Statement of Research

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Past works

Quantum Circuit born machine

Generative modeling is at the frontier of deep learning research and real-world applications. For example, see openai's image generation example and the wavenet example of audio generation. In contrast to much simpler discriminative tasks, one needs to model high-dimensional probability density and generate samples efficiently in generative modeling. Generative models with implicit output probabilities and discrete data are crucial for applications such as natural language processing, decision making, and chemical structure design. However, it remains an open research challenge to perform scalable training of these models since most of the deep learning technique relies on the differentiable learning of the objective functions.

We argue that generative modeling via projective sampling on qubits is a killer application of quantum circuits, which shows "quantum supremacy" for **useful tasks**. While compared to more widespread discriminative tasks, the inherent probabilistic and unitary nature of quantum circuits offer unique and even greater opportunities to outperform the classical approaches.

Manuscript PhysRevA.98.062324 presents a fresh approach to quantum machine learning by using the quantum circuits as probabilistic generative models. We call this approach Born Machines since they exploit the Born's rule of the quantum mechanics. With the differentiable training strategy presented in the manuscript, the quantum circuit Born machine exhibits clear quantum advantage over classical neural networks. The proposed training approach is both practical for near-term quantum devices and scalable for future large-scale real-world applications.

Tensor network inspired quantum circuits

Solving the ground state of a quantum many-body system is one of the killer applications of a near-term noisy intermediate scale quantum computer. These studies are crucial for understanding the physical and chemical properties of strongly correlated quantum matter. Classical simulation approaches such as quantum Monte Carlo and tensor network algorithms have faced fundamental issues such as the negative sign problem and unfavorable computational efforts. While performing variational optimization of a quantum circuit ansatz has high potential in offering a long-sought answer to these questions.

To date, there have been several experiments on this so-called variational quantum eigensolver (VQE) on various quantum hardware platforms including works from the Google team O'Malley et al PRX '16 and the IBM team Kandala et al, Nature '17. However, these experiments are restricted to small toy problems due to the limited number of qubits on the devices.

Manuscript PhysRevResearch.1.023025 presents an algorithmic solution to this pressing problem of scaling up the VQE experiment. In the proposed qubit efficient VQE scheme, one can study the ground state property of a large quantum system using a smaller number of qubits. The approach exploits the relative low entanglement entropy property of typical physics and chemistry problems. As a concrete example, we have obtained the ground state of a frustrated Heisenberg model on a 4 x 4 square lattice up to fidelity 97To solve the same problem with exact diagonalization, one probably needs a server (although the precision of results is higher). With our new ansatz, a faithful simulation of the quantum algorithm requires only a GPU card. A quantum computer is able to provide an exponential speedup in terms of tensor contraction comparing with a classical device, which demonstrates quantum advantage.

Yao.jl: a variational quantum simulator

We introduce Yao, an extensible, efficient open source software framework for quantum algorithm design. Yao focuses on differentiable programming on near-term quantum circuits. We introduce a quantum block intermediate representation, which represents quantum circuits as hierarchical tree structures. Yao realizes a constant memory automatic differentiation which exploits reversible feature of quantum computing. Moreover, Yao utilizes Single Program Multiple Data design to exploit data parallelism and GPU acceleration for the simulation of variational quantum circuits and quantum machine learning tasks. The Yao framework is not only powerful for representing and manipulating quantum circuits, but also efficient for practical simulation tasks.

The above benchmark shows that with extensible specialization on different pattern of quantum blocks, the performance of circuit emulator written in abstract and generic style with pure Julia can acheive similar single gate performance and better circuit performance comparing to manual tuned C++ emulator qulacs [**?**] . For large number of qubits, since the simulation complexity of an arbitrary full amplitude quantum state grows exponentially, the overhead become less significant. To acheive the best performance on above benchmarks, one needs to handle Single Instruction Multiple Data (SIMD), cache locality on CPU correctly while implementing corresponding specialized algorithms. We implement these requirements by writing SIMD friendly Julia code, carefully designed classical register data structure and compiler specialization based on QBIR. The CUDA backend is also written in pure Julia with `CUDAnative.jl` [**?**]. Thus although our symbolic backend, CUDA backend and CPU backend share most of the infrastructure and implementation, we can still acheive similar and even better performance than manual tuned C++ and CUDA C implementation.

Research plan