



Contribution ID: 55

Type: Oral

Quantum neural networks force fields generation

Tuesday, 25 October 2022 17:20 (20 minutes)

Accurate molecular force fields are of paramount importance for the efficient implementation of molecular dynamics techniques at large scales. In the last decade, machine learning methods have demonstrated impressive performances in predicting accurate values for energy and forces when trained on finite size ensembles generated with ab initio techniques. At the same time, quantum computers have recently started to offer new viable computational paradigms to tackle such problems. On the one hand, quantum algorithms may notably be used to extend the reach of electronic structure calculations. On the other hand, quantum machine learning is also emerging as an alternative and promising path to quantum advantage. Here we follow this second route and establish a direct connection between classical and quantum solutions for learning neural network potentials. To this end, we design a quantum neural network architecture and apply it successfully to different molecules of growing complexity. The quantum models exhibit larger effective dimension with respect to classical counterparts and can reach competitive performances, thus pointing towards potential quantum advantages in natural science applications via quantum machine learning.

Significance

We propose a quantum neural network (QNN) for to computation of molecular energy and forces and use it to drive molecular dynamic simulations. While QNNs have already been proposed in quantum chemistry, our reaches better accuracy and computes the forces as well.

References

<https://arxiv.org/abs/2203.04666>

Experiment context, if any

Primary author: KISS, Oriel Orphee Moira (Universite de Geneve (CH))

Co-authors: Dr TACCHINO, Francesco (IBM Research Zürich); TAVERNELLI, Ivano (IBM Research - Zurich); Dr VALLECORSIA, Sofia (CERN)

Presenter: KISS, Oriel Orphee Moira (Universite de Geneve (CH))

Session Classification: Track 3: Computations in Theoretical Physics: Techniques and Methods

Track Classification: Track 3: Computations in Theoretical Physics: Techniques and Methods