Chapter 7

The variational quantum eigensolver

In this chapter, we discuss the variational quantum eigensolver (VQE). The VQE is a heuristic approach to solving various problems with a combination of quantum and classical computation. As we will see later, the QAOA of the preceding chapter can be considered a special case of the VQE.

The content of this chapter is mostly based on the review in Ref. [Moll et al., 2018]. We first outline how the VQE works and then discuss details of some of the steps in the algorithm.

7.1 Outline of the algorithm

The VQE is designed to solve problems that can be cast in the form of finding the ground-state energy $E_{GS}$ of a Hamiltonian $H$. The ground-state energy is the smallest eigenvalue of the Hamiltonian,

$$ H |\Psi_{GS}\rangle = E_{GS} |\Psi_{GS}\rangle. \quad (7.1) $$

How hard is this problem in general? If the Hamiltonian is $k$-local, i.e., if terms in $H$ act on at most $k$ qubits, the problem is know to be QMA-complete for $k \geq 2$. The general problem would thus be hard even for an ideal quantum computer. However, it is believed that physical systems have Hamiltonians that do not correspond to hard instances of this problem, and a heuristic quantum algorithm could still outperform a classical one.

A general Hamiltonian for $N$ qubits can be written

$$ H = \sum_{\alpha} h_{\alpha} P_{\alpha} = \sum_{\alpha} h_{\alpha} \bigotimes_{j=1}^{N} \sigma_{\alpha_j}^{(j)}, \quad (7.2) $$

where the $h_{\alpha}$ are coefficients and the $P_{\alpha}$ are called Pauli strings. The latter are products of single-qubit Pauli matrices (including the identity matrix).

The steps of the VQE algorithm are the following (see also Fig. 7.1):

0. Map the problem that you wish to solve to finding the ground-state energy of a Hamiltonian on the form in Eq. (7.2).

1. Prepare a trial state $|\Psi(\theta)\rangle$ set by a collection of parameters $\theta$.

2. Measure expectation values of the Pauli strings in the Hamiltonian, i.e., measure $E[\Psi(\theta)] P_{\alpha} \Psi(\theta)$.

3. Calculate the energy $E$ corresponding to the trial state, $E = \sum_{\alpha} h_{\alpha} E[\Psi(\theta)] P_{\alpha} \Psi(\theta)$, by summing up the results of the measurements in the preceding step.
3. Exploring Hilbert space with the VQE
To exploit near-term quantum devices, applications and algorithms have to be tailored to current quantum hardware and used for measuring the expectation values needed. These are combined on a classical computer to calculate the ground-state energy. In the following sections, we discuss steps 0, 1, and 4 in more detail.

4. Update the parameters \( \theta \) based on the result (and results in previous iterations).

Steps 1 and 2 are run on a quantum computer, which can handle the quantum states more efficiently than a classical computer. Steps 3 and 4 are done on a classical computer. The algorithm is iterative, i.e., it starts over from step 1 after step 4, and continues to iterate until some convergence criterion is met, indicating that the ground-state energy has been found. In the following sections, we discuss steps 0, 1, and 4 in more detail.

7.2 More on step 0 – mapping to a Hamiltonian

Broadly speaking, the VQE is currently mostly being considered for two types of problems: optimization problems, where \( H \) is a cost function for the problem, and many-body fermionic quantum systems, e.g., molecules (quantum chemistry). The first type of problems was discussed extensively in Chapter 6, where we saw several examples of how optimization problems can be mapped to a Hamiltonian. In this chapter, we therefore focus on quantum-chemistry problems.

Even though a Hamiltonian can be written down for a molecular system, that is not the Hamiltonian that is used in VQE. In classical simulations of molecular systems, there are many different methods, e.g., density functional theory (DFT), where the actual system of interacting electrons is described as non-interacting electrons moving in a modified external potential. An approach more suited to VQE is to describe the system in second quantization. This requires calculating a number of spatial integrals on a classical computer, but that task can be accomplished efficiently. The Hilbert space consists of electron orbitals. The Hamiltonian is

\[
H_F = \sum_{i,j} t_{ij} a_i^\dagger a_j + \sum_{i,j,k,l} u_{ijkl} a_i^\dagger a_k^\dagger a_l a_j,
\]

(7.3)
where $a_i$ ($a_i^\dagger$) annihilates (creates) an electron in the $i$th orbital. The coefficients $t_{ij}$ and $u_{ijkl}$ describing one- and two-electron interactions are calculated from the spatial integrals mentioned above.

The operators in Eq. (7.3) are fermionic. They thus obey the fermionic anti-commutation relations, e.g., $\{a_i, a_j^\dagger\} = \delta_{ij}$. These are not the relations that the qubit Pauli operators obey. We thus need to translate the Hamiltonian in Eq. (7.3) to a form that can be implemented on the quantum computer. One well-known mapping from fermionic operators to qubit operators is the Jordan-Wigner transformation:

$$a_i^\dagger \rightarrow 1 \otimes \sigma_- \otimes \sigma_z^\otimes N-i,$$  \hfill (7.4)

where $N$ is the number of orbitals and qubits. This mapping is not well suited to the VQE, because it creates highly non-local terms in the qubit Hamiltonian. In actual applications of VQE to quantum chemistry, other mappings are used (Bravyi-Kitaev, parity, ...). There is ongoing research on finding more suitable mappings.

### 7.3 More on step 1 – the trial state

The trial state $|\Psi(\theta)\rangle$ can essentially be parameterized by $\theta$ in two ways: to form states that have a form that is suggested by the problem Hamiltonian, or to form states that are easy to create with the available quantum-computing hardware.

#### 7.3.1 Problem-specific trial states

In quantum chemistry, a common class of trial states are created using a so-called coupled-cluster approach, often the unitary coupled-cluster (UCC) one. Here, the unitary operator $U(\theta)$ creates the trial state:

$$|\Psi(\theta)\rangle = U(\theta) |\Phi\rangle = \exp\left[T(\theta) - T^\dagger(\theta)\right] |\Phi\rangle,$$  \hfill (7.5)

where $|\Phi\rangle$ is a simple state formed by the Slater determinant for low-energy orbitals. The operator $T(\theta)$ is known as a cluster operator. It is given by

$$T(\theta) = \sum_k T_k(\theta),$$  \hfill (7.6)

$$T_1(\theta) = \sum_{i\in \text{occ}, j\in \text{unocc}} \theta_{ij}^i a_j^\dagger a_i,$$  \hfill (7.7)

$$T_2(\theta) = \sum_{i,j\in \text{occ}, k,l\in \text{unocc}} \theta_{ijkl}^i a_l^\dagger a_k^\dagger a_j a_i,$$  \hfill (7.8)

where the sums go over occupied and unoccupied orbitals. The coefficients of the higher-order cluster operators decrease rapidly as more orders are included. For this reason, the expansion is usually truncated at the second, “double”, order (UCCSD) or the third, “triple”, order (UCCSDT).

#### 7.3.2 Hardware-efficient trial states

On an actual quantum computer, particularly a NISQ one, implementing the cluster operators can be hard, especially since the fermionic operators in the cluster operators must be mapped to qubit operators first. Therefore, hardware-efficient trial states are preferred. In the work of Ref. [Kandala et al., 2017], where the H$_2$, LiH, and BeH$_2$ molecules were simulated using 2, 4, and 6 qubits, respectively, the trial states were of the form

$$|\Psi(\theta)\rangle = U_{\text{single}}(\theta) U_{\text{ent}}(\theta) U_{\text{single}}(\theta) U_{\text{entr}}(\theta) \ldots U_{\text{single}}(\theta) U_{\text{ent}}(\theta) U_{\text{single}}(\theta) |00\ldots0\rangle.$$  \hfill (7.9)
Here, $U_{\text{single}}(\theta)$ represent arbitrary-single qubit rotations on each of the $N$ qubits (different rotations in each of the $d+1$ steps) and $U_{\text{ent}}(\theta)$ represent two-qubit entangling operations (same in each step) that were easy to implement in the available hardware. For the single-qubit operations alone, there are $N (3d + 2)$ independent rotation angles in the parameter vector $\theta$ (an arbitrary single-qubit rotation can be characterized by 3 Euler angles).

Already for relatively small molecules, $d$ needs to be more than just a few repetitions to reach accuracy that can compete with classical methods. However, a larger $d$ means that the quantum circuit takes longer to run, and thus decoherence will limit the achievable $d$. Recently, researchers are exploring “error mitigation” to get around this problem. In one type of error mitigation, the experiment is rerun several times with varying levels of added noise. From this, one can extrapolate the answer towards what it would have been for zero noise.

Note that the form of Eq. (7.9) is that of the QAOA in Eq. (6.24). This shows that the QAOA is an example of the broader class of algorithms that is the VQE.

### 7.4 More on step 4 – updating the parameters

Just like the other steps in the VQE that we have discussed so far, step 4 is also the subject of ongoing research. When searching for the ground-state energy of the problem Hamiltonian, there are several pitfalls that the update step must deal with. For example, the parameter landscape may have local minima. Furthermore, there is evidence that the landscape for larger problems can contain “barren plateaus”. Both these problems are hard to deal with if one uses a standard gradient-descent-based search for the optimal parameters. Also, the value of $E$ obtained in step 3 is noisy, since it is based on limited sampling of the expectation values for the Pauli strings making up the Hamiltonian (at some point, it becomes too costly to run the quantum computer enough times to sample all strings enough time eliminate the noise). The search method used needs to be robust against this noise. Another issue is that the number of parameters will be large for a larger problem. One possibility is to use gradient-free algorithms like Nelder-Mead.

There are many considerations that go into choosing the right method for updating the parameters. Yet another is that it can take non-negligible time to change all parameters and set up the instructions (pulse shapes, etc.) needed to implement step 1 on the quantum computer again.

Although VQE is an interesting heuristic hybrid quantum-classical algorithm for NISQ devices, it is clear that there is still much to be understood about the different steps of the algorithm. It is still unclear how well the VQE will scale with the size of the problems it is applied to.
Bibliography


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