Variational Quantum Eigensolver

Research Prelude

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1 Introduction

Before understanding the VQE (Variational Quantum Eigensolver), lets first understand what a traditional Eigenvector is. An eigenvector ($\vec{x}$) is a vector that upholds the property A$\vec{x}$ =$\lambda\vec{x}$ for some N * N matrix A, such that $\vec{x}$ only scales (grows longer or shorter) along its eigenvalues (λ) when multiplied by A. Eigenvectors are used to find solutions to systems of equations that deal with the least amount of outside variables. In the context of quantum mechanics, these help us with measuring the energy of some target.

The VQE is a hybrid quantum optimization algorithm which aims to find the minimum set of quantum operations that find the lowest energy state of some target. More simply put, the VQE blends both classical and quantum computing, aiming to find the eigenvectors for some quantum system of equations by optimizing the quantum circuit to use as few quantum gates possible. This algorithm is part of the NISQ (Noisy Intermedia Scale Quantum) era, which aims to deal with lower level quantum computation, up to at most 1000 qubits. This is due to the lower fault tolerance of modern day quantum computing

The general form of the VQE is:

$$\hat{H} = \sum_i \alpha_i \hat{P}_i,$$

Application Steps:

1. To begin, first we express the quantum sytems Hamiltoniain $\hat{H}$, as the sum of the tensor of all Puali Operators $\hat{P}_i = \{I, X, Y, Z\}^{\otimes n}$ multiplied by some coefficient α_i.

2. Next we produce our "Ansatz State" by making some quantum circuit which will prepare a "Trial Quantum State" denoted by $|\psi(\theta_1, \cdots, \theta_n)\rangle$ with parameters $\{\theta_i\}_{i=1}^{N}$,.

3. After computing our Ansatz State, we can measure our qubit output state given by:

$$E(\theta_1, \cdots, \theta_i) = \langle \hat{H} \rangle = \sum_i \alpha_i \langle \psi(\theta_1, \cdots, \theta_i) | \hat{P}_i | \psi(\theta_1, \cdots, \theta_i) \rangle$$

4. After completing our measurement, we load all values into an array $\vec{\theta}$ and

shift over to a classical computer

5. We iteratively pass θ_i into a gradient descent function $U(\vec{\theta})$ to optimize our parameters (the Pauli Gates applied)

6. Repeat step 5 until the Hamilton output converges towards the ground state denoted by $|\psi(\theta^*)\rangle$

7. Evaluate the eigenvectors of the matrix representation of the Hamiltonian

Sample Computation:

A single-qubit gate is defined as $U(\theta) = e^{-i\frac{\theta}{2}P}$, where $P \in \{X, Y, Z\}$. The derivative of U with respect to θ is:

$$\nabla_\theta U = \frac{\partial U}{\partial \theta} = -\frac{i}{2} P e^{-i\frac{\theta}{2}P} = -\frac{i}{2} PU = -\frac{i}{2} UP$$

Now, define $f(\theta) = \langle\phi|U^\dagger A U|\phi\rangle$. The gradient of f is:

$$\nabla_\theta f(\theta) = \frac{\partial}{\partial\theta}\langle\phi|U^\dagger A U|\phi\rangle = \langle\phi|\left(\frac{i}{2}P\right)U^\dagger A U|\phi\rangle + \langle\phi|U^\dagger A\left(-\frac{i}{2}P\right)U|\phi\rangle$$

This becomes:

$$= \frac{1}{2}\left[\langle\phi|U^\dagger(\theta+\frac{\pi}{2})AU(\theta+\frac{\pi}{2})|\phi\rangle - \langle\phi|U^\dagger(\theta-\frac{\pi}{2})AU(\theta-\frac{\pi}{2})|\phi\rangle\right]$$

Or more compactly:

$$\nabla_\theta f(\theta) = \frac{1}{2}\left(f(\theta+\frac{\pi}{2}) - f(\theta-\frac{\pi}{2})\right)$$

Real World Applications:

There are variations of the VQE which change depending on the field worked with. The term α_i will represent the energy contribution of each term and $\hat{P}_i$ will represent the tensor of the Pauli gate at each term. The index i is generally speaking our index of summation, but directly corresponds to a different property depending on which context the VQE is used. Under Quantum Chemistry, i represents number of qubits required to model the orbitals of a molecule. The more complex a molecule is, the more orbitals it will have, which will require more qubits to represent. The index i represents something else entirely when modeling for Nuclear Physics, Quantitative finance etc. Inorder to find out what our i should be, we can apply other quantum algorithms such

as Fermionic operators, Jordan-Winger, Bravyi-Kitaev and Parity transformations depending on our real world use case.

A particular use of the VQE is to solve the ground state of a molecule. The VQE tries to find the lowest possible energy (the ground state) of a Hamiltonian, which represents the energy operator of system. A Hamiltonian is the total energy of a system. The Hamiltoniain tells us how a system (like a molecule) will behave over time, and the Eigenvector's of a Hamiltonian tell us the possible energy levels of the system at each time. The VQE approximates for the Hamiltoniain of a molecule, helping build models to simulate the behaviour of different chemical bonds.

Example of the Hamiltonian expansion for a Hydrogem Atom H_2 :

$$\hat{H} = \alpha_1 \hat{I} \otimes \hat{I} + \alpha_2 \hat{Z} \otimes \hat{I} + \alpha_3 \hat{I} \otimes \hat{Z} + \alpha_4 \hat{Z} \otimes \hat{Z} + \alpha_5 \hat{X} \otimes \hat{X}$$

Other applications of the VQE include:

1. Modeling complex protein bonds in medical scans
2. Modeling nuclear fision, nuclei and deutreon

3. Modeling enzyme-substrate bonds in pharmaceuticals

4. Predicting magnetic properties of complex systems

5. Modeling stochastic investments in banking

6. Developing quantum machine learning models

2 The History

The VQE is still in its infancy, originally published in a paper in 2014 titled "The Thoery of Variational Hybrid Quantim-Classical Algorithms" by authors Jarrod McClean, Jonathan Romero, Ryan Babbush, Alberto Peruzzo, Alan Aspuru-Guzik and Jerem O'Brien. The team was built of IBM and Harvard researcher's aiming to create a quantum algorithm that can compute in tandem with a classical computer. The motivation for this approach was due to quantum computers boasting poor fault tolerance (the ability to reduce the likelihood of making mistakes). By using a hybrid algorithm, the team hoped to combine the strengths of classical computing (stronger fault tolerance) and quantum computing (powerful computational capabilities). The algorithm has

shown success in its deployment, but is not yet complete. It has been observed that there still exists a margin of error in its computation and needs to be refined to reduce the risks of miscalculations. Due to this, the VQE is currently used for modelling in biology and chemistry, where its typical computations can still be checked by classical computers, and is not favoured in the field of nuclear physics, where the bounds of computation are too difficult for the classical computer aspect, or have much too risk to entrust any margin of error. In the future, given fine-tuning to its model, the VQE has the potential to grow into the fields of nuclear sciences and help create more accurate models for efficient energy resources, contributing towards saving the environment as well as producing better vaccines.

3 Quantum Tools

The VQE employs tools and techniques from both Quantum Computing and Classical Computing.

Quantum Computing Tools	**Classical Computing Tools**
Parameterized quantum circuits (Ansätze)	Classical optimizers (COBYLA, SPSA etc.)
Pauli operator decomposition of the Hamiltonian	Gradient function evaluation (numpy, autograd etc.)
Quantum state preparation using R_x, R_y, R_z and entangling gates (e.g., CNOT)	Gradient estimation methods (e.g., parameter-shift rule, finite differences)
Expectation value measurement of Pauli terms	Hamiltonian construction using quantum chemistry packages (e.g., PySCF, Qiskit Nature)
Basis transformations for measurement (e.g., using Hadamard or R_x gates)	Fermionic operation mapping programgs (Jordan-Wigner, Bravyi-Kitaev)
Execution of circuits on quantum backends (hardware/simulators)	Circuit management and job submission (Qiskit, PennyLane)

4 Interests in Research

I decided to study the VQE since I knew I really liked linear algebra, so the "Eigen" in its name called out to me immediately. Before I began my research, I thought that tackling this topic would allow me to dive deeply into linear algebra once again, but was pleasantly surprised to see the implementation of calculus and quantum chemistry. I had a hard time initially understanding how to derive meaning from newer terminology such as "Hamiltonians" and

"Molecule Orbitals", aswell as some of the more intimidating math such as the variational gradiency functions. I made the best of my math background in understanding these subjects wherever I could, I hope that in the future I can continue looking into VQE and learn about its applications in machine learning models and learn more about new ways they can be applied that researches have not done yet.

5 Citations

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Related Topics: To find out more about how to calculate the number of orbitals of a molecule and compute the prerequisite information requierd for applying the VQE in Quantum Chemistry, other quantum algorithms and topics include: Fermionic operators, Jordan-Winger, Bravyi-Kitaev and Parity transformations. These were not discussed in this paper due to their complexity.