Analysis of Classical Optimization Routines used in the Preparation of Quantum States in Variational Quantum Eigensolver Algorithms

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Variational Quantum Eigensolver (VQE)

In many applications, it is important to find the minimum eigenvalue of a matrix. For example, such problems arise very frequently in many areas such as optimization, quantum simulations, and quantum chemistry. The **Variational-Quantum-Eigensolver** (VQE) is a hybrid quantum-classical algorithm that is used to resolve such problems. It is an efficient and effective alternative to the Quantum Phase Estimation (QPE) algorithm in the present Noisy Intermediate-Scale Quantum (NISQ) era of Quantum Computing.

For the purposes of this conference and our study, we define VQE's functionality formally as follows:

Given a Hermitian Matrix, H, with an unknown minimum eigenvalue, λ_{min}, associated with the eigenstate, $|\psi_{min}\rangle$, VQE provides us an estimate, λ_θ, bounding λ_{min}:

$$\boldsymbol{\lambda_{min} \leq \lambda_\theta \equiv \langle\psi(\theta)|H|\psi(\theta)\rangle}$$

Where $|\psi(\theta)\rangle$ is the eigenstate associated with λ_θ. The algorithms works by parameterized circuit, $U(\theta)$, to some arbitrary initial state, $|\psi\rangle$, to obtain an estimate $U(\theta)\ |\psi\rangle \equiv |\psi(\theta)\rangle$ on $|\psi_{min}\rangle$. This estimate is iteratively optimized by a classical controller altering the parameter, θ, to minimize the expectation value of $\langle\psi(\theta)|H|\psi(\theta)\rangle$.

As evident, the VQE algorithm uses a quantum subroutine **inside** a classical minimization task. The quantum subroutine consists of two parts: ***Ansatz based Quantum State Preparation*** and ***Measurement of the Expectation Value of H.***

Ansatz Selection

The ansatzes used in VQE are parameterized circuits, also known as *Variational Forms.* There are three main criterion to keep in mind while defining an ansatz for a VQE problem set up:

1. Ideally, our n qubit variational form would be able to generate any possible state $|\psi\rangle$ where $|\psi\rangle \in \mathbb{C}^N$ and $N = 2^n$.
2. The circuit depth for such ansatzes should be shallow to ensure maximum effectiveness in the NISQ era.
3. The number of parameters are as few as possible.

Parameter Optimization

Once an efficiently parameterized variational form has been selected, in accordance with the variational method, its parameters must be optimized to minimize the expectation value of the target Hamiltonian. There is no universal optimization scheme, and an appropriate optimizer should be selected by considering the requirements of the application.

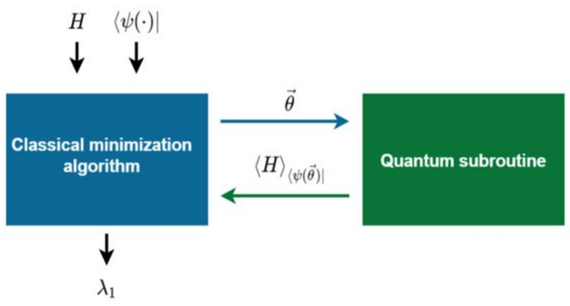

Fig 1: High level schematic of the VQE algorithm

Abstract

Variational Quantum Eigensolver (VQE) circuits are an application of the variational method of quantum mechanics used to solve problems of finding the eigenvalues of Hermitian operators in systems, where the dimension of the problem space grows exponentially. The circuit model is based on the VQE algorithm which uses an ansatze based state preparation technique through the use of parameterized circuits. The important property of such variational form is to be able to span the set of attainable states which is solely dependent on the ansatz and the classical optimizer utilized. We present a study on the various gradient based and gradient free optimizers that can be fitting to this regime and report on the efficiency and accuracy of the overall VQE operation for a standardized problem of calculating the smallest eigenvalues of a given Hamiltonian. We further explore how the effectiveness of such routine is affected by varying circuit depths. We aim to present our efforts in this conference and discuss the planned progression of our study.

Methodology

In our study, we explore the dynamics of changing each component used in the VQE routine by conducting sensitivity analyses on two performance metrics – *time taken to solve the problem* and *accuracy of the solution.* The principle problem that we investigate is that of finding the lowest eigenvalue of a Hamiltonian that is in the form of a 4 by 4 Hermitian matrix. We use *pyquil* and *qiskit* as our primary tools for conducting the simulation experiments and *matplotlib, numpy,* and *scipy* for the ensuant data analysis.

The following section describes the various test cases we considered in our study. Each scenario was tested independently of others keeping all other components set to a defined constant (base regime) to ensure validity and fairness of results.

Hamiltonian and Variational Forms:

We consider Hamiltonians as 4 by 4 Hermitian matrices. The type of Matrices we cover are *Sparse, Dense, Symmetric,* and *Skewed.* The Hamiltonian's are broken down into their Pauli term summations in the VQE circuit. Moreover, we also examine variational forms that utilize $\boldsymbol{U3(\theta,\phi,\lambda), R_X, R_Y, R_Z}$ and $\boldsymbol{\text{Swap}R_Z}$.

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = 0.5\sigma_i \otimes \sigma_i - 0.5\sigma_x \otimes \sigma_x - 0.5\sigma_y \otimes \sigma_y + 0.5\sigma_z \otimes \sigma_z$$

Fig 2: Example of one of the Hamiltonians used

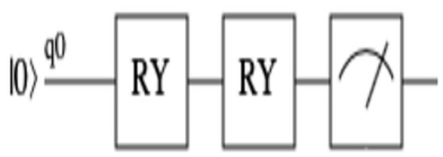

Fig 3: Example of one of the variational forms used

Circuit Depth and Optimizers:

We define circuit depth in this work as the number of repeating units of the ansatz. For certain problems this circuit depth becomes a parameter that needs to optimized and needs to be known a priori. Table 1 shows the classical optimizers used in our study.

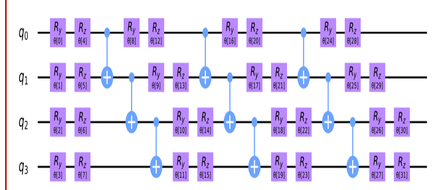

Fig 4: Example showing a variational circuit depth of 3

Gradient Free	Gradient Based
Nelder–Mead Simplex	Gradient Descent
Simulated Annealing	SLSQP
Genetic Algorithms	SPSA
Exhaustive Search	COBYLA

Table 1: Optimizers used in the study

Preliminary Simulation Results

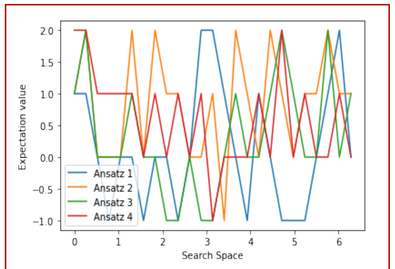

Fig 5: Varying Ansatz in base regime

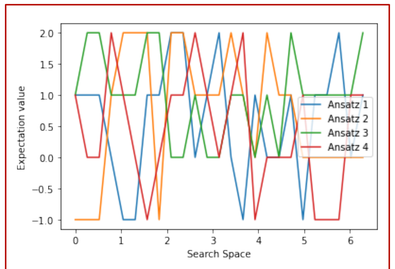

Fig 6: Varying Circuit Depth in base regime

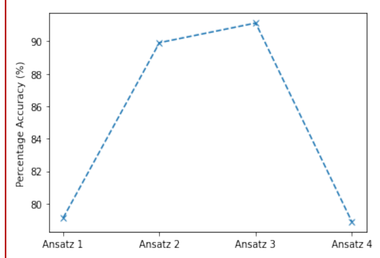

Fig 7: Percentage Accuracy while varying Ansatz

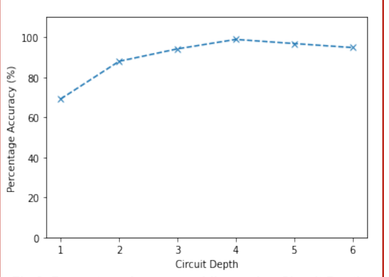

Fig 8: Percentage Accuracy while varying Circuit Depth

The plots above show some of our preliminary work we conducted as a part of the study. For a base regime (default set up of the study), we vary the variational form utilized (ansatz) and analyze the phase space and base optimizer accuracy. We do the same but for different circuit depths. For the base regime, it is evident that the search space is very bumpy, and that certain Ansatz and circuit depths perform better than others (as expected).

Future Work

This study is a work in progress. We are still implementing and running multiple of the test cases that we have discussed about in this conference. After all the scenarios have been simulated and analyzed, we plan to create a normalized *performance-compatibility* metric function that leverages the implications of the study and distinguishes best performing and most compatible components needed for a given application of the VQE algorithm. Depending on the results of our simulation experiments, we, also, plan on developing a comprehensive VQE regime that can be recommended for Hamiltonians of one of the given forms studied in our work. Furthermore, we plan on conducting similar studies on higher dimensional Hamiltonians and then repeat both studies with the Quantum Approximate Optimization Algorithm (QAOA).

References

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