Variational Quantum Algorithms

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Background

- Two approaches to quantum algorithm design
- NISQ algorithms
- Variational quantum algorithms

Background

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) + V(\vec{r},t)\Psi(\vec{r},t) = i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

$$H\Psi = E\Psi$$

The Schrodinger equation is an eigenvalue equation!

Linear Algebra Representation

With n qubits:

- $|\psi\rangle$ is a 2^n normalized complex column vector
- $\langle\psi|$ is its conjugate transpose
- Hamiltonian H is a 2^n by 2^n hermitian matrix

Exponential scaling means ψ and H are hard to store on a classical computer.

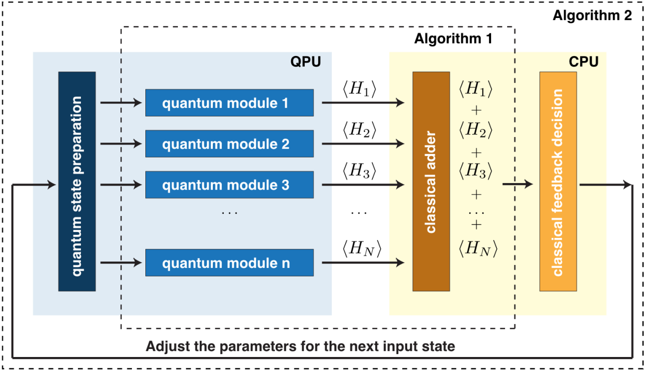
Objective

With VQE, the goal is to find the minimum eigenvalue of a Hamiltonian H and its corresponding eigenvector: E_0 and ψ_0. To do so, we minimize an upper bound on E_0:

$$\min_{\theta} \langle H_\theta \rangle$$

where $$\langle H_\theta \rangle \equiv \langle \psi_\theta | H | \psi_\theta \rangle = E_\theta \geq E_0$$

Algorithm Overview



1. State Preparation (Quantum)
2. Expectation Value Computation (Hybrid)
3. Iterative minimization (Classical)

Variational Quantum Deflation

To calculate the K-th eigenvalue:

$$\min_{\theta} F(\theta)$$

where $$F(\theta) \equiv \langle\psi(\theta_k)| H |\psi(\theta_k)\rangle + \sum_{i=0}^{k-1} \beta_i \, | \langle\psi(\theta_k)|\psi(\theta_i)\rangle \, |^2$$

Can be seen as minimizing $\langle H_\theta \rangle$
s.t. $|\psi(\theta_k)\rangle$ orthogonal to $|\psi(\theta_0)\rangle \ldots |\psi(\theta_{k-1})\rangle$

Subspace-Search VQE

To calculate the K-th eigenvalue:

1. Search for lowest energy k-dimensional subspace
2. Search subspace for highest energy eigenvector

Algorithm:

1. Construct an ansatz circuit $U(\boldsymbol{\theta})$ and choose input states $\{|\varphi_j\rangle\}_{j=0}^{k}$ which are mutually orthogonal $(\langle\varphi_i|\varphi_j\rangle = \delta_{ij})$.
2. Minimize $\mathcal{L}_1(\boldsymbol{\theta}) = \sum_{j=0}^{k} \langle\varphi_j|U^\dagger(\boldsymbol{\theta})HU(\boldsymbol{\theta})|\varphi_j\rangle$. We denote the optimal $\boldsymbol{\theta}$ by $\boldsymbol{\theta}^*$.
3. Construct another parametrized quantum circuit $V(\boldsymbol{\phi})$ that only acts on the space spanned by $\{|\varphi_j\rangle\}_{j=0}^{k}$.
4. Choose an arbitrary index $s \in \{0, \cdots, k\}$, and maximize $\mathcal{L}_2(\boldsymbol{\phi}) = \langle\varphi_s|V^\dagger(\boldsymbol{\phi})U^\dagger(\boldsymbol{\theta}^*)HU(\boldsymbol{\theta}^*)V(\boldsymbol{\phi})|\varphi_s\rangle$.