NISQ algorithm implementation inspired from Universal Quantum Algorithms

Quantum_Questers

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1 Introduction

Our primary goal through this project was to simulate open-quantum systems suitable for the Noisy Intermediate-Scale Quantum (NISQ) era and the Intermediate-Scale Quantum (ISQ) era. Since certain special algorithms are implemented as Universal Quantum Algorithms (UQAs) for Fault Tolerant Quantum Computing (FTQ), which are currently not realized. Furthermore, Quantum Error Correction as mentioned in Laurent Prost's presentation is not currently quite practical since it requires additional qubits (logical qubit formulation), though one can use cat qubits, which we have also incorporated in one of our framework (state preparation), but that too would be feasible in the ISQ era. Hence, there is absence of existing VQA framework for specific problems like "direct estimation of energy difference between two structures in chemistry". The paper [1], discusses about the need for a UQA inspired framework with shallow circuit depth for NISQ devices (essentially a VQA algorithm) for such special problems. In this project, we aim to implement the framework in Python while also introducing our own innovations to enhance its robustness and expand its usability. We will not only utilize these innovations but also test the framework across various scenarios to showcase its usability and discuss the future implications of our work.

2 Problems

There are four major problems,

1. Firstly, we require the approximate mapping of the dynamics of open quantum systems into a stochastic Schrödinger equation with a non-Hermitian Hamiltonian, essentially in terms of the density matrix $\rho(t)$. Furthermore, since the Hamiltonian is non-Hermitian, approximation is required to express the Hamiltonian and the dissipative terms as linear combinations of unitary operators (LOU).

2. Secondly, the preparation of the initial state will involve creating a unitary operator U_{in} to transform $|0\rangle$ into $|\phi_{in}\rangle$.

3. Thirdly, we need to create an evolution unitary operator U_e, which describes the short-term evolution of the system.

4. Lastly, devising a measurement protocol which mitigates learning to reduce the amount of quantum resources.

3 Proposed Solutions

1. The first problem is addressed by "Choi-Jamiolkowski isomorphism technique" with Markovian Approximations. Case 1 of the Variational Quantum State Preparation (VQSP) algorithm will determine the parameters of the Parameterized Quantum Circuit needed to construct the unitary operator for the initial state. Furthermore, the Hamiltonian and the dissipative operators can be expressed as easily implementable LOU with scaling in terms of n qubits having $N = 2^n$ states as $\mathcal{O}((\log N)^a)|\mathcal{O}(n)^a)$. Lastly, the non-unitary evolution operator is approximated using a first-order Taylor expansion, with a sufficiently small Δt to make it expressible as a LOU. A specific cost function is then employed to determine the parameters required to construct the approximate evolution unitary operator.

2. The second and third problems are addressed by learning two PQCs through their VQSP (using **BFGS optimizer**) method which finds the optimal parameters, namely θ_{opt} and β_{opt} for approximating the respective unitary operators. Though the latter V(β) is exponentially fragile based on it's cost function described in equation 28 of [1], and is hence less suitable for higher dimension systems. Lastly, algorithm 4 mentioned in the paper reduces the depth further than algorithm 3, but increases sampling complexity.

3. The last problem is addressed by removing projector $\mathcal{P}$ after the implementation of the evolution unitary. The authors try to find the expectation value through a new observable $\tilde{\mathcal{M}}$ consisting of LOU and finding it through circuit Figure 3b [1].

4 Github Repository

`https://github.com/Hirmay/Qhack`

5 Proposed Innovations

- Cat qubits are a type of qubit that relies on encoding quantum information in the superposition of two coherent states of a quantum oscillator, such as a harmonic oscillator or a superconducting circuit. These states are referred to as "cat states" due to their resemblance to Schrödinger's famous thought experiment involving a cat in a superposition of alive and dead states. Cat qubits offer advantages in terms of coherence times and error rates compared to traditional qubit implementations, making them attractive candidates for quantum information processing tasks [2]. Inclusion of a couple of Cat qubits in our framework could enable us to simulate higher dimension and longer durability of the systems, which

were the limitations in the previous framework [1]. Furthermore, we observed that even for a very low cost function value, there were inaccuracies seen in Section 6, hence in such a scenario using Cat qubits becomes a natural choice. To test the framework, we used the previously obtained trained angles for a specific data from approach 1 and tested the fidelity of those angles using Logical Cat qubits ("EMU:15Q:LOGICAL_EARLY"). Results obtained can be seen in the Cat Qubits folder in the Github Directory. It is important that the fidelity of initial state to be as high as possible, since algorithms like the Harrow–Hassidim–Lloyd (HHL) algorithm relies on Quantum Phase Estimation (QPE) and Quantum Fourier Transform (QFT), which are sensitive to errors in the input state and if the initial state has low fidelity, the algorithm may produce inaccurate or incorrect results, or fail to converge to a solution [3]. Hence, utilizing the Cat-Qubits framework would be crucial in complementing the VQSP algorithm if it is used in the preparation of initial states.

- We have also experimented with various ansatz, including the hardware-efficient ansatz [4], which gave better results, reducing computation time and improving accuracy. However, since the Variational Quantum Algorithms (VQAs) can exhibit barren plateaus, sufficiently random ansatz under certain conditions helps in exponentially decaying the cost gradient with number of qubits [5]. Utilizing the results and strategies discussed in Ref. [6], we create a modified ansatz specifically for computing the evolutionary unitary to increase the probability of finding a near-optimal solution, since even with lower cost values we observed unstable system behaviour. We utilized random single-qubit rotations and ladders of C-Phase operations based on [6] accompanied with Scipy's "differential_evolution" method. We observed faster convergence compared to the other two ansatz structures for complicated cost functions requiring exponential number of calls like unitary evolution, but for state preparation we observed slower convergence.

- Significant scaling up is performed to study the VQSP approaches in more detailed manner. We used the NVIDIA's CuQuantum library to efficiently parallelize the quantum circuit and perform the optimization. Scaling was performed upto 20 qubits and performance is analyzed.

- Implemented the VQSP algorithm to perform state preparation for a real world dataset for drug target prediction for Alzheimer's disease and experimented the barren plateau issues involved in conventional amplitude embedding due to the circuit depth and the efficient VQSP state preparation scheme which has significantly lower depth.

6 Numerical Results

6.1 Open System: A two-level system with an amplitude damping channel

We simulated Example 1 as mentioned in the paper, Ref. [1], in order to make comparisons. However, our graphs are not as accurate as those presented by

the authors [1]. We used a lower depth of 10, with $G(\beta) \approx 10^{-2}$. The authors showcased scenarios with $G(\beta) \approx 10^{-1}$, which are prone to errors, indicating that the system is fragile. This susceptibility to errors may have contributed to the inaccuracies observed in our simulation, as seen in Figure 1.

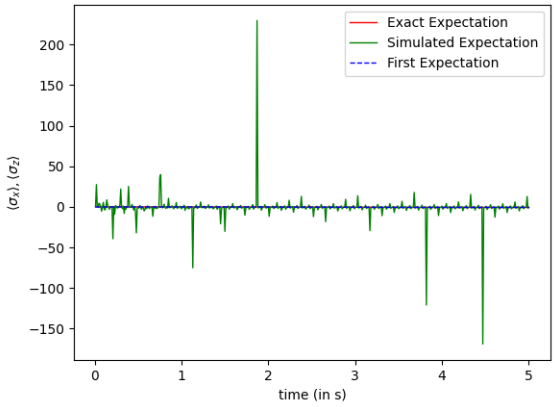


Figure 1: The training process of evolution unitary consisted of depth 10 with random ansatz, resulting in the cost function value of 10^{-2}. The training process of preparing initial state was done with circuit depth 4 with the hardware-efficient ansatz. The dynamics of a two-level system with an amplitude damping channel with $\delta = \omega = \gamma = 1$ and small time $\Delta t = 0.01$.

6.2 State Preparation

In this subsection, we address state preparation approaches, covering two distinct methods. Both approaches necessitate a normalized state vector, which can subsequently be reintroduced in post-processing. The first approach focuses on either all positive or all negative values, while the second approach incorporates both positive and negative values. Regrettably, we were unable to implement the third approach involving both real and imaginary values due to time constraints; however, we intend to include it in future work.

6.2.1 Approach 1

This approach of state preparation using VQSP focuses on the dataset with only all positive values or all negative values. The VQSP embeds these normalized data points into the amplitude values of the state vector.

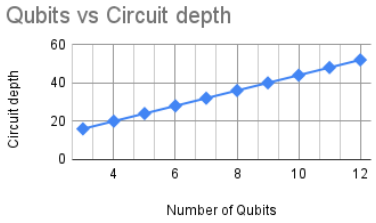
The VQSP algorithm used in this case contains of an ansatz with a repetition of 4 as the PQC. The ansatz is a structure with trainable Ry gates and CZ gates connected in cyclic fashion.

The various performance metrics including circuit depth, fidelity and training time have been analyzed for various number of qubits.

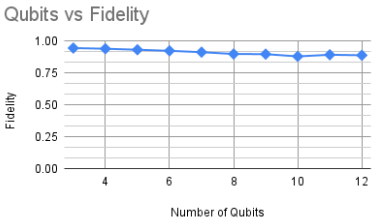
We have also experimented the robustness of the VQSP algorithm by scaling up the number of qubits and observing the performance in terms of fidelity. We have utilized the NVIDIA A100 GPU's to train the VQSP algorithm for random

data points. Varying the number of qubits from 3 to 12 we measured the fidelity, circuit depth and the training time. The results have been plotted below.

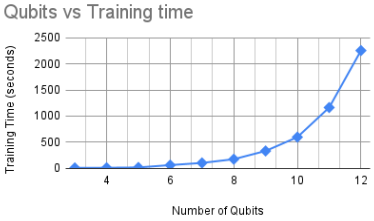
From the below plots, we can see that the circuit depth increases linerly as compared to number of qubits. In conventional amplitude embedding the circuit depth increases exponentially as with number of qubits. Thus, VQSP has a significant advantage in creating amplitude embedded state.



(a) Qubits vs Circuit depth



(b) Qubits vs Fidelity



(c) Qubits vs Training time

Figure 2: The three figures are provided, where Qubits are plotted with respect to Circuit depth, Fidelity and Training time using Approach 1.

Additioanlly, we tested our VQSP approach for a real world dataset. We obtained a drug target dataset from ChEMBL [7], comprising molecular feature descriptors and their corresponding bioactivity related to the inhibition of Alzheimer's disease progression.

After variance thresholding, the molecular features were reduced to 140 input features, and binary classification was performed on this dataset. Representing the 140-qubit system required 8 qubits using amplitude embedding. However, the depth of conventional amplitude embedding, when combined with the trainable ansatz depth, adversely affected convergence due to the presence of Barren plateaus.

To address this challenge, we employed Variational Quantum State Preparation (VQSP) to train a Parametrized Quantum Circuit (PQC) to generate the dataset values. Subsequently, these angles were utilized to construct the corresponding state of the amplitude embedding. This approach reduced the depth of the embedding component to 36, thereby mitigating the impact of Barren plateaus.

The Approach 1 is extensively stress testing to understand the robustness of the VQSP algorithm. A subset of previous dataset containing around 700 data points have been taken and the fidelity is measured. The results can be seen in the Figure 3.

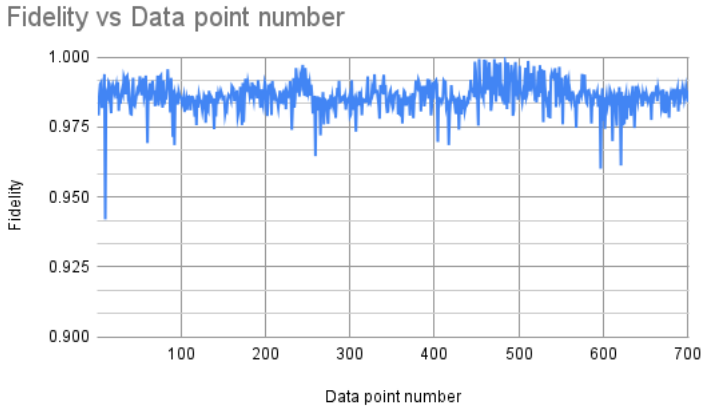


Figure 3: Each data point means a different state vector. We computed 700 data points and obtained an average fidelity of 96% using Approach 1.

We have also plotted the convergence curve of the cost function for various qubits and the results can be seen in the Figure 4. We have also been able to test the embedding angles provided by the above training the Real quantum computers provided by AWS Braket. We tested state embedding in Cat Qubits system as well as IonQ Aria 1 device. The source code and results have been added in GitHub Repository.

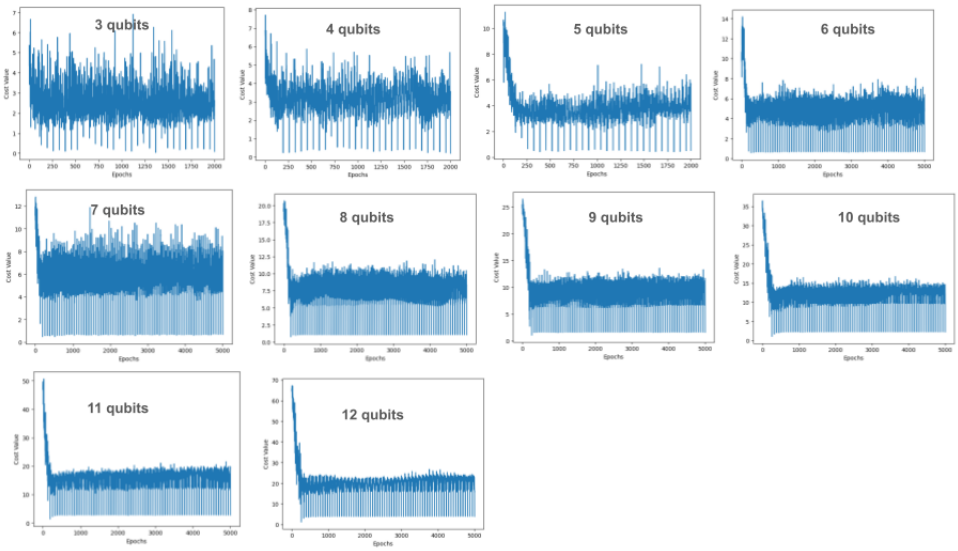


Figure 4: Approach 1 convergence plots with various qubits using random state vectors.

6.2.2 Approach 2

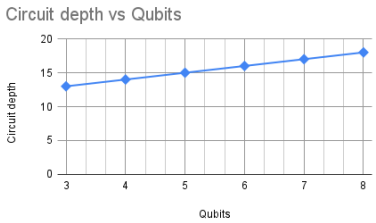
This approach of state preparation using VQSP focuses on the dataset with any positive or negative real values. The VQSP embeds these normalized data points into the amplitude values of the state vector.

The VQSP algorithm used in this case contains of an ansatz with a repetition of 4 as the PQC. This PQC uses a single ancillary qubit to distinguish between positive and negative values. The ansatz is a structure with trainable Ry gates and CZ gates connected in linear fashion. Finally, we have a Hadamard gate in zeroth qubit to distinguish between positive and negative values.

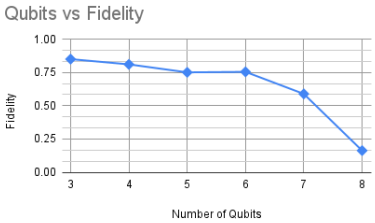
The various performance metrics including circuit depth, fidelity and training time have been analyzed for various number of qubits.

We have also experimented the robustness of the VQSP algorithm by scaling up the number of qubits and observing the performance in terms of fidelity. We have utilized the NVIDIA A100 GPU's to train the VQSP algorithm for random 4 data points. Varying the number of qubits from 3 to 8, we measured the fidelity, circuit depth and the training time. The results have been plotted in the below Figure 5.

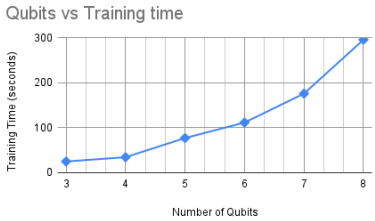
It can be seen that we obtain lower fidelity compared to approach 1. The reason is because of the optimization approach which we have used. We were able to improve the performance to around 95% fidelity using Dual annealing based optimization technique. The work has been posted in GitHub Repository.



(a) Qubits vs Circuit depth



(b) Qubits vs Fidelity



(c) Qubits vs Training time

Figure 5: The three figures are provided, where Qubits are plotted with respect to Circuit depth, Fidelity and Training time using Approach 2.

Additioanlly, we have also added the cost function convergence plot for various qubits in the below Figure 6.

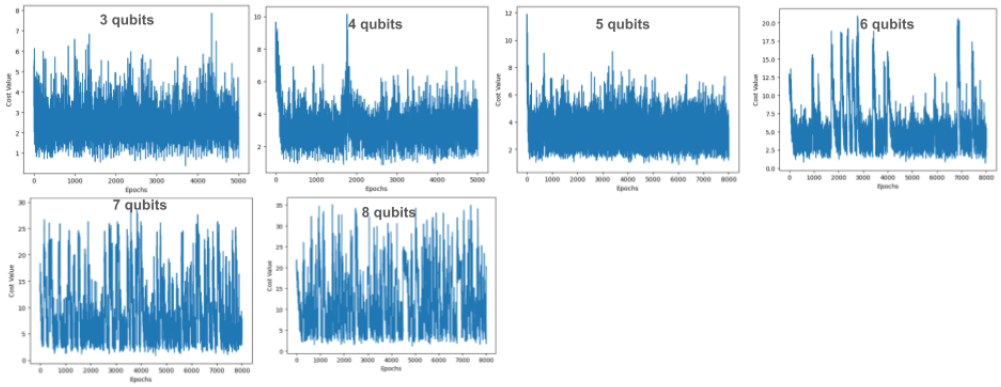


Figure 6: Approach 2 convergence plots with various qubits using random state vectors.

7 Discussion

- Another area worth exploring is the potential application of quantum-assisted algorithms like HHL (or similar important algorithms) with their VQSP framework. For instance, in [8], quantum conditional logic is proposed as a replacement for QPE for estimating the eigenvalues. In this context, the only remaining expensive component is the preparation of the right-side vector $|b\rangle$.

- A better cost function which addresses some of the problems like exponential calls required for $V(\beta)$ circuit or better approximations which reduces circuit depth and/or sampling complexity to make it more suitable for more strongly correlated problems. The sampling variance could be reduced by training an approximate Restricted Boltzmann machine (RBM) [9], which is an issue in Algorithm 4 [1].

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