Lecture 10: Unitary coupled cluster and VQE
Reading: O Malley et al PRX:6 031007 (2016)

1 VQE - unitary coupled-cluster

1.1 Introduction

Phase estimation is in principle a good method to get out energy eigenvalues, but the gate depths required are out of reach even any but the simplest Hamiltonians which are not physically very interesting. An alternative approach is to use a parametrized wave function (ansatz) as a guess, hoping that it is of a form close to the actual ground state wavefunction, and figure out the parameters that minimize the energy. The energy measurement is done on a quantum computer, where we take advantage of the ability to represent the entire Hilbert space, while the optimization of parameters in ansatz is done with a classical routine.

This method is based on the Rayleigh-Ritz variational principle, which says the following. Say we have a parametrized state $|\phi(\vec{\theta})\rangle$ where $\vec{\theta}$ is a vector of parameters that specify the wavefunction. Then,

$$\frac{\langle\phi(\vec{\theta})|H|\phi(\vec{\theta})\rangle}{\langle\phi(\vec{\theta})|\phi(\vec{\theta})\rangle} \geq E_0 \tag{1.1}$$

where E_0 is the ground state energy. You can prove this in a few lines by expanding H in its eigenbasis and looking at the terms in the sum. Therefore, we can find an estimate of E_0 within the wavefunctions allowed by the ansatz by finding $\vec{\theta}$ that minimizes the above functional.

Of course, we can and do perform this procedure classically. The advantage of quantum computers is that we are no longer restricted by memory limitations to a polynomial number of states over which to perform the expectation value. The QC can perform averages over the entire Hilbert space and represent states with high degrees of entanglement with only a polynomial number of operations.

The question then becomes with ansatz to use. One of the earliest ones to be suggested was the unitary coupled cluster method [1]. Coupled cluster is an ansatz originating in nuclear physics that is derived from many-body perturbation theory from the HF state $|\Phi_0\rangle$ (a single Slater determinant). It is now widely used for quantum chemistry. It expresses the wavefunction $|\Psi\rangle$ as:

$$|\Psi\rangle = e^T |\Phi_0\rangle \tag{1.2}$$

where $T = T_1 + T_2 + ...$ is an excitation operator. The individual operators have the following forms:

$$T_1 = \sum_{pr} t_p^r a_p^\dagger a_r \tag{1.3}$$

$$T_2 = \sum_{pqrs} t_{pq}^{rs} a_p^\dagger a_q^\dagger a_r a_s \tag{1.4}$$

We think of T_1 as a single excitation operator and T_2 as a double excitation operator. If we continue excitations to T_N, we reach the exact FCI limit. Of course we always have to truncate the series, often at double excitations.

While coupled-cluster is highly successful on classical computers, it cannot be directly implemented on a QC since e^T is not unitary. An alternative that fixes this problem is the unitary coupled cluster method where the excitation operator is defined as $T - T^\dagger$. This operator is anti-Hermitian and thus when exponentiated yields a unitary operator. Classically, UCC is not tractable because it leads to a series that does not converge. Fortunately, unitaries can be implemented on a QC with no trouble, and so UCC therefore is a good candidate for an ansatz for VQE.

1.2 Example: minimal basis H_2

We will not go into all the details of implementing UCC for an arbitrary problem. Instead we will focus on minimal basis H_2. In this case, the parametrization of the wavefunction is especially easy because there is only one parameter:

$$|\phi(\theta)\rangle = e^{-i\theta X_0 Y_1} |01\rangle \tag{1.5}$$

For any θ this unitary is easy to apply. We then need a way to get the energy expectation value. We don't want to use phase estimation since it requires large gate depth, and the whole point of VQE was to decrease gate depth!

The approach we can use is called Hamiltonian averaging. A local Hamiltonian H (after an appropriate transform) can generally be expanded as:

$$H = \sum_\gamma H_\gamma g_\gamma \tag{1.6}$$

where $H_\gamma = \sigma_0^a \otimes \sigma_1^b \otimes ... \otimes \sigma_n^x$ where the superscripts indicate X, Y, Z, or I Pauli matrix and the subscript indicates qubit number. Each subterm is individually a Hermitian operator, and so it has a spectral decomposition:

$$H_\gamma = \sum_i \lambda_i |\lambda_i\rangle \langle\lambda_i| \tag{1.7}$$

Therefore,

$$\langle\phi(\theta)|H_\gamma|\phi(\theta)\rangle = \sum_i \lambda_i \langle\phi|\lambda_i\rangle \langle\lambda_i|\phi\rangle = \sum_i \lambda_i |\langle\phi|\lambda_i\rangle|^2 \tag{1.8}$$

Recall how measuring a qubit works. When we measure, the system collapses into an eigenstate with probability $|\langle\phi|\lambda_i\rangle|^2$. Therefore, measuring the probability to observe a given eigenstate by repeated measurement gives us the probability and hence the term $|\langle\phi|\lambda_i\rangle|^2$. We can get the eigenvalues for a Pauli string, and therefore get the expectation value as:

In a little more detail, say we need to obtain the expectation value of the string $X_0 Z_1 Y_2$. After applying the unitary to get to the state $|\psi(\theta)\rangle$, we should rotate our basis so that each operator is diagonal. Explicitly, we would apply $H = R_y(-\pi/2)$ to qubit 0 and $R_x(-\pi/2)$ for qubit 2. We don't need to do anything to qubit 1 since Z is diagonal in the computational basis. We then measure in the computational basis, getting bit strings with certain probabilities corresponding to the overlap of the state with the various eigenstates. These probabilities are what we need for computing the expectation value. Note that the number of eigenstates scales exponentially with the length of the

Pauli string so we hope the strings are not too long. The nice log scaling of the length of Pauli strings with the BK transform is helpful here.

With each term determined, we get the expectation value of the Hamiltonian as:

$$\langle H \rangle = \sum_{\gamma} \langle H_\gamma \rangle = E(\theta) \tag{1.9}$$

Finally, once we have $E(\theta)$, we use a classical optimization routine to find the parameters that minimize the energy. That final value is an estimate for the ground state energy. In the HW, you will try this algorithm out following [2].

References

[1]A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'Brien, "A variational eigenvalue solver on a photonic quantum processor.", Nature Communications **5**, 4213 (2014).

[2]P. O'Malley, R. Babbush, I. Kivlichan, J. Romero, J. McClean, R. Barends, J. Kelly, P. Roushan, A. Tranter, N. Ding, B. Campbell, Y. Chen, Z. Chen, B. Chiaro, A. Dunsworth, A. Fowler, E. Jeffrey, E. Lucero, A. Megrant, J. Mutus, M. Neeley, C. Neill, C. Quintana, D. Sank, A. Vainsencher, J. Wenner, T. White, P. Coveney, P. Love, H. Neven, A. Aspuru-Guzik, and J. Martinis, "Scalable quantum simulation of molecular energies", Physical Review X **6**, 031007 (2016).