Differentiable Simulation of Variational Quantum Eigensolver

Jin-Guo Liu, May 22, 2019

cacate0129@gmail.com

Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Differentiable programming provides a fresh new approach for quantum simulations. [**JG: The following text in this paragraph is copied from my previous paper [9], please change the description to avoid potential issues.**] Studying ground state properties of quantum many-body systems is a promising native application of quantum computers. Given limited qubit resources and noisy realizations of near-term quantum devices [1, 2], a practical approach is to employ the variational quantum eigensolver (VQE) [3–9], which runs in a classical-quantum hybrid mode. In this scheme, a parameterized quantum circuit provides a variational ansatz for the ground state. A classical optimizer tunes the circuit parameters to reduce the expected energy of the target Hamiltonian of the output quantum state. Recent progress on unbiased gradient estimation on quantum circuits [15? –17] breaks the information bottleneck between classical and quantum processors, thus providing a route towards scalable optimization of circuits with a large number of parameters.

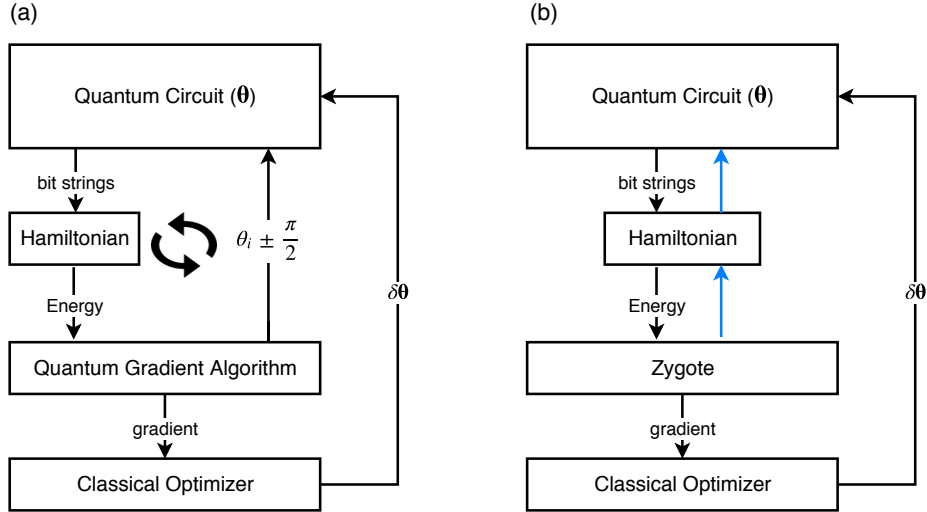The VQE algorithm can be summarized as the following diagram

FIG. 1. A schetch of VQE algorithm, boxes are objectives and lines indicates data flow. (a) the quantum algorithm, (b) the classical simulation approach with Zygote.

The goal of VQE is obtaining the ground state wave function of a model Hamiltonian. As concrete example, we apply our automatic differentiation approach on the anti-ferromagnetic Heisenberg model defined one a chain (a toy model that all physicists like). Its hamiltonian is

$$H = \frac{1}{4}\left[\sum_{\langle i,j\rangle} \sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y + \sigma_i^z\sigma_j^z\right], \tag{1}$$

where $\langle i,j\rangle$ denotes nearest neighbors pairs, $\sigma_i^{\alpha=x,y,z}$ is a Pauli operator.

To obtain the gradient of parameters $\boldsymbol{\theta}$ inside a quantum circuit, the quantum differentiable programming approach in Fig. 1 employs the relation [16]

$$\frac{\partial}{\partial \theta_i}\langle H \rangle_{\boldsymbol{\theta}} = \frac{1}{2}\left(\langle H \rangle_{\boldsymbol{\theta} + \frac{\pi}{2}\boldsymbol{e}_i} - \langle H \rangle_{\boldsymbol{\theta} - \frac{\pi}{2}\boldsymbol{e}_i}\right). \tag{2}$$

This formula has a similar form to finite difference, but it is exact. Its algorithm complexity a $O(N^2)$. In classical simulation, we are able to manipulate the wave functions directly, back propagation would help in decreasing the algorithm complexity to $O(N)$.

```julia
using Yao
using YaoFlux
using LinearAlgebra
using QuAlgorithmZoo: heisenberg, random_diff_circuit, pair_ring

# define a AFM-Heisenberg Model Hamiltonian
nbit = 4
h = mat(heisenberg(nbit))
v0 = statevec(zero_state(nbit))
function energy(circuit)
    v = mat(circuit) * v0
    (v'* h * v)[] |> real
end

# Generate a circuit as a wave function ansatz
circuit = random_diff_circuit(nbit, 2, pair_ring(nbit))

using Flux: ADAM, Optimise
function train!(lossfunc, circuit, optimizer; maxiter::Int=200)
    dispatch!(circuit, :random)
    params = parameters(circuit)
    for i = 1:maxiter
        # collect gradients from returned structured data
        grad = collect_gradients(lossfunc'(circuit))
        Optimise.update!(optimizer, params, grad)
        dispatch!(circuit, params)
        println("Iter $i, Loss = $(lossfunc(circuit))")
    end
    circuit
end

using Random
Random.seed!(5)
EG = eigvals(Matrix(h))[1]
println("$nbit site Heisenberg model, exact ground state energy = $EG")
train!(energy, circuit, ADAM(0.1); maxiter=200)
```

Here, `mat(circuit)` returns a complex valued `SparseMatrixCSC` matrix, then we back propagate through this sparse matrix, it will return an adjoint with data structure that mimics the block tree in the original `Yao.jl` structure. Then we are able to collect gradients easily with `collect_gradients` function. The training uses the Adam optimizer in `Flux.jl`
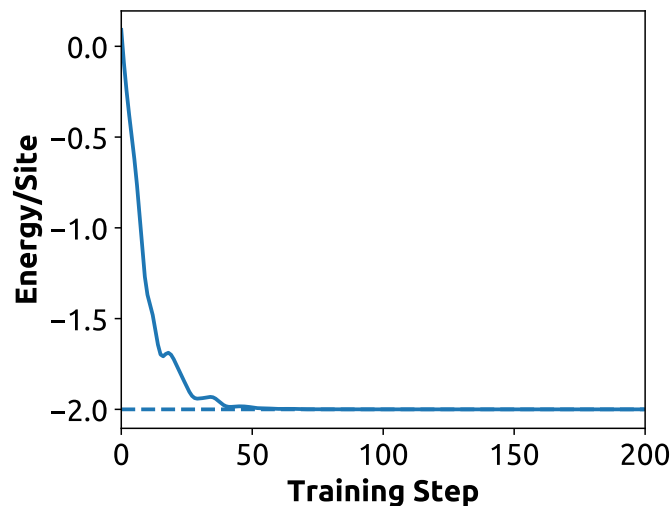
FIG. 2. Energy as a function training step. The dashed line corresponds to the exact ground state energy.

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