Variational Quantum Eigensolvers

VQE allows us to find an upper bound of the lowest eigenvalue of a given Hamiltonian. It is a hybrid, quantum-classical algorithm.

Hamiltonian:

Hamiltonian — the Hamiltonian is a matrix which describes the possible energies of a physical system. If we know the Hamiltonian, we can calculate the behaviour of the system, learn what the physical states of the system are etc. It's a central piece of quantum mechanics.

Eigenvalue:

A given physical system can be in various states. Each state has a corresponding energy. These states are described by the eigenvectors and their energies are equal to the corresponding eigenvalues. In particular, the lowest eigenvalue corresponds to the ground state energy.

Ground state:

This is the state of the system with the lowest energy, which means it's the "most natural" state — i.e. a given system always tend to get there, and if it is in the ground state and is left alone, it will stay there forever.

Conditions needed for VQE to work:

-[] Hamiltonian for system is known

The Variational Principle:

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< Psi_{lamda} | H | Psi_{lamda} > >= E_{0}
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VQE Circuit:

It consists of three parts:

- Ansatz - it prepares the state we need in order to apply variational principle.
- Hamiltonian - Hamiltonians constructed as a sum of Pauli operators (X, Y, Z) and their tensor products.
  - We don't actually put any of the corresponding X, Y, Z gates into the circuit. We use them to choose in which basis we want to do a measurement.
- Measurement

Hybrid Model:

So the idea is that we use a quantum computer (sometimes called QPU — quantum processing unit) for one thing only — to get the energy value for a given set of parameters. Everything else — so the whole optimization part — happens on a regular computer.

The parameters to optimize the Ansatz is classical and the rest of the procedure is quantum.

Quantum Processing Unit (QPU):

Role of a QPU:

- Given a set of parameters, returns us a set of measurements.
- What a classical computer does:
- Given a set of measurements calculates the energy value (it's usually some kind of averaging)
- Performs optimization procedure
- Calculates what a new set of parameters should be
- Checks whether we have reached the minimum
- Makes sure we don't make more iterations than we should have done

VQE Algorithm

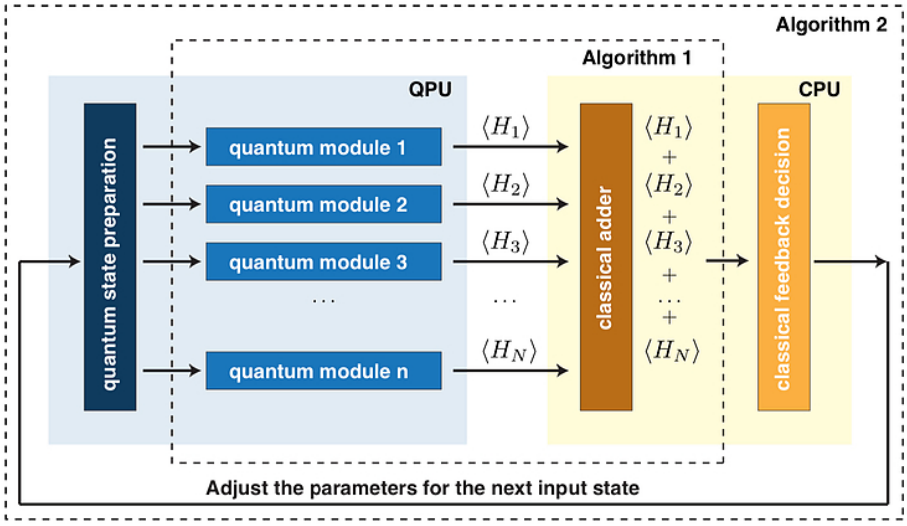

Figure 1: vqe