiveness of message passing due to repeated compression of information. Effects related to this trade-off have been identified as over-squashing, under-reaching, over-smoothing [3]. To improve the learning abilities of SGCNs, we need to properly mitigate these effects. A promising first step might be mitigation layers.

Scalability: Large graphs come with large memory requirements and inefficient gradient updates. Several studies (e.g., [4, 5]) propose different sampling algorithms to solve this. However, depending on the application and the prediction task, sampling may decrease the predictive performance. Considering the mesh-based representation of geometries of parts, we could think about a better sampling algorithm in which the resolution of the representation varies depending on the "relevance" of the corresponding geometry region. Such an adaptive resolution could bring a runtime advantage.

Domain knowledge: Incorporating domain knowledge may improve the performance and runtime of the model. For instance, we could add important process parameters (e.g., melt temperature) and search for relevant domain-specific features (e.g., velocity data profile).

Thus, the focus of this thesis is on how to accelerate and improve the learning abilities of GCNs, by considering the mentioned multi-faceted aspects individually. This results in the following tasks:

- Literature review on Graph Neural Networks.
- Design and implementation of an appropriate approach addressing the issues above.
- Systematic evaluation of the approach and generalizations for other GNN use cases.

For this work, you will get access to data for the case study as well as to domain knowledge as we collaborate with materials scientists from the KIT institute "FAST".

To successfully conduct this thesis project, you must have a basic knowledge of Python, the ability to plan and work independently as well as a high level of motivation, enthusiasm and curiosity. To support you with this task, we offer thorough mentoring and recurrent meetings with your advisor as well as access to our institute's computing infrastructure.

[1] T. Danel et al. "Spatial Graph Convolutional Networks". In: *Neural Information Processing*. 2020.
[2] A. Sanchez-Gonzalez et al. "Learning to Simulate Complex Physics with Graph Networks". In: *PMLR 119*. 2020.
[3] U. Alon and E. Yahav. "On the Bottleneck of Graph Neural Networks and its Practical Implications". In: *ICLR*. 2021.
[4] W. Hamilton et al. "Inductive Representation Learning on Large Graphs". In: *Advances in Neural Information Processing Systems*. 2017.
[5] J. Chen et al. "FastGCN: Fast Learning with Graph Convolutional Networks via Importance Sampling". In: *ICLR*. 2018.

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