Project Report

Abstract

A short summery about the ansatz in variational quantum algorithm

Requirements for ansatz There are various kinds of ansatz in the VQA, which should have the desired feature:

- It should be very convenient to construct (especially on a quantum circuit form). That is, to have a modest circuit size and depth.
- It should have a strong representation power:, which means that it should contain a large range of the Hilbert space, thus having a positive probability to arrive at the target apace

Some methods to construct ansatz Under the demand above there are some methods:

- Ansatz from quantum chemistry:
  - FCI: full configuration interaction
  - UCC: unitary coupled cluster

$$|\psi(\theta)\rangle = e^T|0\rangle = (1+T)|0\rangle \tag{1}$$

  The methods use operators $c_i^+ c_j$ and $c_i^+ c_j^+ c_k c_l$ to simulate electron transition. It expands the ansatz with more basis functions and meanwhile keeping the symmetry and other properties unchanged. But it always has its' chemical limits in accuracy and most time is not easy to make a decomposition into elementary gates.
- Hardware-efficient method: Once we got the Hamiltonian we can analyse it from the view of quantum computation
  - Direct search: It uses a multi-layer blocks acting a initial state with each block consistent of general rotation and general correlation.

$$|\psi(\theta)\rangle = \prod_{i=1}^{n} U(\theta_{(i)})|0\rangle \tag{2}$$

  - symmetry-preserved: It directly constructs quantum superposition state:

$$|\psi(\theta)\rangle = \sum_i \theta_i |i\rangle \tag{3}$$

It's more "direct" and sometimes has a easier way to realize such function. But in this way we need more information before we construct the ansatz.

Discussion We see that even there are many kinds of ansatzz, their construction methods are just to satisfy the need of the one's desire. That is, the more information you know the more specific ansatz you can construct.

On the other hand, there are also some encoding functions that can realize simulation quantum chemistry on a quantum circuit that can reduce the qubit or quantum gate requirement, but most of them need to change almost everything that is different with our usual process, which is caused by the computational details. There are two examples:

- To prepare the spin-preserved matrix we need to encode the qubits for spin-up with the first half and spin-down for the others, which is disagree with the conventions that rank the orbitals from low to high in HF energy. Therefore the Hamiltonian should be adjusted and at the end we should make a transformation back to get the wavefunction.
- The problem is caused by our computational process. That is in the second-quantized Hamiltonian we don't compute the one- and two-electron integrals by ourselves limited by our knowledge but use the computational package such as OpenFermion and PyQuante. If we can do this better we can get desired Hamiltonian, which can help realized more functions.