Differentiable Programming for Analytic Quantum Simulation

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Overview

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We are currently in the NISQ (Noisy Intermediate Scale Quantum computing[Pre18]) era: we only have access to quantum computers with50-100 qubits with noise.

A strategy that makes the best use of NISQ devices must account for:

- Limited numbers of qubits;
- Limited connectivity of qubits;
- Coherent and incoherent errors that limit quantum circuit depth.

To solve variational quantum algorithms more efficiently, we would like to develop ways to automatically compute the analytic gradients of quantum simulations and use gradient-based methods to optimize the problems.

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[SBG^{+}19] and [MNKF18] propose a way to compute the gradients on pulse sequences.

However, since pulses discretize the physics process on the time domain, the number of parameters can grow very huge when the system evolve for a long time.

Besides, their discretization of time forces them to use the product of each time interval to approximate the evolution realized by the pulse sequence, which makes the loss function deviate from the reality. Choosing other formulation may relieve this problem.

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Quantum advantage with NISQ devices

Considering the limitation of the existing differentiation techniques on the pulse-based representation, we would like to come up with another representation and its corresponding gradient formulation that is more suitable for the analytic simulation process.

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There are many optional formulations. For example, we can use Fourier transformation to parametrize the system in the spectral domain by

$$\hat{H}_j(a_0, a_1, b_1, ..., a, N, b_N)(t) = \left(\frac{1}{2}a_0 + \sum_{k=1}^{N}(a_k \cos(kt) + b_k \sin(kt))\right) H_j,$$

where H_j is a time-independent Hamiltonian and $\hat{H}_j$ is its time-parametrized version. Then we try to derive the derivatives for each a_k and b_k with the evolution controlled by $\sum_j \hat{H}_j$, and represent the derivatives using another evolution.

Another possibility is using wavelet series to represent the pulses. The formulation is similar to the above one for Fourier series.

Overview

Nov. 20, 2021 Finish the theoretical derivations.

Dec. 10, 2021 Finish some experiments and applications.

Reference I

- Kosuke Mitarai, Makoto Negoro, Masahiro Kitagawa, and Keisuke Fujii, *Quantum circuit learning*, Physical Review A **98** (2018), no. 3, 032309.
- John Preskill, *Quantum computing in the nisq era and beyond*, Quantum **2** (2018), 79.
- Maria Schuld, Ville Bergholm, Christian Gogolin, Josh Izaac, and Nathan Killoran, *Evaluating analytic gradients on quantum hardware*, Physical Review A **99** (2019), no. 3, 032331.