Lecture 10: First circuit, the variational quantum eigensolver

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Our first quantum citcuit

Today we discuss our first quantum circuit. We will use the *variational quantum eigensolver* (VQE) to find the lowest eigenvalue of a 2×2 matrix. The VQE was one of the first quantum algorithms applied to problems in physics, chemistry, and elsewhere. Now more sophisticated algorithms are being developed. The VQE is still an important starting point.

The Rayleigh-Ritz variational theorem

We rely upon the Rayleigh-Ritz variational theorem, which can be found in most books on quantum mechanics (but not our *Starter Kit*) or in many texts on linear algebra.

The theorem is simple. Consider a finite Hermitian matrix $\mathbf{A}$, which must have real eigenvalues. Let E_0 be the lowest eigenvalue. Then for any vector $|v\rangle$, we have

$$E_0 \leq \frac{\langle v|\mathbf{A}|v\rangle}{\langle v|v\rangle}$$

This means we can put an upper bound on the lowest eigenvalue. If $\mathbf{A}$ is a Hamiltonian, which measures the energy of a system, this is an upper bound on the ground state energy.

The Variational Quantum Eigensolver

The VQE is straightforward. We parameterize some wave function $|\psi(\lambda_i)\rangle$ as a function of parameters $\{\lambda_i\}$, make sure it is normalized $\langle\psi(\lambda_i)|\psi(\lambda_i)\rangle = 1$, and then compute

$$E(\lambda_i) = \langle\psi(\lambda_i)|\mathbf{A}|\psi(\lambda_i)\rangle$$

We then vary the parameters $\{\lambda_i\}$ until we get a minimum value. (This method also works on classical computers.)

The VQE has two tasks we must master:

1. Prepare the variational wave function (also called an *ansatz* or 'guess') $|\psi(\lambda_i)\rangle$
2. Evaluate the expectation value $\langle\psi(\lambda_i)|\mathbf{A}|\psi(\lambda_i)\rangle$

2×2 matrices

For this problem consider a real 2×2 matrix

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

where all the a_{ij} are real and $a_{12} = a_{21}$ so Hermitian. We write this in terms of the matrices $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ (also called the Pauli matrices) and $\mathbf{I}$.

$$\mathbf{A} = \frac{a_{11} + a_{22}}{2}\mathbf{I} + a_{12}\mathbf{X} + \frac{a_{11} - a_{22}}{2}\mathbf{Z}$$

To simplify things, we use our knowledge that a real Hermitian matrix has real eigenvectors.

Preparing the trial state

To simplify things, we use our knowledge that a real Hermitian matrix has real eigenvectors. Then the most general normalized two-dimensional real vector is

$$|\chi(\lambda)\rangle = \begin{pmatrix} \cos\lambda \\ \sin\lambda \end{pmatrix} = \cos\lambda|0\rangle + \sin\lambda|1\rangle$$

We can form this from an initial $|0\rangle$ qubit (which is the usual starting point for quantum computers) by applying $\mathbf{R}_y(\theta)$ from last time:

$$|\chi(\lambda)\rangle = \mathbf{R}_y(2\lambda)|0\rangle$$

(the factor of 2 comes about because of how we defined rotation in terms of spin-1/2 matrices).

Evaluating the expectation value

Next, we have to evaluate three expectation values:

$$\langle \mathbf{I} \rangle, \quad \langle \mathbf{Z} \rangle, \quad \langle \mathbf{X} \rangle,$$

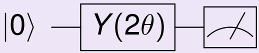
$\langle \mathbf{I} \rangle$ is the easiest, as it always = 1.

$\langle \mathbf{Z} \rangle$ is easier than it looks, as the eigenvectors of **Z** are the elements of the computational basis $|0\rangle, |1\rangle$. We can see that $\langle \mathbf{Z} \rangle = P(0) - P(1)$ where P is the probability.

To evaluate this on a quantum computer, we have to prepare $|\chi(\theta)\rangle$ many time and then measure **Z** which is just to find the probability of 0 and 1.

Evaluating the expectation value

The circuit to measure $\langle Z \rangle$ is



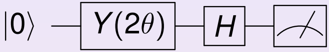
To evaluate this on a quantum computer, we have to prepare $|\chi(\theta)\rangle$ many time and then measure **Z** which is just to find the probability of 0 and 1.

(If you want to draw your own quantum circuits in LaTeX, go to "Course resource materials" files folder on Canvas and and get `qcircuit.sty` and a tutorial in `qcircuit.pdf`. In your LaTeX file you must have at the top

\includepackage{qcircuit.sty}

Evaluating the expectation value

The circuit to measure $\langle X \rangle$ is



Why this? It turns out the Hadamard gate transforms eigenstates of **X** to eigenstates of **Z**, that is

$$\mathbf{H}|x=+1\rangle = |z=+1\rangle = |0\rangle, \quad \mathbf{H}|x=-1\rangle = |z=-1\rangle = |1\rangle$$

To evaluate this on a quantum computer, we have to prepare $|\chi(\theta)\rangle$ many time and then measure **Z** which is just to find the probability of 0 and 1. (It turns out that generally, no matter what we want to measure, we first transform to the **Z**-basis.)

Evaluating the expectation value

After all this, we vary θ and then compute (by averaging over many 'experiments')

$$\langle \mathbf{A} \rangle = \frac{a_{11} + a_{22}}{2} + a_{12} \langle \mathbf{X} \rangle + \frac{a_{11} - a_{22}}{2} \langle \mathbf{Z} \rangle$$

and plot $\langle \mathbf{A} \rangle$ vs. θ.

Next time:

Next time we start looking at tensor products and 2-qubit systems.

- QC:GI. Chapter 3, especially 3.1.2-3.1.3
- *QM starter kit*: intro to Ch 3, up to eqn (3.2)