Quantum Machine Learning - VQLS

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Abstract

This project uses a variational quantum algorithm to approximate the inverse quantum Fourier transform (QFT). We investigate the algorithm's accuracy based on the number of qubits and layers, using the matrix A as the QFT operation. The performance is assessed using numerical simulations, with a focus on how increasing qubits and circuit ansatz influence the approximation. The findings provide insights into optimizing the variational technique for quantum Fourier transforms with limited resources.

1 Introduction

A key component of many quantum algorithms, the Quantum Fourier Transform (QFT) is essential for tasks like phase estimation and period discovery, which are essential to Shor's algorithm and other quantum computational procedures. The direct implementation of QFT can be resource-intensive despite its significance, especially as the number of qubits increases. The goal of this project is to investigate a variational method for estimating the inverse quantum Fourier transform (IQFT), taking advantage of parameterized quantum circuits' flexibility to produce effective approximations with less processing overhead and faster run-time.

Because they can be executed on noisy intermediate-scale quantum (NISQ) devices, variational quantum algorithms (VQAs) are attractive options for near-term quantum computing. By minimizing a predetermined cost function and achieving a desired output, these algorithms iteratively update the parameters of quantum circuits using classical optimization techniques.

The Variational Quantum Linear Solver (VQLS) is an innovative quantum algorithm designed to solve systems of linear equations. It builds upon the Variational Quantum Eigensolver (VQE) framework, offering a more efficient solution compared to classical methods. The VQLS aims to find a vector $|x\rangle$ satisfying $A|x\rangle = |b\rangle$, where A is a given matrix and $|b\rangle$ is a known vector. While the VQLS produces results similar to the HHL (Harrow-Hassidim-Lloyd) algorithm, it has a crucial advantage: it can operate on Noisy Intermediate-Scale Quantum (NISQ) devices. This makes the VQLS more practical for near-term quantum computing applications, as it requires fewer qubits and less robust hardware than HHL. The VQLS typically outputs a vector proportional to $|x\rangle$, which is often sufficient for many applications. This approximation, combined with its NISQ compatibility, makes the VQLS a valuable tool in quantum computing.

In this project, to approximate the IQFT in this setting, we design a variational quantum algorithm (VQLS) that strives for a trade-off between computational resources, such the amount of qubits and circuit depth, and precision. The accuracy of the variational IQFT is examined in this work by analyzing the error in relation to the number of qubits. By tackling these, we hope to shed light on the scalability and resource optimization of quantum Fourier transforms and find out how variational approaches can effectively simulate the IQFT. Furthermore, we examine the circuit's data encoding process and the training strategies employed to maximize the variational parameters for a range of input data sets.
please, view the project presentation in this link

2 Research Question

The primary focus of our research is to determine whether our approach, utilizing the Variational Quantum Linear Solver (VQLS) algorithm for computing the inverse Fourier transform, aligns with the theoretical framework we have established. Specifically, we aim to evaluate the algorithm's efficiency in terms of runtime, potential speedup, and other performance metrics. Additionally, this study will seek to investigate the limitations and potential drawbacks of the algorithm, conducting a comprehensive analysis across various experimental scenarios.

3 Mathematics of the VQLS and IQFT

As said in the article, a variational quantum solver is used to clear up a line of equations of the form $\hat{A}|x\rangle$. Setting an ansatz based on a set of parameters $|x\rangle = \hat{V}(\alpha)|0\rangle$ and calculating a cost function $1 - |\langle b|\psi\rangle|^2$, where $|\psi\rangle = \hat{A}|x\rangle$, leads to a state $|\tilde{x}\rangle$ that is close to the exact solution of the set of equations, $|x\rangle = \hat{A}^{-1}|b\rangle$. By setting $\hat{A} = Q\hat{F}T$ and using the variational quantum linear solver (VQLS) several times, we were able to compute the inverse matrix of the QFT operator for a range of qubit counts using the techniques described in the paper. We computed each time with different $|b\rangle$: $(1, 0, 0, ...), (0, 1, 0, ...), ...$ in order to generate the $Q\hat{F}T^{-1}$ columns.
There are many option for the cost function, but in the paper they chose to present:

$$C_G = 1 - |\langle b|\psi\rangle|^2$$

when $|\psi\rangle = A|x\rangle$ so the cost function gets lower as $A|x\rangle = |b\rangle$ we can define A as sum of unitary matrices $A = \sum_l c_l A_l$ and then $\langle\psi|\psi\rangle = \sum_{l,l'} c_l c_{l'} \langle 0|V^\dagger A_{l'}^\dagger A_l V|0\rangle$ and $|\langle b|\psi\rangle|^2 = \sum_{l,l'} \langle 0|\hat{U}^\dagger A_l V|0\rangle\langle 0|\hat{U} A_{l'}^\dagger V^\dagger|0\rangle$. for simplification assuming A is a unitary matrix then we get that $\langle\psi|\psi\rangle = \langle 0|V^\dagger V|0\rangle$ because $A^\dagger A = I$ furthermore, we can calculate $|\langle b|\psi\rangle|^2$ by measuring the probability of outcome zeros of the state $\hat{U}^\dagger AV|0\rangle$

We say $N = 2^n$, $\omega = e^{i\frac{2\pi}{N}}$, therefore, for n qubits, the QFT matrix has the following form:

$$\frac{1}{\sqrt{N}}\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega & \omega^2 & \cdots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \cdots & \omega^{2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \cdots & \omega^{(N-1)^2} \end{bmatrix}$$

notice, that for 1 qubit, the matrix is Hadamard.

$$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

4 Results

We developed Python code in a Jupyter Notebook (`.ipynb` format) using the Qiskit package to estimate the Inverse Quantum Fourier Transform (IQFT) matrix for 1, 2, 4, and 8 qubits, based on the corresponding Quantum Fourier Transform (QFT) matrix, utilizing the Variational Quantum Linear Solver (VQLS) algorithm.
Initially, we experimented with a simple ansatz featuring rotations around the y-axis. However, this approach resulted in significant errors. We then tried a more complex ansatz using controlled-X (CNOT) gates and U-gates, which provide rotations along all axes. Despite this improvement, the errors remained substantial. Finally, we adopted the EfficientSU2 ansatz with two layers, which yielded a smaller error. Although the U-gate ansatz was not necessary, we retained it for comparison.
Next, we defined the cost function as outlined in the introduction and created an optimization function using the COBYLA optimizer and the VQLS algorithm. This function was designed to find the optimal parameters for the ansatz given A and b, resulting in an unnormalized quantum state vector $|x\rangle$.
Our approach then involved creating a function to:

1. Construct the QFT matrix and identity matrix for each number of qubits.
2. Define the ansatz.
3. Enumerate through each column of the identity matrix.
4. Apply the VQLS algorithm to determine the corresponding column in the IQFT matrix.

Since the columns of the resulting matrix were not normalized to the correct phase, we implemented a function to adjust the phase of each column, ensuring that the first element in each column of the IQFT matrix is 1. This adjustment produced the correct IQFT matrix. For each number of qubits, we printed the IQFT matrix obtained from the VQLS algorithm, along with the error relative to the correct matrix and the ansatz used. The error was calculated using the following formula, which is the norm of the matrix of the differences matrices using np.linalg.norm:

$$\text{error} = \sqrt{\sum_{i,j} \left\| IQFT_{i,j}^{\text{VQLS}} - IQFT_{i,j}^{\text{Real}} \right\|^2}$$

Here are the results note that the matrices for 4 and 8 qubits are not printed here due to their size; they can be reviewed in the code file.

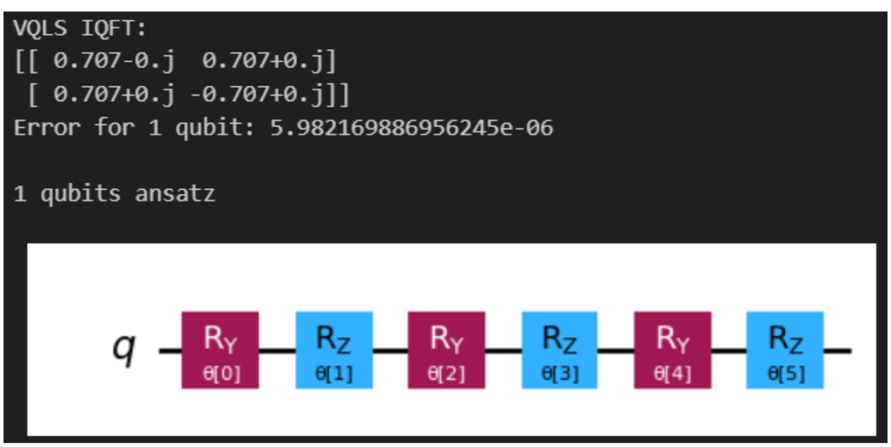

Figure 1: result of the VQLS to construct the IQFT for 1 qubit

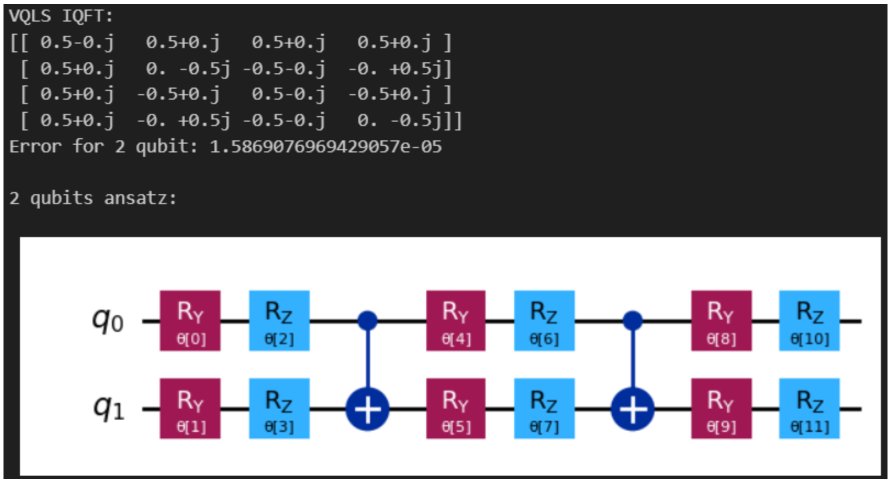

Figure 2: result of the VQLS to construct the IQFT for 2 qubits

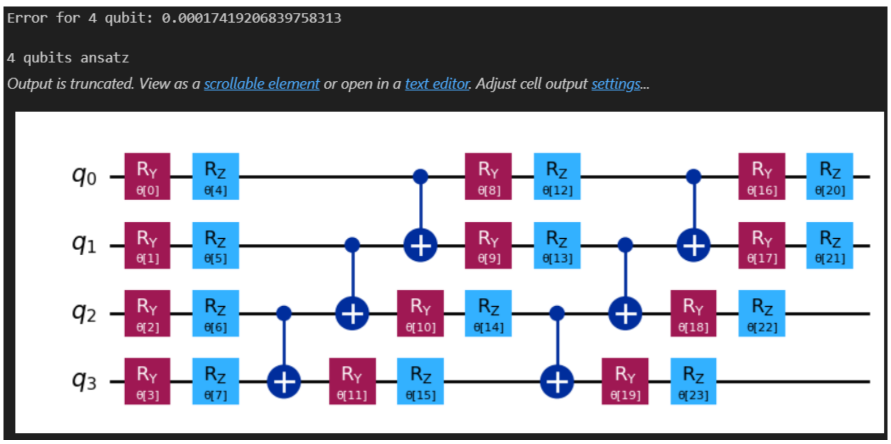

Figure 3: result of the VQLS to construct the IQFT for 4 qubits

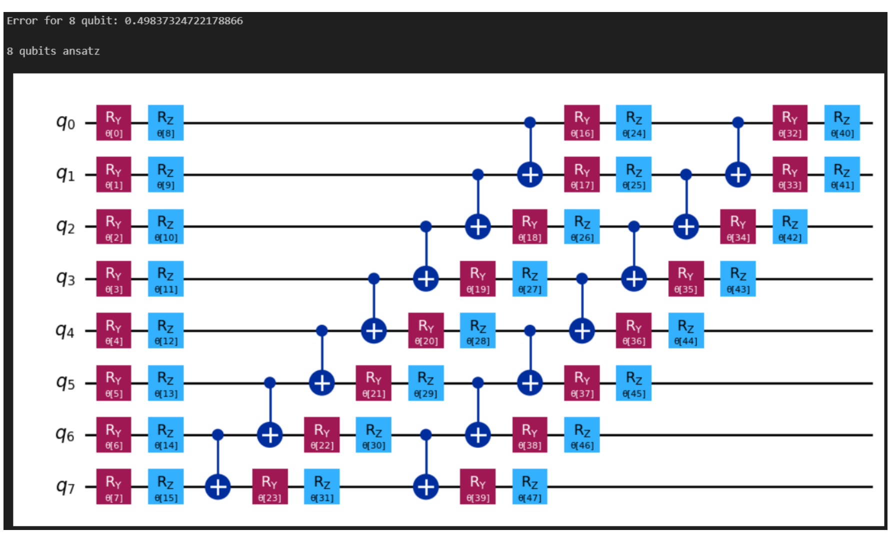

Figure 4: result of the VQLS to construct the IQFT for 8 qubits

There was no precise method to measure the accuracy, so we measured only the error. We observed that the error grows exponentially as the number of qubits increases. However, this does not necessarily imply that the accuracy decreases. Notice that the way we defined the error did not involve taking the average error of the matrix; instead, we summed the error of each element. Therefore, as the matrix size grows, we expect the total error to grow accordingly. This brings us to the following graph:

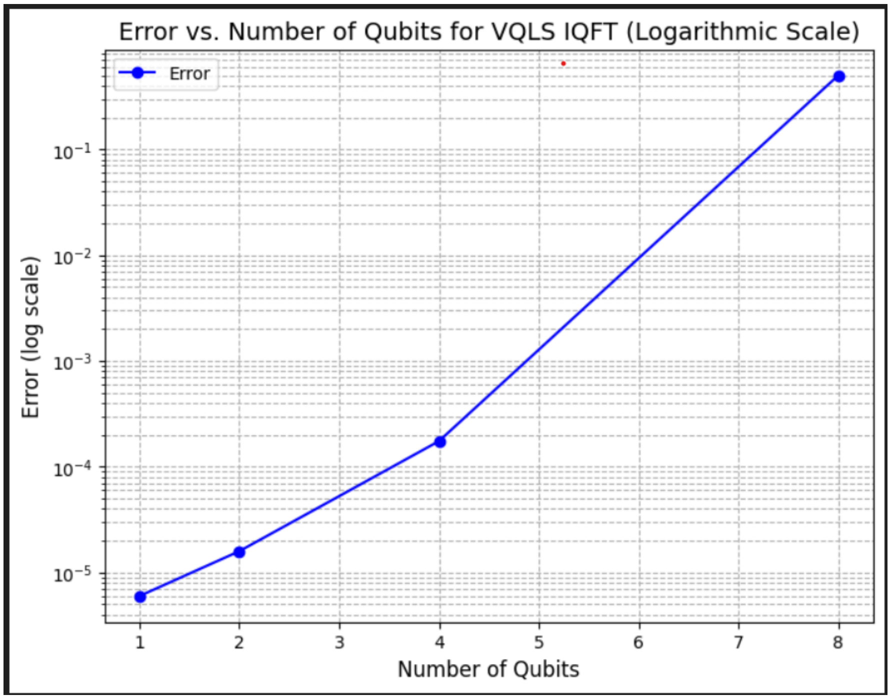

Figure 5: plot of the norm error vs. the number of qubits. the graph is in logarithmic scale in the y-axis and the plot grows linearly, therefore the error grows exponentially by the number of qubits.

From the graph, we can see that as the number of qubits increases, the error grows exponentially. This is expected because the size of the matrix grows exponentially with the number of qubits, and so does the total error. However, if we were to compute the average error per element in the matrix, we would find that **the error of the VQLS remains constant with respect to the number of qubits**.

5 Discussion

In this work, we demonstrated how to efficiently obtain the inverse of a unitary matrix using a NISQ algorithm known as the Variational Quantum Linear Solver (VQLS). Our approach builds upon the method described in [1], which addresses solving linear systems of equations. The primary distinction is that while [1] focuses on solving equations to find the vector resulting from multiplying a matrix by a given vector $|b\rangle$, our goal was to determine the actual inverse matrix. To achieve this, we utilized VQLS iteratively to compute each column of the inverse matrix by defining the output vectors $|b_i\rangle$ as the standard basis vectors. Additionally, a key difference lies in the matrix properties: in general linear systems, the defining matrix may not be unitary, requiring decomposition into a sum of unitary matrices. However, since the Quantum Fourier Transform (QFT) matrix we needed to invert is unitary, our calculations were significantly simplified.
We successfully applied the Variational Quantum Linear Solver (VQLS) algorithm to determine the Inverse Quantum Fourier Transform (IQFT) for various numbers of qubits, achieving consistent overall error. Our project utilized a Qiskit simulation rather than actual quantum hardware. While this approach provided reliable error metrics, the computational time increased exponentially with the number of qubits. This is because the VQLS algorithm was executed classically rather than on real quantum hardware, leading to longer calculation times compared to the theoretical performance of VQLS. As a future direction, we plan to test VQLS on actual quantum hardware, which should be

feasible using IBM's Qiskit packages. We anticipate that this will significantly reduce the computational time to a polylogarithmic complexity relative to the matrix size. However, we must consider that hardware noise could impact the accuracy of the VQLS results.

Because of the time complexity issue of using VQLS classically instead of on a real hardware, we used only EfficientSU2 ansatz with 2 layers and did not check what would happen has the layers increased, but we suspect that in real hardware the errors will just grow larger since the error is already small and more layers provide more noise.

Looking ahead, as noted in [1], advancements in quantum hardware—specifically improvements in noise reduction and qubit count—are expected. These advancements could lower the errors in VQLS computations and enable the use of algorithms like HHL (Harrow-Hassidim-Lloyd) for solving larger linear systems using quantum technology. Consequently, VQLS might become less prominent in the landscape of major quantum computing companies. In conclusion, we believe this algorithm offers significant quantum gains, with potential applications across various areas of mathematics has it can solve on real quantum hardware large-scale linear systems, and we have demonstrated its effectiveness. However, as we discussed, these advantages may diminish over the next 20 years as more powerful hardware is developed. At that point, algorithms like HHL, which will also be able to handle linear systems, may become preferable once again.

6 Contributions

Erel Dekel - Wrote the entire code for the project and ensured it met all requirements, Wrote the result and discussion sections in the paper and slides number 2,4,5,6 in the presentation.

Dolev Shmaryahu - Mainly wrote the introduction for this project

Aviv Gabay - Conducted research for the background section of the project, and contributed to the implementation of the algorithm. Also assisted in proofreading the entire paper.

David Swissa - main contributor in writing the research question, presented the background of the project and the motivation, and was active in the discussions.

References

[1] C. Bravo-Prieto *et al.*, "Variational quantum linear solver," Sep 2019.