Hybrid quantum tensor networks for aeroelastic applications

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Simulations of aeroelastic phenomena involve modelling complex fluid dynamics and the structural behaviour of components. Data driven implementations using machine-learning algorithms for aerodynamic simulations are currently under development as possible solutions. Recently there has also been an increasing interest in utilising quantum computations and tensor network approaches (both on classical and quantum hardware) for machine learning (ML). Therefore, we investigated the prospect of using hybrid quantum tensor network based algorithms for aeroelastic problems.

Tensor networks were initially developed to reduce the computational cost of lowly entangled multi-particle quantum states. Nevertheless, they are able to efficiently approximate a wide variety of large tensorial objects using a regular, less complex structure. Thus, providing a convenient approach to quantum machine learning (QML) [6].

A wide variety of QML approaches employing quantum circuits with tunable parameterised gates, so called variational quantum circuits (VQCs), have recently been proposed [4]. Quantum tensor network for ML can be realised by VQCs using a tensor network inspired internal gate structure [6].Unlike for general VQCs, the dimension of the space of possible weights can be adjusted easily by varying the bond dimension between each tensor node. This allows for access to the full Hilbert space and a set of product spaces. Thus allowing the tuning of the expressivity of the circuit [2].

QML is still in very early stages of development, therefore when designing a quantum circuit, choices on a very basic level must be made, e.g. the data encoding circuit, entangling schemes and the measurement processes. As it is not clear to date which choices are the most relevant we carried out multiple hyperparameter searches to find optimal configurations.

Classical tensor networks have various applications within aeroelastics, such as aeroelastic system identification. The goal is to derive data driven models which enable the prediction of aeroelastic characteristics including the stability behaviour of the system [1].

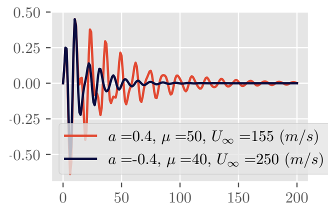

Fig. 1. Stable aeroelastic response.

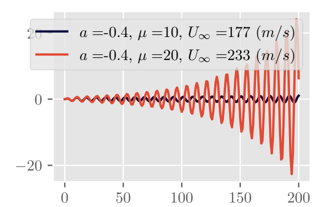

Fig. 2. Unstable aeroelastic response.

We used a simplified aeroelastic configuration including a low-dimensional aerodynamic model for investigating the potential of QML for estimating the flutter stability of the system, based on [5]. The stability is represented by time series for different combinations of aerolastic parameters (a, μ, U_∞), examples are shown in fig. 1 and 2. The goal of this application case is to apply hybrid quantum algorithms to the complete time series and on one hand determine the binary stability classification and on the other to regress the generating aeroelastic parameters from the time series.

The data has a wide range of values, therefore we clipped outlier values and then applied a ± 1 normalisation. Due to the one dimensional structure of the time series, tensor networks and specifically Matrix Product States (MPS) are well suited to express this type of data [6]. However, due to the computational power needed to simulate quantum circuits we first needed to carry out a dimensionality reduction. We used classical 1D convolutional neural networks [3] to reduce the data from 201 to an 8-dimensional compressed feature vector. Which was then used as input for the MPS inspired quantum neural networks.

We found that the simple binary time-series classification could be easily solved by our algorithm. Achieving a maximum F1-score of well above 0.9, averaged over 5 repeated training runs. The best model achieved a F1-score of 0.999 as shown in the confusion matrix (CM) in fig. 3. We carried out a small hyperparameter search since we quickly found good performing configurations.

For the regression task we used the same tensor networks inspired VQC algorithm as in the previous task, up to the number of qubits measured. In the first task we measured only 1 qubit to get the binary classification probability, but for the regression task we needed to measure 3 expectation values to get the regression values. This also increased the minimal bond dimension.

We carried out an extensive hyperparameter search and found that overall the runs are less stable, especially when considering each dimension of the regression vector separately as shown in fig. 4. This can be explained by the different granularity of each component: a has 9 distinct values, μ has 5 and U_∞ has 201. The score difference between a and μ could be explained by the former having enough values to better cover the normed target value range, so that the errors between predictions and targets in the mean are less than for the more separated values of μ.

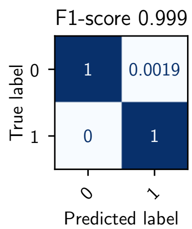

Fig. 3. Best test CM for the classification task.

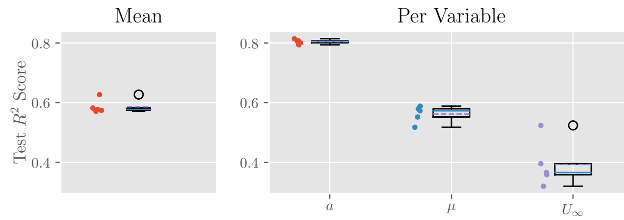

Fig. 4. Test regression score for the best model for the regression task, averaged over 5 runs.

The regression task is considerably harder to solve since the prediction of discrete variables with multiple possible values using expectation values of observables is far more challenging than a binary classification, where only a certain threshold has to be surpassed.

In conclusion, we found that hybrid quantum tensor network based algorithms can be successfully applied to aeroelastic problems. Nevertheless the appropriate choice of hyperparameters is still a challenge. At the moment, we have achieved outstanding results for the time series classification task, and promising results for regressing parameters from the time series.

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