The Variational Quantum Eigensolver

In Quantum Chemistry

What is the Variational Quantum Eigensolver?

The Variational Quantum Eigensolver (VQE) is a near term hybrid quantum-classical quantum machine learning algorithm that is used to find the minimum eigenvalue of a matrix, *H*. *H* is usually a very large matrix, and finding its eigenvalue is very difficult using classical computers. In quantum chemistry, the molecule's minimum eigenvalue of its Hamiltonian matrix corresponds to the ground state energy of the system. This has applications in material design, drug discovery and fundamental science.

How does it work?

1. Transform the molecule Hamiltonian to a qubit Hamiltonian which can be represented as a matrix. The larger the molecule will result in a larger matrix, causing a need for more qubits.
2. A "trial wavefunction" is encoded into the quantum computer and the quantum computer creates an ansatz that represents the molecule.
3. Measuring aspects of the ansatz that was created, we estimate the energy of the "trial wavefunction".
4. The estimated value of the energy is put onto a classical computer. Based on the energy, the computer creates new parameters for a new "trial wavefunction" with lower energy.
5. We continue doing this until the energy converges to a minimum. This value corresponds to the ground state energy of the molecule.
6. To find the bond length, we repeat steps 2-5 for different interatomic spacing Hamiltonians. The Hamiltonian with the minimum energy would correspond to the equilibrium configuration.

Other uses of VQE

Combinatorial optimization
VQE is great at finding optimal combination of things, such as the shortest route for visiting a list of cities. This is called the Traveling Salesman Problem.

Principal Component Analysis
VQE can be used to enhance principal component analysis, which has applications in bioinformatics, neuroscience, image processing, and quantitative finance.

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