Usage Report for Fiscal Year 2021

Project Title:

Deep Learning of Quantum Matrix

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1. Background and purpose of the project, relationship of the project with other projects

Deep learning is transforming many areas of physics and engineering. Deep neural networks can be used as universal approximations to simplify the analysis of several physical systems, from materials to the brain.

In quantum physics we are often interested in computing the wave function of a collection of degrees of freedom (a configuration, or a state). From this point of view, the wave function can be seen as a map from quantum states to a probability amplitude (a complex number related to the Born probability).

Neural networks are naturally suited to represent such mappings in a parametric way: the parameters of the neural network can then be adjusted to obtain the desired wave function.

This project applies the aforementioned idea to a quantum system of matrices used to describe the low-energy dynamics of certain string theories. Extracting the ground state wave function of a quantum matrix model can be useful to study how information is encoded in a black hole. For this reason, this project is deeply connected to quantum information science and quantum gravity.

2. Specific usage status of the system and calculation method

We had started our study before applying for time on Hokusai BIGWATERFALL, but we have used the system to finish the study by using 4% of the total allocated resources, amounting to 100665 core-hours. We used a single-node multi-threaded code based on python and on the tensorflow deep learning framework.

The calculation method starts by identifying the Hilbert space of the quantum matrix model and defining a base of states over which to compute the wave function. Then we define a neural network taking any quantum state as input and returning a probability density. For this purpose, we use normalizing flows which have a flexible but tractable density.

The parameters of the neural network/flow are optimized iteratively under the objective of minimizing the expectation value of the energy: this process is called Variational Monte Carlo, because the expectation values are computed stochastically over a set of sampled states according to the parameterized probability density.

3. Result

We have tested this Variational Monte Carlo method with parameterized wave functions using neural networks. The first test was to compute the energy of the ground state for a bosonic quantum matrix model and compare the results to an exact result obtained using the diagonalization of the Hamiltonian in qutip (a python package developed by our group at

RIKEN). The results achieve a precision higher than 99%.

We have also tested the method on a supersymmetric quantum matrix model and obtained similar encouraging results.

Our results have attracted attention from the media, with a calculated attention score of over 300 in just a few weeks (Link to Altmetric)

4. Conclusion

Deep learning paired with Variational Monte Carlo methods is a very promising avenue to study quantum many-body systems, from spin glasses to matrix models. Our project demonstrates the accuracy of this method on different quantum matrix models and also compares this method to recent quantum algorithms.

5. Schedule and prospect for the future

We expect to continue this project in the next fiscal year and study more complicated wave functions. For example, we plan to study how to create wave functions of localized states in quantum matrix models as well as investigate their properties at finite temperature.

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Fiscal Year 2021 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

Enrico Rinaldi, Xizhi Han, Mohammad Hassan, Yuan Feng, Franco Nori, Michael McGuigan, Masanori Hanada, "Matrix Model simulations using Quantum Computing, Deep Learning, and Lattice Monte Carlo", PRX Quantum 3, 010324, 2022

[Conference Proceedings]

Enrico Rinaldi, Xizhi Han, "Neural quantum states for supersymmetric quantum gauge theories", 4^{th} workshop on Machine Learning and the Physical Sciences at NeurIPS 2021, December 13th

[Oral presentation]

Enrico Rinaldi, "A deep learning and hybrid quantum-classical approach to matrix quantum mechanics", EPFL, Computational Quantum Science group seminar, Lausanne, September 2021

Enrico Rinaldi, "Quantum gravity in the lab: quantum computing and deep learning solutions", Infineon, Machine Learning Reading Seminar Series, Munich, October 2021

Enrico Rinaldi, "Quantum gravity in the lab: matrix quantum mechanics meets quantum computing", FRIB, Nuclear Science Seminar Series, East Lansing, October 2021

Enrico Rinaldi, "Quantum gravity in the lab: matrix quantum mechanics meets quantum computing", University of Liverpool, Nuclear Theory Seminar Series, Liverpool, November 2021

Enrico Rinaldi, "Quantum gravity in the lab: matrix quantum mechanics meets quantum computing", QTML2021, Quantum Techniques in Machine Learning, Online, November 2021

[Poster presentation]

Enrico Rinaldi, "A deep learning and hybrid quantum-classical approach to matrix quantum mechanics", Applied Machine Learning Days, Physics & AI, September 2021

Enrico Rinaldi, Xizhi Han, "Neural quantum states for supersymmetric quantum gauge theories", 4^{th} workshop on Machine Learning and the Physical Sciences at NeurIPS 2021, December 13th

[Others (Book, Press release, etc.)]

Enrico Rinaldi, Morgan Sherburne, "What's inside a black hole? U-M physicist uses quantum computing, machine learning to find out", Michigan News

YouTube video: Link