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Title : Role of data-embedding in equivariant quantum convolutional neural networks.

Abstract: The subfield of geometric quantum machine learning gives rise to Equivariant quantum neural networks (EQNNs), which are parametrized quantum circuits (PQCs) designed to respect *label symmetry* viz. the invariance of the class labels of data points under the action of a symmetry group. Therefore, these networks perform optimization over a smaller parameter space, and have shown faster training and better generalization compared to a general non-equivariant QNN. We specifically study an Equivariant quantum convolutional neural network (EQCNN). An EQCNN is composed of a sequence of equivariant convolutional and pooling layers. Each of these layers is constituted of locally acting two-qubit parametrized ansatze. Moreover, the translation invariance condition demands that in a particular convolutional or pooling layer, all locally acting ansatze must share the same parameters.

In our work, we investigate the role of classical-to-quantum data embedding on the performance of an EQCNN. Our motivation comes from the fact that- in any EQNN the PQC belongs to the space of commutators of the group representation, and the representation in turn can vary with changing data-embedding methods. For example- when using amplitude embedding, the representations corresponding to spatial transformations on classical images, eg. reflection or rotation, are tensor products of single-qubit unitary operators acting locally on each qubit. On the other hand, for qubit embedding, the representations corresponding to the these transformations act non-locally on a group of qubits.

In the former case, an EQCNN can be designed by making sure that each of the two-qubit convolutional and pooling ansatze commute with the locally acting two-qubit component of the representation. However, as we discuss in our manuscript, due to translation invariance constraint, these two-qubit ansatze can be made equivariant with respect to only a subset of all locally acting components of a representation. Moreover, in some cases the choice of initial representation may affect the reduced representations after each pooling layer, which in turn affect the expressibility of the full PQC corresponding to the EQCNN. These observations point to the importance of choosing a suitable data-embedding for EQCNNs for an optimum performance.

To numerically verify the above arguments for amplitude embedded classical images, we use reflection-symmetric datasets Fashion MNIST and Cifar10, and 180°-rotation-symmetric dataset Blood MNIST. As different data embeddings- we use standard amplitude embedding (AE), and another embedding obtained by permuting the basis of standard AE. These embeddings give rise to different group representations corresponding to above symmetries. We explicitly show the construction of EQCNNs for all the above symmetry groups, and perform binary classification on each of the datasets using Pennylane quantum simulator. Our results show the following.

1. The test set classification accuracy clearly varies depending on the data embedding. This behaviour is more prominent during the initial training iterations. Particularly, we find that when the representation is a tensor product of Pauli-X matrices acting on each qubit, the accuracy significantly lags behind those for other representations.

2. The improvement in classification accuracy for EQCNN over a non-Equivariant QCNN may be present or absent depending on the particular dataset and embedding used.

Turning our attention now to qubit embedding, the label symmetries for reflection or rotation of classical images are manifested as subgroups of the Symmetric group S_n which acts non-locally on the qubits. However, due to the local and translation-invariant nature of convolutional layers and qubit-reducing feature of pooling layers in a QCNN, it is not straightforward to incorporate equivariance in these layers for non-local representations. We argue that depending on the symmetry, it is important to hand-pick a particular order in which the pixels are embedded into the qubits for designing equivariant convolutional layers. We explicitly demonstrate these constructions for reflection group, as well as the case when both reflection and 180°-rotation symmetry is present in labels of classical images. Our numerical simulations using Pennylane show improved test set accuracy of these EQCNNs compared to non-equivariant QCNNs.

Quantum convolutional neural networks have been successfully applied to classify topological phases of quantum many-body Hamiltonians, as well as classical images. They are free of barren-plateau problem, implying an efficient trainability. Our results conceptually and numerically show the importance of choosing a suitable encoding and strategies to build the corresponding architecture to ensure an improved performance of EQCNN compared to a non-equivariant QCNN. We believe that the results will contribute to the understanding of the growing field of geometric quantum machine learning.