Guided Graph Compression for Quantum Graph Neural Networks

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Abstract

Graph Neural Networks (GNNs) are a set of Machine Learning (ML) models that are very powerful for analyzing graph-structured data [1, 2]. However, classical GNNs suffer from limitations when handling large graphs, since the memory requirements are high [3] and they require sparse matrix operations, which are not efficient in classical GPUs [4]. Additionally, GNNs are also limited in expressiveness by the Weisfeiler-Lehman test [5].

Due to this, there is a motivation to use Quantum Computing (QC) to overcome these limitations [6], since it is known to surpass classical methods in terms of speed for some problems [7, 8]. Furthermore, Quantum Machine Learning (QML) aims to enhance classical ML methods. Recently, guarantees about the generalization capabilities, expressivity and trainability of QML models have been studied [9, 10, 11], showcasing their potential.

One of the most popular QML frameworks is the Variational Quantum Classifier (VQC) [12]. Within this framework, Quantum Neural Networks (QNNs) serve as the quantum analogs to classical Neural Networks (NNs). General QNN circuits or ansatzes have already been used for a number of ML tasks [13, 14]. However, these types of general ansatzes suffer from barren plateaus [15], where the gradients of the quantum circuit tend to zero. To overcome this problem, more specialized ansatzes are needed. Quantum Graph Neural Networks (QGNNs) [16] emerged with this motivation to be able to analyze graph-structured data with quantum computers.

Nevertheless, quantum hardware is subject to noise and error correction protocols are still far from being implemented. This limits the dimension of the data that can be effectively encoded on current quantum computers. For graph-structured data, recent works manually preprocess and simplify the datasets based on domain knowledge [17] or create small synthetic datasets that have little practical use [18]. For non-graph data, autoencoders have been used in the context of QML to reduce the dimensionality of the datasets [19]. Moreover, the Guided Quantum Compression (GQC) framework introduced in [20] proposes an enhanced way to reduce the dimensionality of the datasets by simultaneously guiding the compression towards improving the performance of a complex classification task taken from high energy physics. This is done by combining the reconstruction loss function of the autoencoder with the classification loss function of the quantum classifier. This is applied to the task of classifying Higgs bosons and demonstrates an improvement in comparison to training the autoencoder as a separate preprocessing step.

In this work, the GQC framework is generalized to graph-structured data, proposing the Guided Graph Compression (GGC) framework. In it, a graph autoencoder named SAG model [21] is used. The model uses a combination of the GraphSAGE architecture [22] with Self-Attention Graph (SAG) pooling [23] to obtain compressed graphs in terms of the number of nodes and node feature dimensionality. The reconstruction and classification loss functions are coupled and controlled by a weight hyperparameter to be able to guide the compression towards improving the final classification performance. This framework enables the possibility of designing novel QGNN ansatzes and be able to apply them to practical tasks with the aim of obtaining a quantum advantage.

Here, the GGC framework is applied to the jet tagging task [24], which consists on classifying jets as being originated from a quark or a gluon. Jets are a set of particles that can be represented as graphs. To validate the performance of the framework, the following training paradigms are evaluated. First, a classical GNN baseline classifier is used without compressing the data. Then, the graph autoencoder is trained as a separate preprocessing step, and the compressed graphs are fed to the classical GNN classifier and to a QGNN classifier introduced in [25]. Lastly, the GGC framework is tested on both the classical and quantum classifiers.

Results show that compressing the graph as a separate step for the classical and quantum classifiers significantly degrades the performance compared to training with the uncompressed data in the classical case. However, using the GGC framework, the classical and quantum classifiers outperform the uncompressed classical baseline. Both the guided classical and quantum classifiers obtain similar results in terms of the ROC AUC score.

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