Differentiable Simulation of Variational Quantum Eigensolver

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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

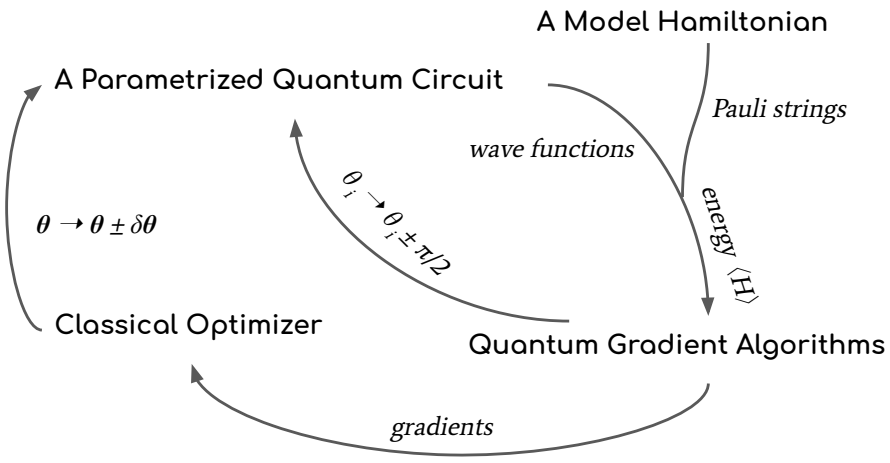

FIG. 1. A schetch of VQE algorithm, nodes are objectives and lines indicates information flow.

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 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`

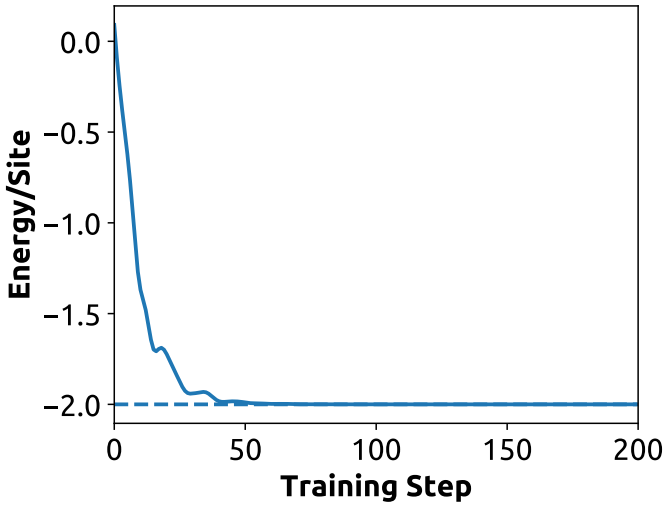

FIG. 2. Energy as a function training step. The dashed line corresponds to the exact ground state energy.

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