Bridging Research and Applications in Quantum Machine Learning with the Qsun universal platform

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Abstract

Quantum virtual machine (QVM) for simulating a quantum computer on classical computers is an important platform to write and test quantum algorithms before running them on real quantum computers. We are pleased to introduce Qsun, which functions as a QVM founded upon quantum state wavefunctions. The platform also has a set of native tools for VQAs, especially with the parameter-shift rule to implement quantum differentiable programming (QDP) for gradient-based optimization. In summary, Qsun is a powerful QVM to solve machine learning problems.

Introduction

We introduce Qsun as a wavefunction-based QVM platform specifically designed to support QML applications. A quantum register in Qsun is described by a wavefunction, and quantum gates are simulated directly by updating the wavefunction's amplitude. The measurement results are derived by the probability of the wavefunction. With our simple implementation, our project has a faster computation speed with a small number of qubits when compared to other QVMs such as Qiskit, ProjectQ, or Pennylane. Based on this general purpose QVM, we will try to take advantages from QDP with parameter-shift rule as a core engine towards the practical QML application. Qsun is compared with standard programs: Qiskit, ProjectQ, and Pennylane, as well as classical algorithms in applicable aspects. In these comparisons, Qsun generally performs a bit better in quantum differentiable programming (QDP), Quantum Regression (QR), and quantum neural network (QNN). In summary, Qsun is an efficient and effective integration of QVM and QDP for the machine learning problem-oriented.

Structure

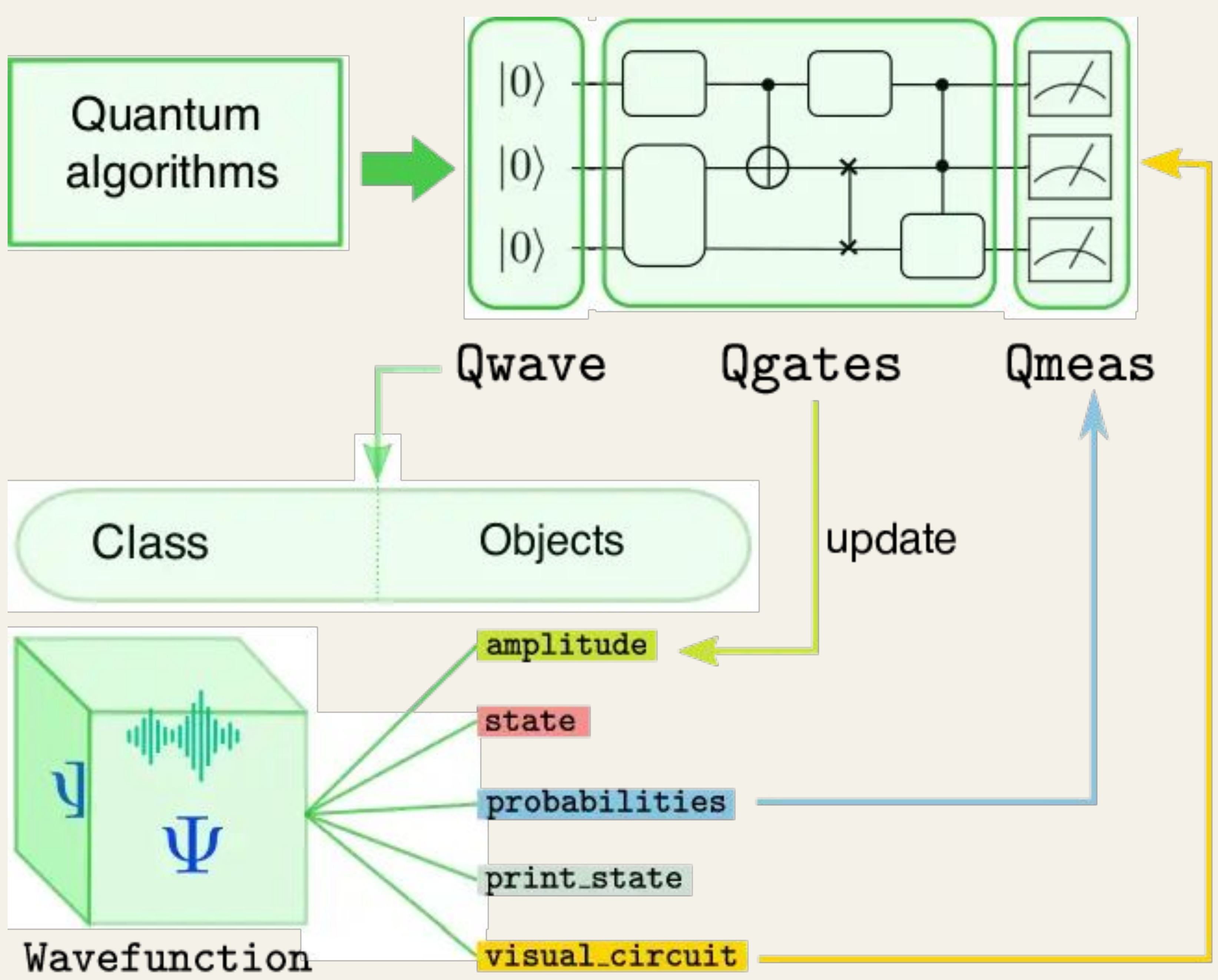

Figure 1. Qsun quantum virtual machine (QVM) [1] consists of three main modules: `Qwave`, `Qgates`, and `Qmeas`, to simulate quantum circuits with a quantum register (qubits), quantum gates, and quantum measurements, respectively. A quantum register is built through its wavefunction by the `Wavefunction` class and its constituent objects in Qsun, as shown in the figure. Qsun also contains `Qkernels` and `Qencodes` for quantum kernel methods.

Results and Discussion

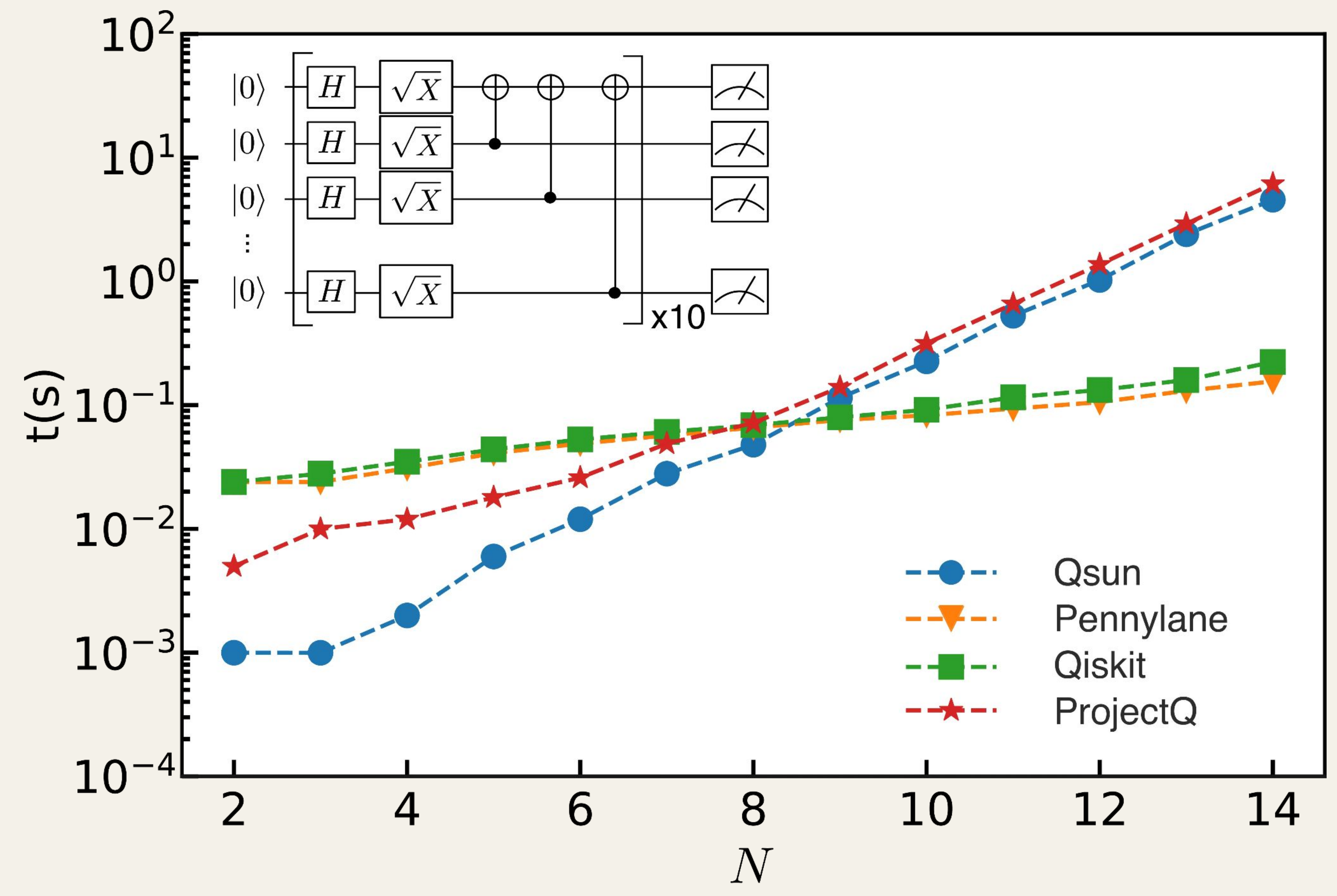

Figure 2. Computational time t (seconds) for different QVMs as a function of increasing number of qubits N. Inset: the testing circuit consisting of an H, an $X^{1/2}$, and a CNOT gates acting on each qubit. The depth is fixed to be 10, and the number N of qubits is varied to test the performance of QVMs.

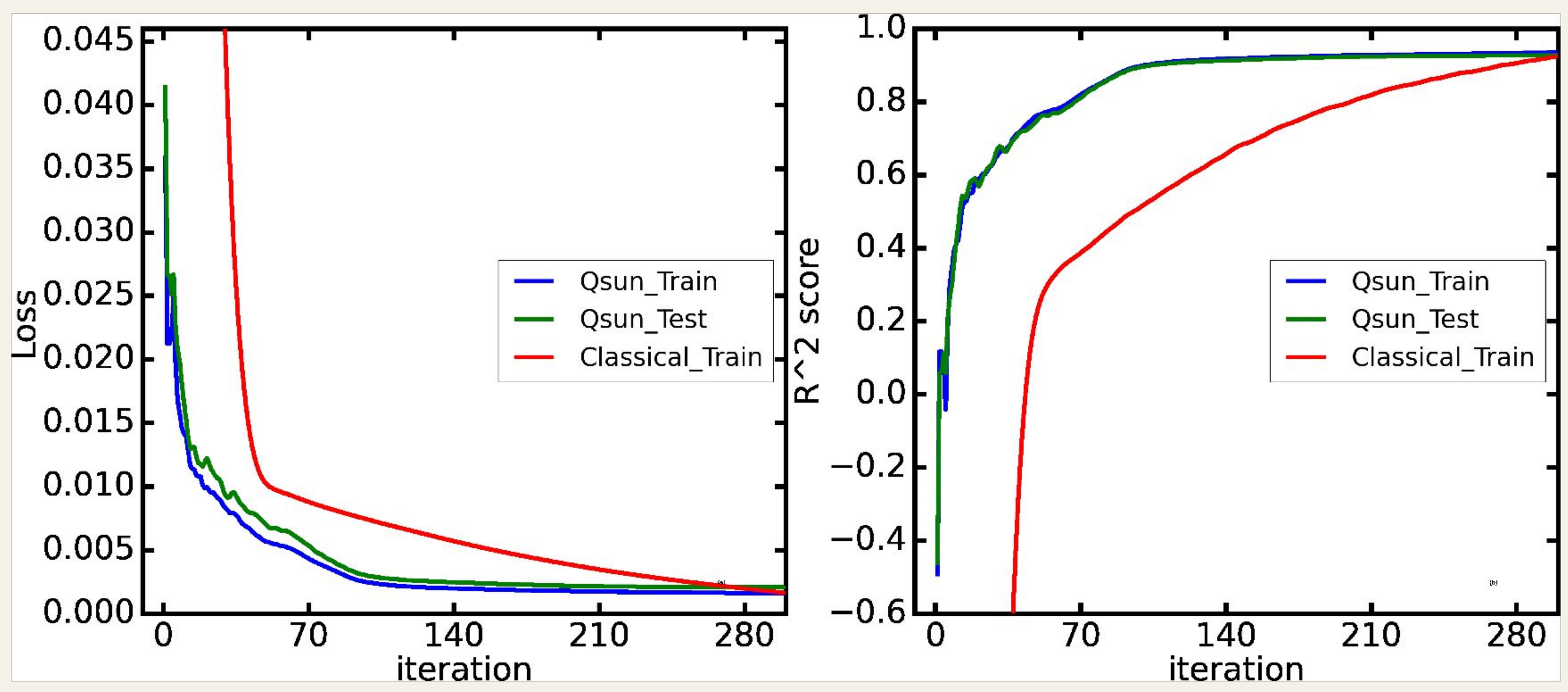

Figure 3. We created a novel computational dataset derived from pyCALPHAD calculations [2]. We have 656 data points (half for training) for binary and ternary alloys, which describe phase diagrams of 16 alloy systems. The alloys include two or three elements chosen from Fe, Ni, Co, Cr, and Al, with composition ratios in steps of 0.05. By using the same circuit structure in [3], we show that Qsun has a better convergence rate and can extract more correlations than the classical model with the same approximate number of nodes and layers (20 nodes in each layer and 3 layers in the classical neural network).

Conclusion

We have developed Qsun, an open-source implementation of QVM, that emulates the working of an actual quantum computer by using the wavefunction approach. The current version of Qsun can perform standard tasks orders of magnitude faster than other platforms in the case of a small number of qubits. We implemented QDP as an intrinsic function of Qsun to run QML applications. In fact, Qsun has been primarily designed to tackle QML problems; however, as a general QVM, it could be utilized for several other applications, for instance, to develop and test VQAs for electronic structures or quantum information. Qsun, being a lightweight, is suitable for personal use. We are currently improving it to encompass a broad scope of content in machine learning. Our code is open source and publicly available on GitHub [4].

References

[1] **DOI**: 10.1088/2632-2153/ac5997
[2] **DOI**: 10.1016/j.mtcomm.2025.112287
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[4] https://github.com/ChuongQuoc1413017/Quantum_Virtual_Machine/tree/main