IQRG PROGRAMME

Introduction to Quantum Research for Girls 2024, Inaugural Cohort Proceedings

A programme led by ThinkingBeyond
in collaboration with Girls in quantum

Proceedings of the Introduction to Quantum Research for Girls Programme

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August 2024

Preface

Welcome to the proceedings of the 2024 inaugural cohort of the *Introduction to Quantum Research for Girls* (IQRG) programme run by ThinkingBeyond in collaboration with Girls in Quantum from 29th April until 28th June 2024.

This year's programme brought together thirty-six talented young women aged 15-22 from across the globe. Each of our young researchers had to pass a rigorous selection process. Having stood out amongst 309 applicants from more than 50 countries, they must also successfully complete the Course Stage of the programme before proceeding to conduct a research project under the guidance of an academic mentor.

During the four-week Course Stage, the participants learned about the basics of Quantum Computing, received an introduction to the foundations of Quantum Mechanics, had the option to explore the mathematics underlying Quantum Mechanics, and were introduced to the world of academic research. In a series of workshops they also started to develop important soft skills of a researcher like scheduling and time management, effective learning, personal knowledge management, project management, paper-writing, and poster-making. Throughout the programme, they had to complete and submit work, either individually, or in a team.

Participants who successfully completed the Course Stage moved on to the five-week-long Research Stage. After choosing a Quantum Computing project, they worked in teams of two under the guidance of a mentor, while attending talks by academics and industry experts on advanced topics and applications in the subject.

Quantum Computing stands poised as a state-of-the-art technology to revolutionise numerous sectors, from drug discovery and material science, to financial modeling and artificial intelligence. The programme served as a vital platform to introduce talented young women to this multifaceted field, as well as to the world of research. It has been our focus to empower our participants and give them a head start to become future subject experts by educating them on the basics, equipping them with the essential skills to excel, and offering them their first research experience, where they could apply what they had learnt.

We extend our sincere gratitude to our co-organizers and many volunteers for their tireless efforts in making this programme a success. Our special thanks extend to our academic mentors Prof. Dr. Gerhard Hellstern, Dr. Filip Bár, Manuel Rudolf, MSc, Kathrin König, MSc, Vanessa Dehn, MSc, Andreea Iulia Lefterovici, MSc, Victoria Hazoglou, MSc, Jannes Stubbemann, MSc, Mohammed Alabdullah, MEng, Sanskriti Oza, BSc and Juweria Sayed, BSc. Their guidance and patience were essential for our participants' success. We also acknowledge our participants whose contributions form the backbone

of these proceedings.

The research projects showcased in these proceedings span a diverse range of topics and applications, from fundamental Quantum Computing concepts to Quantum Machine Learning. These projects represent a significant advancement beyond the Course Stage of the programme, posing a considerable challenge to our participants - many of whom were newcomers to Quantum Computing by the time of their application.

We commend all participants for their remarkable dedication and success in overcoming these challenges, and invite you, the reader, to appreciate the culmination of their intellectual labour and curiosity within these pages. We are proud to present their accomplishments and trust that their work will inspire countless young minds aspiring to become researchers in STEM.[1] We are confident that these young women will continue to make significant contributions to the fields of STEM, and we look forward to witnessing their future accomplishments.

Chairs of IQRG

Dr. Filip Bár and María Delgado Álvarez

August 2024

[1] The code for each project can be found on https://github.com/ThinkingBeyond/IQRG-2024.

Contents

VQE for Ground State Energy Optimisation of H_2

IQRG 2024 Project 10B
By Keisha Kwok and Inés Martín - Mentor: Jannes Stubbemann

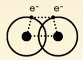
1) Problem Statement + why it is hard

"How to find a molecule's ground state energy?"

Motivation for finding it
A quantum system's **ground state energy** is the energy in its **most stable** state. This is useful as it tells us how a molecule behaves in low temperatures (where quantum effects are the strongest).

Potential real-life use-cases
- Simulating molecules
- → Studying new drugs
- → Studying superconductors

Consider the simple molecule: H_2



Its total energy consists of:
- Kinetic energy
- Potential energy electrostatic potential energy amongst 2 nuclei & 2 electrons
- Gravitational potential energy (negligible)

In quantum language:

$$\hat{H} = \hat{T} + \hat{V} \quad (1)$$

Hamiltonian (energy operator) — Kinetic energy — Potential energy

Our intention: To find the minimum energy by solving for the **eigenvalue** of H in the **Schrödinger equation** (SE) for the two-electron wavefunction.

Energy between the 2 electrons: $V_{e-e} = \frac{e^2}{4\pi\epsilon_0 r}$ (2)
r, the distance between the 2 electrons, is impossible to find since **both electrons are moving** (there is no centre of reference frame). Therefore we cannot find this term's exact value.

Therefore, our original intention cannot be carried out directly. The Coulomb **electron-electron repulsion terms** makes it **impossible** to find an exact solution to the SE for many-electron atoms and molecules, even for a molecule as simple as hydrogen.

2) Computational Estimations

Since we can't find the exact solution, we turn towards computational approaches to make estimations.

Required ideas for an algorithm to estimate a molecule's ground state energy

Idea 1: Enable computation by encoding fermionic information

We need to map **fermionic** (electron) operators to **qubit** operators. A map translates creation and annihilation operators that make up $\phi(\theta)$, into strings of Pauli rotation operators (akin to spin). These, acting on the initial "Hartree-Fock state", encode the electrons' information into the quantum circuits.

Two common maps are the **Jordan-Wigner** and the **Bravyi-Kitaev** mappings.

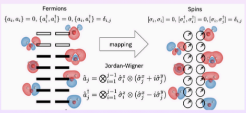


Fig 1. The Jordan-Wigner mapping, visualised.

Idea 2: Enable estimations with the Variational Method

A player in a **1-100 number-guessing game** starts with 50, then (if target is less) guesses 25, then (if target is more) 38, etc. She is **varying** her guesses until the gaps narrow and the guesses get closer and closer, i.e. **converge**, to the target value.

Here, we utilise the same **variational principle**. to estimate the ground state energy. Just like 50 in the 1-100 game, we need a good first guess, a.k.a. **ansatz**, to maximise efficiency.

$$E_{trial} = \frac{\langle\phi_{trial}(\theta)|\hat{H}|\phi_{trial}(\theta)\rangle}{\langle\phi_{trial}(\theta)|\phi_{trial}(\theta)\rangle} \geq E_0 \quad (3)$$

This equation describes that for any **trial** wavefunction ϕ, the **expectation value** of the Hamiltonian E_{trial} is an **upper bound** for the ground state energy. The classical processor evaluates how much the energy has converged by calculating the cost function. Then, it provides $U(\theta)$ to **vary** $\phi(\theta)$.

3) Using VQE

Variational Quantum Eigensolver (VQE) is one computational approach to estimate ground state energies. Again we will use H_2 - it is the simplest molecule to verify VQE with, since the output can be compared to theoretical calculations.

"How does VQE estimate H_2's ground state energy?"

Our VQE uses **Jordan-Wigner** mapping to prepare qubits to represent H_2's electrons' information

U(θ) represents the varied **parameters** θ in ϕ(θ), which varies the **expectation value** of H's energy state

This involves the **classical gradient descent** method to optimise parameters based on obtained expectation value

$|1100\rangle$ is the initial H-F state for H_2

VQE is a **hybrid** algorithm

Iterative process to obtain the best converged value (optimisation)

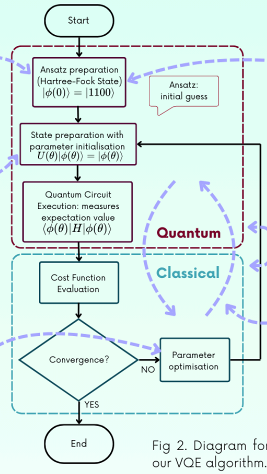
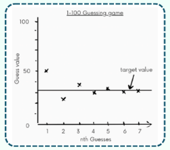


Fig 2. Diagram for our VQE algorithm.

What we expected from our code



Just like how the guess value **converges to the target value** in the number-guessing game, we expect the same to happen for our H_2 energy expectation value.

This was indeed what happened.

Our code's outputs

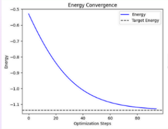


Fig 3: **95** iterations

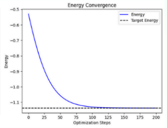


Fig 4: **200** iterations

See the variational method in action: Figs 3 and 4 show the **optimisation** process: the more **iterations** done, the more the expectation value converges to the target energy.

4) VQE's Problems and beyond

Lack of scalability

Current VQE implementations are **limited** by the **number of qubits** available. Moreover, for larger molecules, there are more than one **local minimum** on the energy landscape, so the ansatz sometimes converges to one of them that isn't the desired **global minimum**. This is why VQE in itself can't be used in molecules that have real-life applications, e.g. protein molecules in biochemistry.

Errors

Errors can be caused by hardware **noise**, ansatz **inaccuracy** or **measurement errors**. Mitigation strategies such as zero-noise extrapolation enhances VQE's accuracy within its current limitations.

Ongoing work to extend VQE

Some examples to improve or extend VQE are:
- **ADAPT-VQE**: here the ansatz is dynamically built to improve its accuracy and compactness.
- **Overlap-ADAPT-VQE:** avoids building the ansatz in such a way that the expectation value falls into a local but not global minimum (likely for large-molecule simulations), thus improving the output's accuracy.
- **Quantum Natural Gradient**: uses the quantum Fisher information matrix to perform optimization respecting the geometry of the parameter space

References

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Scan this QR code to access our code:

We would love to hear your questions and feedback on our presentation. Thank you for your interest!

Quantum Complexity & the HHL Algorithm

1 Complexity CLASSES

There are many algorithms to solve different types of problems, categorized into complexity classes. Classes P, NP, and BQP are all in the PSPACE, meaning they can be solved by a Turing Machine, and use a polynomial amount of space.

- P: Polynomial Time--problems that are easy to solve; there is a classical algorithm that efficiently solves them.
- NP: Nondeterministic Polynomial Time--a set of problems that are difficult to solve, but easy to verify.
  - NP-Hard: Problem Y is NP-Hard if X NP-Complete problems can be reduced to Y in polynomial time.
  - NP-Complete: These problems are in NP, and are NP-Hard.
- BQP: Bounded-Error Quantum Polynomial Time--problems solvable by a Quantum Turing machine bound by polynomial time.

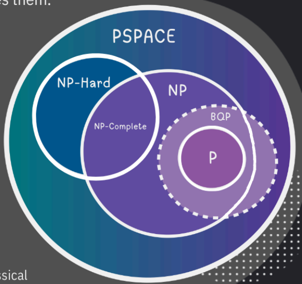
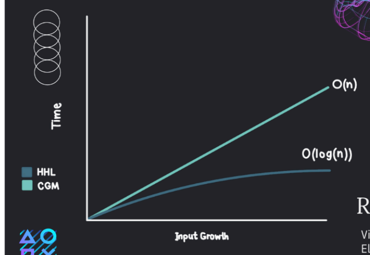


Figure 1. details the relationship between the different classical complexity classes: P, NP, NP-Hard, NP-Complete, BQP, and PSPACE. Up till the point of writing, there is no proof that P = NP, or that PSPACE = NP. However, BQP is believed to contain all of P and some of NP.

2 LSP, CGM, & HHL

Our goal is to solve linear system problems (LSP) with n variables (dimension n). Let A be a Hermitian matrix, $\vec{b}$ be a vector, and $\vec{x}$ be the vector to be solved. Then we can write our LSP as: $A\vec{x} = \vec{b}$.

Many classical algorithms can solve this system, the fastest being the CGM (Conjugate Gradient Method). CGM solves LSP with a complexity of O(n). The quantum algorithm for linear solvers--HHL (Harrow–Hassidim–Lloyd)--can solve these systems with complexity O(log(n)), providing an exponential speedup over the fastest known classical linear solver.

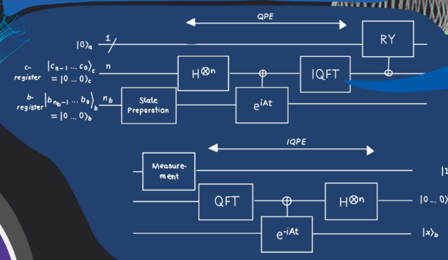


3 HHL Algorithm

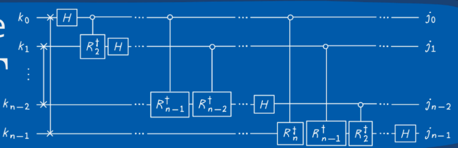
HHL has 4 main steps:

1. HHL estimates the eigenvalues of A^{-1}, λ^{-1} of the matrix, using Quantum Phase Estimation.
2. Performs a controlled rotation on auxiliary qubit in accordance to the eigenvalues estimated.
3. Qubits in the main register are reset to $|0\rangle$
4. The auxiliary qubit is then measured untill the result is $|1\rangle$

4 The HHL Circuit



The IQFT Circuit



A change in basis from computational ($|0\rangle$ and $|1\rangle$) to the Fourier basis: computational basis ($|-\rangle$ and $|+\rangle$)

The IQFT circuit consists of 3 parts:

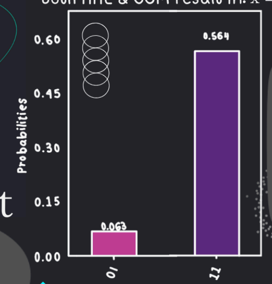
1. The swap gate is applied to 2 qubits to swap their states
2. Rotation gate creates an interference pattern to generate Fourier states
3. Use Hadamard gate to create equal superposition of qubits

5 Numerical Example

This numerical example will solve a sample $A\vec{x} = \vec{b}$ problem for a real $\vec{x}$. We will put both CGM and HHL to the test, and see the results they yield.

$$A = \begin{pmatrix} 1 & -\frac{1}{3} \\ -\frac{1}{3} & 1 \end{pmatrix}, \vec{b} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \vec{u_0} = \begin{pmatrix} \frac{-1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}, \vec{u_1} = \begin{pmatrix} \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

Both HHL & CGM result in: $\vec{x} = \begin{pmatrix} \frac{3}{8} \\ \frac{9}{8} \end{pmatrix}$



Only the $\vec{b}$ register and ancilla qubit are measured, so there are 4 possible outputs. We only care about the $|1\rangle$ results, which are 01 and 11. The ratio between these 2, 0.063 : 0.564→ 1: 8.95, is close to the expected value of 1: 9.

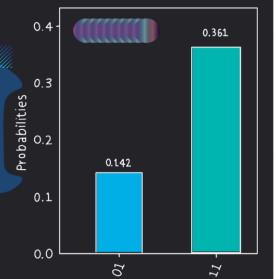
Abstract

In this poster, we present the classical and quantum complexity of linear solvers: we compare CGM and HHL asymptotic complexities (Big-O notation), and lightly explain the components of the HHL algorithm. The goal of this poster is to show how the HHL algorithm solves an LSP and its scaling.

6 Practicality

Current architectures do not support using HHL for large practical LSP, due to a lack of qubits, coherence problems and noise. HHL is well suited for fault-tolerant quantum computers.

Running HHL on quantum hardware yields 0.142 : 0.361→1 : 2.54, far from 1 : 9.



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3. Indranil G. (2021, July 29).“Conjugate Gradient Method
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Visuals by Anagha P
Elements by Sergey Bitos

Our Paper:

Created By: Anagha Padmasola, & Oneka Singh
Mentor: Andreea Lefterovici
Group 1B: Quantum Complexity (and the HHL algorithm)
Introduction to Quantum Research by ThinkingBeyond x Girls in Quantum

Introduction to Quantum Research for Girls 2024 — Gana Gangadharan, Gabriella Xenia Talarico - Mentor: Vanessa Dehn

Optimization problem for QAOA

Abstract: Combinatorial Optimization problems are often NP-hard and therefore hard to solve classically. To tackle this, the Quantum Approximate Optimization Algorithm (QAOA), a case of variational quantum eigensolver, was found, which gives approximate solutions to these problems. To implement the QAOA algorithm for Maxcut, we studied the general QUBO formulation and its similarity to the Ising model. We implemented the algorithm for a six-node Maxcut problem using Qiskit and obtained the expected solutions.

What is a QUBO problem?

QUBO stands for "Quadratic Unconstrained Binary Optimization", it is a mathematical framework which allows to reformulate many Combinatorial Optimization problems (CO), often NP hard, and is widely used in quantum computing. QUBO serves as input for algorithms like QAOA, which has the potential to solve these problems exponentially faster. [1]

Combinatorial optimization problem

Finding the "optimal" combination from set of all combinations

Eg: MaxCut problem

→ *Reformulating*

QUBO

Minimize/Maximize

$$y = x^t Q x$$

Vector of binary variables representing different combinations

Symmetric real-valued matrix

QUBO instance

What is MaxCut problem?

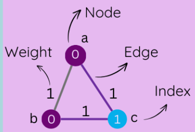


Fig 1: Example for a graph

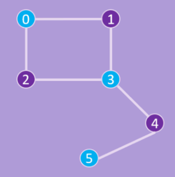
Problem: How to make a partition of nodes into two disjoint subsets (0 and 1), such that total weight of the edges between the two subsets (also called "cuts") is maximized.

Cost Function: $y = \sum_{i,j} w_{ij}[x_i(1-x_j)]$ $\quad w_{ij} = \begin{cases} 1, \text{ nodes i and j are connected} \\ 0, \text{ not connected} \end{cases}$

Cost Value(001) = $\underset{ab}{0(1-0)} + \underset{bc}{0(1-1)} + \underset{ca}{1(1-0)} + \underset{ac}{0(1-1)} + \underset{cb}{1(1-0)} + \underset{ba}{0(1-0)} = 2$

Results for the example problem

As we can see we get as first results either 100101 or 011010 which are equivalent in term of cuts (6 cuts) and so represent the optimal solutions to our example graph.



This is the configuration 011010: it has 6 cuts and it's one of the optimal solution.

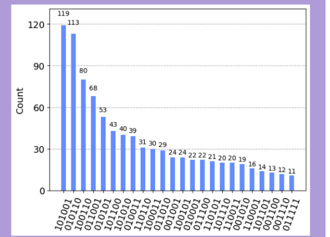


Fig 3: Results: Counts v/s bitstrings

Code & Solution

Correlation to physics

Hamiltonian $|\psi(t)\rangle = U(t)|\psi(0)\rangle = e^{-iHt\hbar}|\psi(0)\rangle$

- Operator which describes the total energy of a system
- Time evolution of the state of a quantum system can be expressed in terms of an hamiltonian acting on it.

Ising Model $H(\sigma) = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j - \mu \sum_j h_j \sigma_j \qquad \sigma \in -1, 1$

- Mathematical model in statistical mechanics to study magnetic dipole moments of atomic "spins".
- The QUBO formulation and Ising formulation are isomorphic. Solving QUBO is equivalent to finding the Ising groundstate: the ground-state configuration of a N-qubit Ising Hamiltonian.

Scan to read our implementation of the QAOA algorithm for MaxCut!

Scan to read our literature review for this project!

QAOA algorithm

QAOA is an algorithm introduced in 2014 [2] which finds approximate solutions for QUBO instances. By encoding the cost function as a Hamiltonian Hc, its ground state would correspond to the solution.

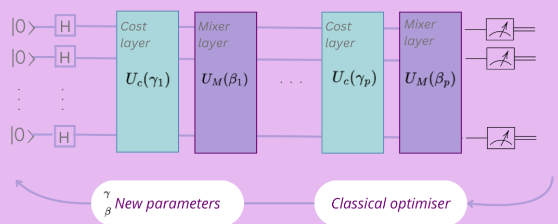


Fig 2:QAOA Circuit

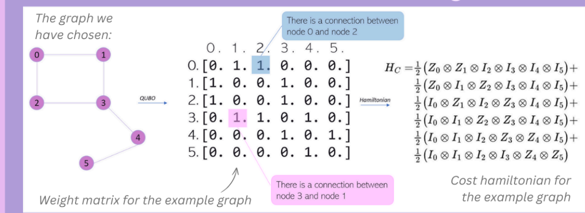
QAOA mimics adiabatic evolution from the ground state of H_M to the ground state of Hc.

Cost layer $U(H_c) = e^{-i\gamma H_c}$

Adiabatic quantum computation is a way to compute the ground state energy. QAOA ansatz is inspired by adiabatic theorem.

Mixer layer $U(H_M) = e^{-i\beta H_M}$

How to solve MaxCut with QAOA



From the QUBO formulation we can construct the Hamiltonian Hc of our instance problem, from it we construct the Cost Layer of the QAOA algorithm.

$$Z(x)|x\rangle = (-1)^x|x\rangle \implies \frac{I - Z_i}{2} = x_i|x\rangle$$

The cost hamiltonian is constructed by mapping the binary variables (0,1) to the eigenvalues of an operator which contains Pauli Z and Identity operator.

References:

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3. Qiskit textbook. "Solving combinatorial optimization problems using QAOA."

SPOTIFY MUSIC RECOMMENDATIONS BASED ON PERSONALITY TRAITS

Mentor: Prof. Dr. Gerhard Hellstern
Student: Iris Vavilov

CHECK OUR RESEARCH HERE:

1.PROBLEM

Even though **the first recommender system was centered on personality traits** and goals of the people (Grundy), most of the **modern ones do not correlate these things with the recommended content**, but rather create a hybrid ecosystem based on **Collaborative Filtering (CF) and Content Based Filtering (CBF)**. This seems a bit counterintuitive, but let's analyze the Netflix case. When Netflix firstly started, they would ask the users many questions related to their ethnicity, gender, movie preferences. They soon removed this feature because it was a burden for the users to complete the survey and the users were not the best at deciding what they like and what they don't. **However, we do know that incorporating personality traits of a user improves their recommendations by 3-28%.**[1]

2.SPOTIFY RECOMMENDER

Spotify uses a combination of CF and CBF when it comes to the recommender system. They get specific data about the user (their liked songs/playlists) and **they build a user "taste profile"**, which they use afterwards for their recommendations, after the CF/CBF was done. (Figure 1)

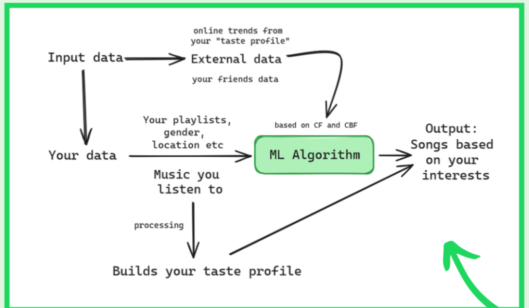


FIGURE 1: ESTIMATED SPOTIFY ARCHITECTURE

3.USERS OPINIONS

On data collected on **27 people about the recommender system of Spotify**, we concluded that the opinions on the recommender system are divided. **8** people said they would prefer **no music suggestions**, **8** said **the system is very efficient**, **6** said that **they would prefer more diversity** in the recommended songs. One study also classifies the Spotify algorithm as the **"least diverse."**[2] (see Table 1)

Table 1: Similarity Coefficients of Music Services

	Input playlists	Recommendation output					
		Spotify	Pandora	Apple	YouTube	Last.fm	Average
Low	0.510	0.681	0.606	0.448	0.446	0.427	0.522
Medium	0.289	0.538	0.282	0.313	0.239	0.236	0.322
High	0.084	0.217	0.195	0.101	0.092	0.266	0.174
Average		0.479	0.361	0.287	0.259	0.310	

4.CAN QUANTUM COMPUTING IMPROVE THE SYSTEM?

Some agree that quantum computers can outperform classical computers in recommendation tasks, due to their lower Big-O complexity (for matrix inversion the complexity for a classical computer is $O(N^2)$, while for a quantum computer $O(\log(N)^2)$ [3]

Others think QML can't outperform existing solutions. Quantum computers usually **struggle with the linearly separable benchmark**. A new study also suggests that **by removing the entanglement between the qubits the models gave better results.** [4]

We concluded that, since quantum machine learning can't outperform machine learning, and Spotify's issue with their algorithm is diversity, the **best approach** to improve the recommendation system of Spotify would be **to leverage the "true randomness" of quantum computers and combining it with the Spotify API.** However, we still tested a QNN to see how it performs.

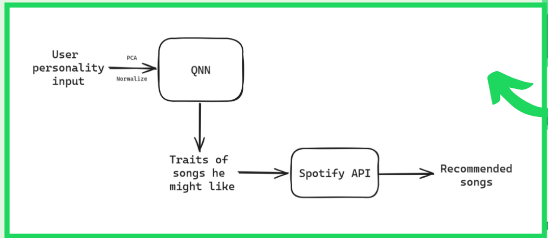
5.METHODOLOGY:

For this we trained our model on a dataset **(PER_dataset)** that connected certain characteristics obtained through the **Big Five personality test** (best test in the field of psychology) to respective song traits (liked by participants in the study with a song reviewing app called "Music Master") [5]

The algorithms were written using **Python** with the necessary modules installed. **(NumPy, Pandas, Scikit-Learn** for data processing, and also **Qiskit** and others for quantum algorithms)

First, **the dimensionality was reduced using a PCA** algorithm. Then we implemented a **quantum circuit (a variational ansatz and measurement) and encoded the classical data using angular encoding (we used Ry gates)**. We initialized the parameters, **built a prediction function that takes user personality input, normalizes and reduces it, then uses the QNN to predict the song features which the user might like. Then these features would be given to the Spotify API for song recommendations based on that.** (see Figure 2) In the end we tested our model by checking the mean square error.

FIGURE 2: ARCHITECTURE FOR OUR RECOMMENDER SYSTEM



6.CONCLUSION:

Although quantum computers promise to revolutionize the engineering world, in the "Spotify case" **we might not be able to see an advantage soon and most of the future recommendations systems would probably use machine learning ran on a classical computer rather than on a quantum computer.** However, quantum computing might give businesses in the music industry an advantage by leveraging the "true randomness" and **recommending "random songs" to users. However, personality of the user integrated in the app was proven effective.**

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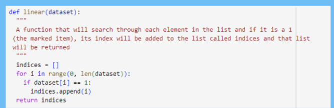
LINEAR SEARCH VS GROVER'S ALGORITHM

1 Time Complexity

Time complexity is a measure of the efficiency of a program. The asymptotic scaling (Big-O) is used to describe how the execution time varies with the size of the problem.

2 Linear Search

How it works:
The first item is checked
If it is equal to the required item, it is returned
If not, the next item in the list is checked
This process repeats until all items have been checked
This is why linear search has an asymptotic scaling (Big-O) of O(n) because as the size of the dataset increases, the time will increase in proportion to that given that in the worst-case scenario where the desired item is the last item in the dataset, every single item will have to be checked.

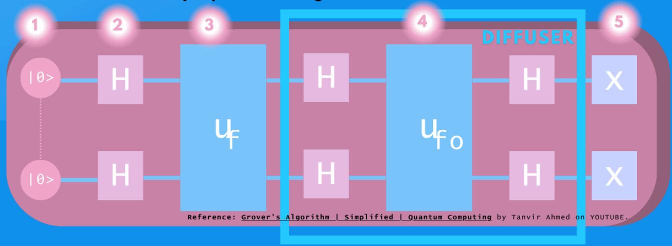


```
def linear(dataset):
  """
  A function that will search through each element in the list and if it is a 1
 (the marked item), its index will be added to the list called indices and that list
 will be returned
  """
  indices = []
  for i in range(0, len(dataset)):
    if dataset[i] == 1:
      indices.append(i)
  return indices
```

A screenshot of the code taken from the Google Colab we created

3 Grover's Algorithm

This is about searching an unsorted database of 2^n elements - this provides a quadratic speed up as Grover's Algorithm performs this by square rooting the number of evaluations.



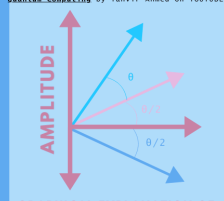
Below provides the difference between classical algorithms and Grover's algorithm when searching an unsorted database.

CLASSICAL:	GROVER:
N/2 = O(N) evaluations	O(√N) evaluations

Reference: Grover's Algorithm | Simplified | Quantum Computing by Tanvir Ahmed on YOUTUBE.

The aim is to increase the probability that the w will be measured.

Reference: Grover's Algorithm | Simplified | Quantum Computing by Tanvir Ahmed on YOUTUBE.



GRAPHICAL EXPLANATION OF GROVER'S ALGORITHM

How does Grover's Algorithm work?

1. The qubits are initialised to a zero state.
2. H-Gate is applied to the qubits creating uniform superposition & sets qubits with an equal amplitude.
3. Qubits are passed through the oracle (uf), this inverses ONLY the phase of "w".
4. The Diffuser performs an inversion operation, shifting "w" by 3/2θ. *The Diffuser performs "r" evaluations.*
5. *At the end, we measure the qubit & obtain our output which should be "w" (because "w" has a higher probability of being measured).*

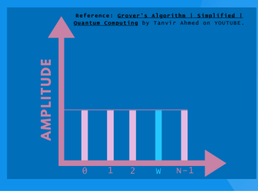
Reference: Grover's Algorithm | Simplified | Quantum Computing by Tanvir Ahmed on YOUTUBE.

EQUATION FOR APPLICATION OF THE H GATE:

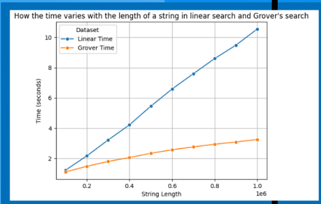
Reference: Grover's Algorithm | Simplified | Quantum Computing by Tanvir Ahmed on YOUTUBE.

$$H^{\otimes n}|0> = \frac{1}{\sqrt{2}}\Sigma_{x\in\{0,1\}^n}|x> = |S>$$

Reference: Grover's Algorithm | Simplified | Quantum Computing by Tanvir Ahmed on YOUTUBE.



AFTER H-GATE APPLIED TO QUBITS



4 How do they compare?

Scan our QR Code!

LINEAR

This is a classical algorithm which as a time complexity of O(n) in the average and worst-case

It works by sequentially checking each element and it is deterministic therefore given that the same dataset and input is given, the same output wil be given every time

Furthermore, it is simple to implement as it works on any classical computer however it is much less efficient for larger datasets

GROVER

It is a quantum algorithm which has a time complexity of O(√n) due to its quadratic speedup

It uses quantum superposition and amplifies the amplitude of the desired item

Moreover, it is probabilistic however the chance of returning the correct output does increase with every evaluation

It is difficult to implement as it requires quantum hardware

It is slower for smaller datasets but it has an exponential speedup for larger databases as evidenced by the graph

A screenshot of the code taken from the Google Colab we created

Advanced Carbon Footprint Forecasting based on Quantum RNNs

Aanya Amit | Fatema Asim

1 Carbon Forecasting CO_2

The issues of carbon emissions and global warming are intrinsically related in such a way that as society has progressed and developed, the environment has gradually downgraded and degenerated to a great extent. Since the Industrial Revolution, humans have emitted over

1.5 TRILLION METRIC TONS OF CARBON DIOXIDE

To properly deal with these issues, it is necessary to gauge an accurate estimate of the amount of carbon emissions in our environment. To do so, a number of Carbon Emission Prediction Models (CEPMs) have been developed, each with increasing accuracy and efficiency. This project intends to explore two such CEPMs and compare them, namely Recurrent Neural Networks and Quantum Recurrent Neural Networks.

2 Methodology </>

This project utilizes Google Colab as the environment to run its code. Both models were trained and tested using data pertaining to carbon emissions from 1958 to 2023 which was obtained from Scripps Institute of Oceonography's CO2 programme (initiated in 1956). The data was split into two parts, with the data for 1958 to 2010 being used to train the models, and the data from 2011 to 2023 being used to test the models. The graph comparing both models' tests is given here. Tensorflow was used as the primary language to develop the Recurrent Neural Network, while the Quantum Recurrent Neural Network was developed using a Pennylane integration into Tensorflow.

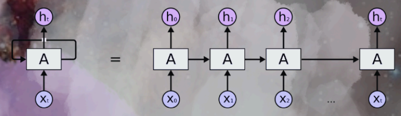
- Input
- LSTM Layer
- LSTM Layer
- LSTM Layer
- Dense Layer
- Output

3 Recurrent Neural Networks

Recurrent Neural Networks (RNNs) are a type of artificial neural network designed to recognize patterns in sequences of data, such as time series. RNNs work by maintaining a hidden state that captures information about previous inputs in the sequence. This hidden state is updated at each time step, allowing the network to retain memory of previous inputs while processing new ones. This feature makes RNNs ideal for tasks like time series prediction, sequential learning, natural language processing, and more. In this project, we implemented a more advanced form of RNN known as a Long Short-Term Memory (LSTM) network. LSTMs are capable of learning long-term dependencies, which is essential for accurate time series forecasting. They help solve the vanishing gradient problem by capturing and saving these dependencies with the help of gates.

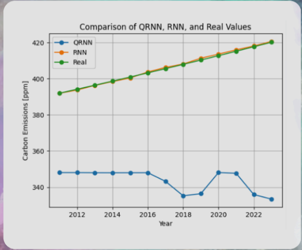
This model begins working when an input is provided to it. Three LSTM layers follow this, which capture dependencies and identify patterns in the data. The final dense layer unifies all the data to a singular output which is provided to us.

For this project, we utilize the Root Mean Square Error (RMSE) metric to judge the accuracy of both models. As seen here, the RNN performs extraordinarily by attaining an RMSE of just 0.07.



6 Further Steps

It is true that, at the moment, the QRNN is being outperformed by the Classical RNN. However, numerous papers and research articles lead us to believe that this outperformance is only due to the lack of research in the field and the presence of noise in quantum hardware. It can be said that, with due advancement and research in the given field, improved quantum hardware, and development of more efficient quantum algorithms, there is a very good chance that QRNNs will provide even much accurate results than their classical counterparts. However, to conclude for this project, currently with the limited available resources, RNNs are more efficient and more accurate than QRNNs for use in CEPMs.



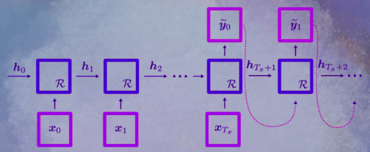
RMSEs	RNN	QRNN
	00.07	60.01

5 Quantum Recurrent Neural Networks

Quantum Recurrent Neural Networks (QRNNs) are similar models to Classical RNNs, but they integrate quantum computing principles to enhance their predictive accuracy. In this project, we developed a hybrid model consisting of a quantum layer and two LSTM layers followed by a dense layer, leveraging the advantages of both types of layers.

First of all, the input is given to the network. The quantum layer encodes the input data into qubits and entangles them so that they become correlated. The next stage of this layer estimates the values of the qubits when Pauli-Z operators are applied to them. Next, the LSTM layers sift through the data and identify dependencies and correlations in it. After learning the trend, the final dense layer combines and unifies all the information that the network has gathered into a single output which is then provided to us.

The QRNN is seen to perform drastically below how the Classical RNN performs. Although the Classical RNN has an RMSE of only about 0.07, its quantum counterpart has one of over 60. The reason for this is the high noise level in current quantum hardware, along with underdeveloped quantum algorithms. With advancement and progress in both of these sectors, a huge improvement can be expected in these results.



- Input
- Quantum Layer
- LSTM Layer
- LSTM Layer
- Dense Layer
- Output

4 Quantum Computing

While the RNN performs tremendously well in these circumstances, this is not always the case. Even with the improved LSTM Network, there are issues of computational complexity, gradient issues and memory limitations. Additionally, even though the LSTM Network is a huge step from Classical RNNs in terms of capturing long-term dependencies, its functionality is still quite limited. A step forward is the implementation of quantum computing concepts into this network. By implementing the principle of superposition, the computer can explore a large number of possibilities at the same time, and the principle of entanglement plays a role in identifying dependencies and correlations. In general, quantum computing concepts can assist the network in being more efficient and making more accurate predictions.

Scan for supplementary material and references!

IQRG PROGRAMME

Introduction to Quantum Research for Girls
2024, Inaugural Cohort

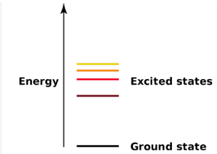


Fig 1: Energy States in an Atom (Wikipedia)

Using VQE and QPE for Chemical Problems

Maitreyi Muralidhar & Verity Greenald

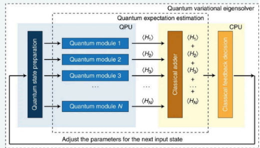


Fig 2: Quantum VQE (Liu et al., 2014)

Classical computers are inefficient in simulating quantum systems such as the atomic structures studied in chemistry. However, using quantum hardware to simulate quantum systems gives good results, for example in finding the ***Ground State Energy of molecules (GSE).*** *We used the* ***Variational Quantum Eigensolver(VQE) and Quantum Phase Estimation (QPE)*** *in finding the* ***GSE*** *of simple molecules.*

The Principles of VQE:

The VQE finds the lowest eigenvalue of a given Hamiltonian of a chemical system. It is based on the Variational Principle:

eigenvalue ← $\lambda_{min} \leq \langle H \rangle_{\psi}$ → expectation value

Eq 1: Variational Principle

The VQE is a hybrid algorithm making it suitable for the NISQ era.

- **Quantum** part is involved in finding the minimum eigenvalue for the matrix.
- **Classical** part optimizes the variational parameters.

By modelling a molecule's **Hamiltonian** for a Hermitian Matrix and making good **ansatzes** for the trial wavefunctions, the algorithm can find the **minimum eigenvalue** at various interatomic **distances** equivalent to the molecule's **ground state energy.**

The Principles of QPE:

The QPE finds the eigenvalue of the eigenvector given the matrix. We can express this as:

$$U|v\rangle = e^{i\theta}|v\rangle$$

matrix (U), eigenvector ($|v\rangle$), eigenvalue ($e^{i\theta}$)

Eq 2: Representation of QPE

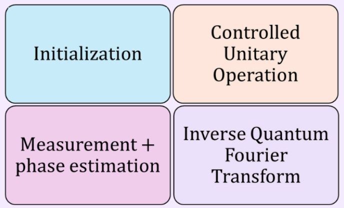


Fig 3: Structure of QPE

Other key uses of QPE include:

- Shor's algorithm
- Quantum simulations
- linear systems of equations algorithms

Code Architecture:

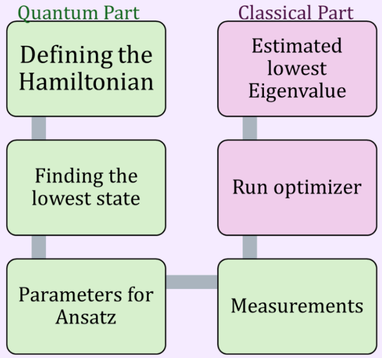


Fig 4: Structure of VQE

VQE

- **Parity Mapper**
- **Pauli Strings** to represent the Hamiltonian
- Ansatz used is **UCCSD**
- True Simulator **AerSimulator**

QPE

1. Create the **molecule** (LiH)
2. Create **hamiltonian** and **restrict it within range** $[0, 1-(\frac{1}{2})^n]$ n = number of ancillary qubits
3. Construct **QPE circuit** using this hamiltonian, run and analyze results of energy and distances

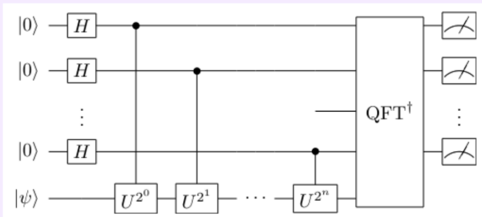


Fig 5: QPE Circuit (LaRose)

Findings:

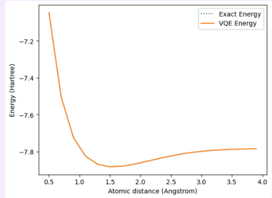


Fig 6 : Energy at various interatomic distances

VQE	QPE
Circuit depth @ interatomic distances = **26**	Circuit depth @ interatomic distances = **43**
Depth depends on **ansatz** and **molecule**	Deep circuits due to **QFT** and **CUT**
Works well with **NISQ** devices because of **hybrid nature**	Needs **Fault tolerant** Quantum Computers
Accuracy depends on **ansatz quality** and **optimization**	More **qubits** leads to more precise GSE approximation

Further exploration:

During the course of our research we encountered obstacles particularly with the code for QPE due to a limited time frame:

- *Import libraries in Qiskit-updated version meant we struggled to fix the code*
- *Diagram inconsistencies for QPE*

To solve these issues we want to now ***build a QPE circuit*** *fully in order to be able to verify our data and get* ***more accurate results****. We are going to take this another step further.*

Bibliography:

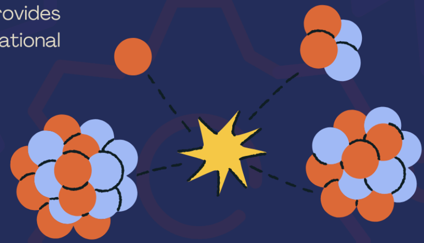
Thanks to the entire **ThinkingBeyond + Girls in quantum** team, **Dr. Filip Bar** and our mentor **Ms. Victoria Hazoglou** for guiding us through the research process!

Scan to view our sources

Alessandra Jablonowska, Luana Kopke
Mentor: Ms. Victoria Hazoglou

USING VQE FOR OPTIMISING CHEMICAL PROBLEMS

Classical computers are inefficient in parametrising quantum systems. Using **quantum hardware** to simulate quantum systems provides **promising results**, particularly in finding the **Ground State Energy** (GSE) of molecules. This poster explores the application of the Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE) in determining the GSE of simple molecules.



1.Abstract

This study focuses on optimally using VQE algorithms to find the GSE of molecules. We focused on the hybrid quantum-classical algorithm, because it is well-suited for the current Noisy Intermediate-Scale Quantum (NISQ) era, while QPE requires more advanced, fault-tolerant quantum computers. We aim to find the most reliable and efficient way of calculating GSE to date.

2.Questions and methodologies

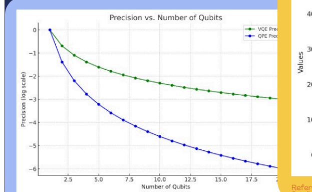
What is the most efficient VQE algorithm to calculate GSE of simple molecules?

How can the accuracy and efficiency of VQE algorithms be improved?

VQE vs **QPE**

- Variational Quantum Eigensolver (VQE)
  - Principle: Based on the Variational Principle, VQE seeks to find the lowest eigenvalue of a Hamiltonian.
  - Hybrid Approach: Combines quantum and classical computations.
  - Quantum Part: Involves constructing and evaluating the trial wavefunction.
  - Classical Part: Optimizes the variational parameters to minimize the energy expectation value.
  - Circuit Depth: Dependent on the ansatz and molecule; typically manageable for NISQ devices.

- Quantum Phase Estimation (QPE)
  - Principle: Uses quantum algorithms to estimate the phase, which is related to the eigenvalue of a unitary operator.
  - Requirements: Requires deep quantum circuits due to Quantum Fourier Transform (QFT) and Controlled Unitaries (CUTs).
  - Precision: More qubits lead to a more precise approximation of the GSE.



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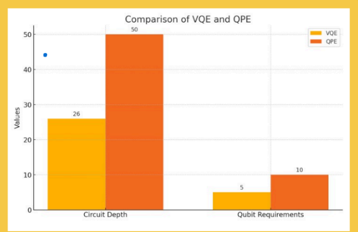
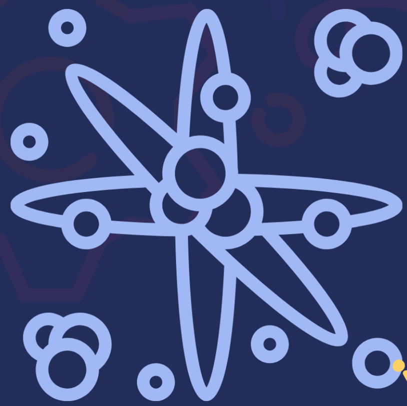


References: [1] Kandala, Abhinav, et al. "Hardware-efficient Variational Quantum Eigensolver for Small Molecules and Quantum Magnets." Nature, vol. 549, no. 7671, 2017, pp. 242-246.



3.Research, code and findings

VQE is a family of algorithms. They can be differenciated by two parameters: the **ansatz** and **basis** used in estimations.
We simulated VQE using different ansatzes and bases to **find the most optimal combinations** - ultimately, to streamline the computational process.
We compared the effects of four algorithms and five basis sets on 4 molecules: **LiH, He, H and Be**. We focused on these molecules because of the ease of calculations and their applicability in the field of fusion energy and engineering.
Our findings are behind the QR code.

More

ansatz **PauliTwoDesign**

basis **"3-21g"**

4.Applications and benefits

- Molecular Energy Calculations
- Finding the GSE of molecules to understand **chemical properties** and reactions.
- Potential applications in drug discovery and material science.
- Optimization Problems
- Application of quantum algorithms to solve **complex optimization problems in chemistry**.
- Quantum Chemistry Research
- Advancement in quantum algorithms to improve the accuracy and efficiency of chemical simulations.
- Use of VQE and QPE as **teaching tools** to illustrate quantum computing concepts in chemistry.

better batteries

cleaner energy

efficient screens

reliable drugs

A programme led by ThinkingBeyond
in collaboration with Girls in quantum

Application of QML to Identify Malicious Login Attempts Based on BETH Dataset

Basmala Sallam - Menna Zaied
Mentor: Jannes Stubbemann

Abstract

In our Project, we're trying to answer the question "How to identify malicious login attempts?", so we focused on using Variational Quantum Circuits (VQC) to identify the malicious login attempts based on BETH dataset, which provides data on successful and failed login attempts, including 14 features such as User ID, Process ID, and Event ID, and includes 2 labels which are Sus, and Evil. We trained the model to detect malicious login attempts and found the correlation between features and labels.
If the features have low-cost values, they have a high correlation with the labels and vice-versa. Features such as User ID and Event ID have a high correlation with the labels, while features such as Uservalue have a low correlation with the labels.

Why VQC?

VQC can be applied to compress and represent high-dimensional data, such as network traffic or system logs in a more compact and meaningful way. This can facilitate the identification of patterns, anomalies, and trends that may indicate potential security threats. They also offer several advantages over classical machine learning algorithms and some quantum algorithms such as Improved Performance, ability to Learn Complex Relationships, improved accuracy, flexibility, robustness to noise, and interpretability.
In the following table, we will compare a classical algorithm (SVM) with a quantum algorithm (VQC)

Comparison

	SVM	VQC
Accuracy	91.2%	93.5%
training time	10.2s	59s
Non-linear classification	limited to kernel	perform it efficiently
feature space	only 10 dimensions	high-dimensional

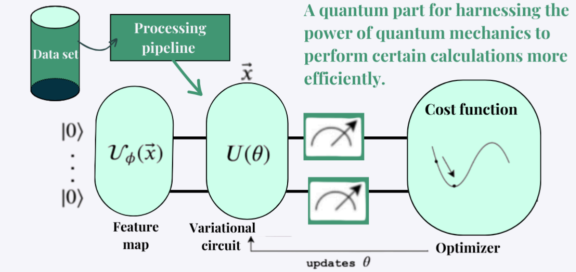
What is VQC?

Variational Quantum Classifiers (VQCs) are a type of hybrid quantum machine learning algorithm that can be used to solve a wide variety of classification problems.

It consists of two parts :

A classical part for pre- and post-processing data

A quantum part for harnessing the power of quantum mechanics to perform certain calculations more efficiently.

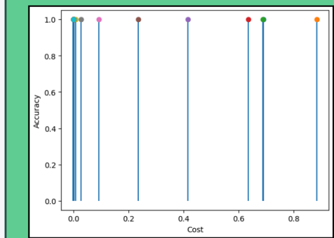


There are some steps to follow to have our output Y:

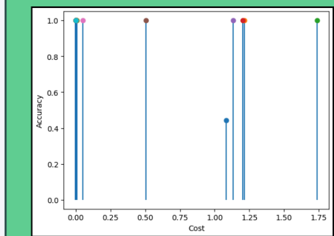
1- Encode Classical Data into a Quantum State
2- Apply a Parameterized Model
3- Measure the Circuit to Extract Labels
4- Optimize Model Parameters

Results

In the code you can see that we cleaned the data before working on it, and after that we trained the model using VQC and it showed different cost results when applied to different features, but in general the accuracy was 1.00.



Plotting of the correlation between Return value, User ID, and labels, which shows high correlation



Plotting of the correlation between Return value, Process ID, and labels, which shows high correlation

The code on GitHub

Future applications

QML can analyze complex data patterns, which makes it ideal for spotting hidden threats in network traffic and user behavior. Future advancements in quantum hardware and QML algorithms and addressing problems such as error correction, noise reduction, and efficient implementation will unlock its full potential for building next-generation cyber security systems

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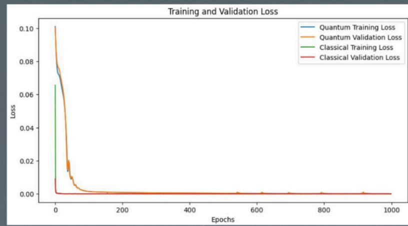
2- Highnam, K., Arulkumaran, K., Hanif, Z., & R. Jennings, N. (2021). BETH Dataset: Real Cybersecurity Data for Anomaly Detection Research.

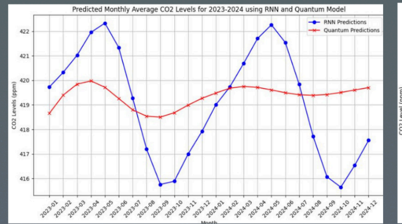
CARBON FOOTPRINT FORECASTING BASED ON QUANTUM RNN

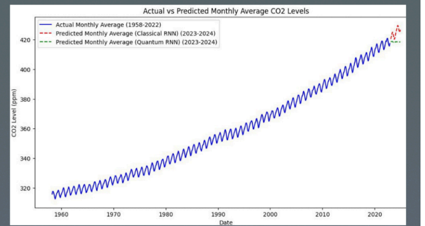
BY AFREEN HOSSAIN AND FARHEEN

Why is Carbon Footprint Forecasting Important ?

- **Fight Climate Change:** Helps us see future pollution levels and take action to reduce them
- **Better Plans and Policies:** Helps governments and businesses create good rules and improve how they work to be more eco-friendly
- **Manage Risks and Innovate:** Helps find financial risks and encourages new, green technologies







METHODOLOGY

Data

Feature Engineering
We selected year, month, average as the relevant features among others giving more emphasis on average

Data Processing
Handling missing values and normalization using MinMaxScaler

Classical RNN Model

Architecture
SimpleRNN with 50 hidden units and a dense output layer

Evaluation
Test loss evaluation and predictions for the next 24 months

Preprocessing
Handling missing values, normalization, and sequence creation

Training
80-20 train-test split, trained for 50 epochs using Adam optimizer and mse loss function

Quantum RNN Model

Model Architecture
Hybrid model combining classical RNN with quantum layer

Training
1000 epochs using Adam optimizer

Preprocessing
Similar to the classical RNN

Quantum Circuit
Angle embedding and basic entangler layers

Evaluation
Validation and test loss evaluation, predictions for the next 24 months

ABSTRACT

Carbon footprint forecasting is essential for climate change mitigation. This study compares traditional Recurrent Neural Networks (RNN) and Quantum Recurrent Neural Networks (QRNN) in predicting atmospheric CO2 levels. The models were trained on historical CO2 data from 1958 to 2022 of California region

DISCUSSION AND RESULT

We have confidence in our RNN model due to its accurate prediction capabilities. Our RNN outperforms others and delivers more precise results. We have fine-tuned our RNN model, with the most suitable optimization and loss functions to adjust weights effectively.

However, Quantum RNNs (QRNNs) have seen less research compared to RNNs. Despite this, we have made every effort to incorporate all available training methodologies.

We are exploring potential enhancements such as integrating quantum layers more effectively and improving the optimization functions to further enhance our model's performance.

FUTURE RESEARCH

- How can the optimization strategies for hybrid models combining classical RNNs and quantum layers be further refined to improve convergence speed and model accuracy?
- What are the optimal circuit architectures and layer configurations within quantum layers that enhance predictive power and resilience to noise?

SCAN FOR REFERENCES

SCAN FOR CODE AND CONTACT INFO.

Quantum Computing Concepts with Qubit Manipulation

Mentor: Ms Sanskriti Oza
Student: Joy Lee, Farah Amr

1 INTRODUCTION

Qubit is a (basic unit of quantum information) it is like a magical bit that can hold both 0 and 1 at the same time, but in a special way, it's more like a quick switch between 0 and 1 that can't be directly observed until measured. In classical computers, logic gates simply flip bits between 0 and 1, like flipping a switch. But quantum gates use the magic of qubits; like superposition (holding both 0 and 1 simultaneously) and entanglement (where one qubit's state depends on another's), These unique properties allow qubits to perform much more complex operations, giving quantum computing its edge over classical bits.

2

To understand and visualize how quantum gates work, we use several tools:
A Bloch sphere is a 3D sphere that shows the state of a qubit. Think of it as a globe where the poles represent the classical states 0 and 1, and any point on the sphere represents a possible qubit state. (see: figure 1)
Matrix Representations as shown in (figure 2). Quantum gates can be described using matrices (arrays of numbers). These matrices show how the gate changes the state of a qubit.
Furthermore, we can use circuit diagrams (see: figure 3). These diagrams show how multiple quantum gates are connected and interact with qubits, similar to how electrical circuits are drawn for classical computers.

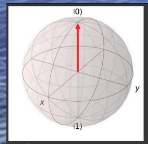


figure 1

figure 2

$$x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

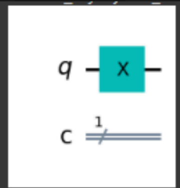


figure 3

3

Using the Bloch Sphere to Show Quantum Gates:
The Bloch sphere is a way to see the state of a qubit in a 3D by seeing where the arrow is pointing
Hence here in (figure 4), we can figure out that the Initial State is $|0\rangle$.
When Applying the X Gate
The X gate flips the qubit's state from $|0\rangle$ to $|1\rangle$ hence the arrow will be pointing at (south pole)as shown in (figure 5).
That is why The Bloch sphere helps us visualize how quantum gates like the X gate manipulate qubit states.

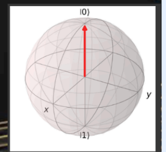


figure 5

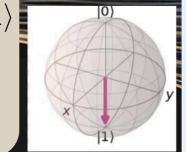


figure 6

4

Quantum logic gates are essentially the building blocks of circuits. These are unitary operators, represented by unitary matrices. To make qubits useful, we need to perform a series of operations which are the quantum logic gates. There are two types of gates: single-qubit gates and mutiple-qubit gates. In this presentation, we focus on the very basics: X-gate, H-gate, Y-gate, Z-gate, CNOT-gate.

WHY DO WE USE QUANTUM LOGIC GATES

Firstly, we use quantum logic gates for complex operations; quantum gates do complicated tasks that classical computer parts can't do. They use quantum mechanics: superposition and entanglement. Secondly, quantum superposition: quantum gates (for example, H-gate) can make qubits exist in many states at once. This means they can do many calculations at the same time, making things faster. Thirdly, quantum entanglement, quantum gates can link qubits together. When qubits are linked, knowing the state of one tells you about the other. This can make computations more efficient. Fourthly, parallel processing, with superposition and entanglement, quantum computers can check many possible solutions at the same time, speeding up problem-solving. Fifthly, building quantum circuits, quantum gates are the building blocks for quantum circuits. By combining them, we can make powerful quantum algorithms. Finally, running quantum algorithms, quantum gates run special algorithms like Shor's for breaking large numbers and Grover's for searching data. These can do things much faster than regular computers, which is very useful for security and data.

SEE THE APPLICATION OF OUR RESEARCH

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Universal Quantum, Quantum gates explained (without the maths), Medium
ThinkingBeyond, GirlsInQuantum, Preparation for the Quantum Computing course - Week 1
figure 1:
ThinkingBeyond, GirlsInQuantum, Preparation for the Quantum Computing course - Week 2
figure 2:
Wikipedia, Quantum Logic Gate
figure 3:
ThinkingBeyond, GirlsInQuantum, Preparation for the Quantum Computing course - Week 2
figure 4:
ThinkingBeyond, GirlsInQuantum, Preparation for the Quantum Computing course - Week 2
figure 5:
Deep Learning University, Qiskit: Bloch Sphere

To code quantum circuits: the free resource, google.colab, is a great way to organise your python coding and is great at showing steps in digestible ways. To use google.colab, you need to understand the essential Python code to download other tools such as Qiskit, which is an open-sourced software development kit used to program quantum computing. However, Qiskit is not the only software you can use, Pennylane, for example, is a cross-platform Python library used to program quantum computing. To use Pennylane, you must have Jupyter Notebooks installed alongside Pennylane, then using the required code, import Pennylane onto Jupyter Notebooks. For Qiskit, you must first install the software using the required Python code to do so.

QR code 1

QR code 2

5

To Apply and code quantum computing concepts, we use platforms such as: Qiskit in Google Colab (QR code 1), IBM Quantum Experience (QR code 2) (Scan the QR codes to access these platforms directly)
These platforms provide tools and resources for running quantum computing experiments and simulations, empowering researchers to explore the potential of quantum computing in solving real-world problems.

SECTION A: QKD PROTOCOL AND ITS IMAPCT

QUANTUM PRINCIPLES

Heisenberg's Uncertainty Principle: Once an eavesdropper measures a quantum state, the quantum state's properties will be affected.

Entanglement: Entanglement is a quantum phenomenon that connects two particles not considering the distance. Any change in one particle directly affects the other particle.

No-Cloning Theorem: This prevents the eavesdropper from being able to replicate the exact quantum state that was sent by Alice

QUANTUM KEY DISTRIBUTION PROTOCOLS

Quantum Key Distribution (QKD) addresses the vulnerability to interception by detecting eavesdropping. There are two kinds of QKD protocols. The prepare and measure QKD protocol uses Heisenberg's uncertainty principle . This protocol depends on the fact that once Eve intercepts and measures the photons, the quantum state will be altered. The second QKD protocol depends on entanglement where an entangled photon is each sent to Alice and Bob . Any changes to one photon will instantaneously affect the other photon.
Quantum Key Distribution can help us to trasmit the key between two users in a secure manner so that no one can intercept it and by extension eavesdrop into the conversation.

SOCIETAL IMPACT

Adopting quantum cryptography can have a lasting impact on our society. For example , banking transactions that rely on classical cryptography can be more susceptible to attacks. Also, in social media accounts, QKD can be used to secure sensitive data and even detect if there is an eavesdropper. Most importantly, the healthcare sector also stores private patient data which on being intercepted can also threaten the lives of these patients.

INTRODUCTION

Classical cryptography relies on mathematical complexity and time consumption to deter decryption. Though in any kind of cryptography method, the key exchange process is vulnerable to interception. Quantum Key Distribution (QKD) detects this eavesdropping (interception), without relying on complex math or long-time requirements to facilitate secure communication.

QUANTUM CRYPTOGRAPHY

BY TRISHA CLARA AND AGNESE FORASTIERI

GLOSSARY

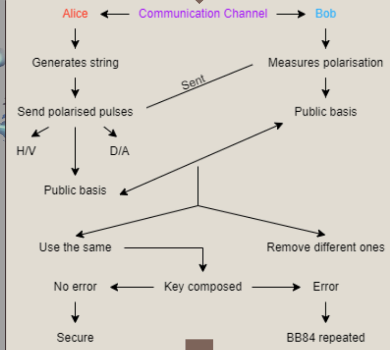
ALICE: sender
BOB: receiver
EVE: eavesdropper

SECTION B: EAVESDROPPING AND BB84 PROTOCOL

BB84 PROTOCOL

BB84 was developed by Bennett and Brassard in 1984 and it was the first quantum key distribution protocol ever designed. It is based on the no-cloning theorem and on the fact that the state is altered when measured. It is provably secure given that information can only be gained by disturbing the signal applied when the two states being distinguished are non-orthogonal, by the no-cloning theorem and the existence of an authenticated public classical channel. Many QKD protocols are based on the BB84. In BB84, Alice prepares quantum states (photons) in one of two bases chosen. Bob randomly chooses a measurement basis to decode the information. If Eve measure this these transmitted photons she cannot replicate the exact ones sent due to the uncertainty principle.

PROCESS



EAVESDROPPING ANALSYSIS

Eavesdropping is a form of cyberattack wherein someone secretly intercepts or modifies the data without awareness of the parts. In BB84 Eve measures the qubits when they are in transmission from Alice to Bob, basically measuring them. This measurement can change the quantum system. By comparing the basis of Alice and Bob we can find if there was an eavesdropper in the conversation by using quantum error detection.

Discover more: code of BB84 protocol and report

SOURCES

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- Fundamentals of Quantum Key Distribution: https://medium.com/@qcgiitr/fundamentals-of-quantum-key-distribution-bb84-b92-e91-protocols-e1373b683ead

Understanding Quantum Teleportation

Prayanshi Garg, Parthavi Chauhan

Mentor:
Ms Juweria Sayed

Introduction

Quantum teleportation is the transfer of an unknown quantum state over long distances without actual physical transfer. This process works on the principles of entanglement. In this research project, we will review the quantum teleportation protocol, applications in secure communication, cryptography and quantum network. Along with this we also employed the quantum flytrap game to visualize the results.

Quantum Protocol [1]

Quantum Teleportation can be implemented by the following process: Generating an entangled pair of electrons with spin states A and B, in a particular Bell state. Measuring bell state of A and C(to be sent). Sending the measurement by classical method of communication. Measuring the spin of state B along an axis as determined by the previous measurement.

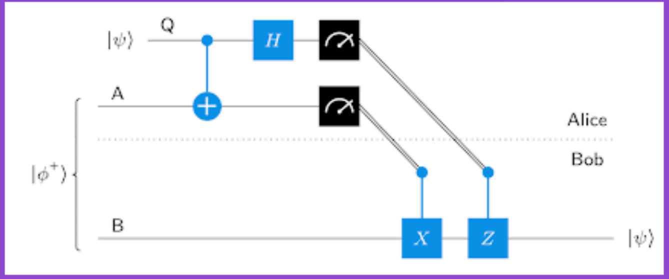


Fig. 1: Quantum Teleportation circuit

Applications

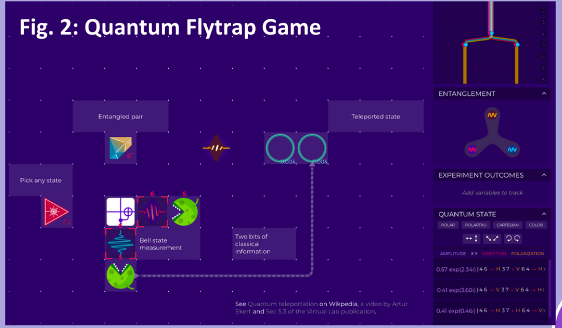
Secure Communication

Quantum Teleportation provides unbreakable encryption and is immune to classical computational attacks. It can detect eavesdropping as interception disturbs entangled particles and triggers alerts. Quantum Key Distribution (QKD): Secure Key Creation: Establishes cryptographic keys via quantum entanglement. Quantum secure communication protocols, such as BB84 and B92, utilize the principles of quantum mechanics to establish secure and unbreakable communication channels.

Quantum Networks and Cybersecurity

As quantum computing threatens traditional cryptographic systems, post-quantum cryptography (PQC) offers a robust solution. PQC uses algorithms resistant to quantum attacks for secure authentication, digital signatures, and encryption. Integrating quantum networks with PQC ensures data integrity and confidentiality, safeguarding against future quantum threats and advancing cybersecurity.

Fig. 2: Quantum Flytrap Game



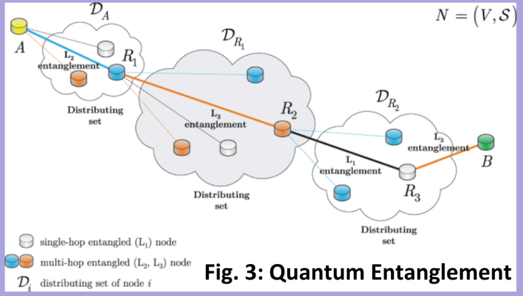


Fig. 3: Quantum Entanglement

Conclusion

Quantum Teleportation has immense potential to significantly advance quantum communication and computing. The essential elements include quantum entanglement, the initialisation of the state to be teleported, and a classical communication channel.

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5. Andy Matuschak and Michael A. Nielsen, "How Quantum Teleportation Works", https://quantum.country/teleportation, San Francisco (2019)

SPOTIFY MUSIC RECOMMENDATION SYSTEM USING QUANTUM MACHINE LEARNING

Research Student: Roshani Vijayan
Mentor : Dr. Gerhard Hellstern, Professor, Duale Hochschule Baden-Württemberg, Germany

ACKNOWLEDGEMENT

I would like to thank my mentors Dr. Gerhard Hellstern and Dr. Filip Bar for all their help on this project. I would also like to thank all team members and students of PhysicsBeyond (ThinkingBeyond) and Girls in Quantum for their unwavering support.

GITHUB LINK

01. INTRODUCTION

Spotify, the world's largest on-demand music service, is best known for its user experience, music recommendation that is constantly getting improved.

02. OBJECTIVE

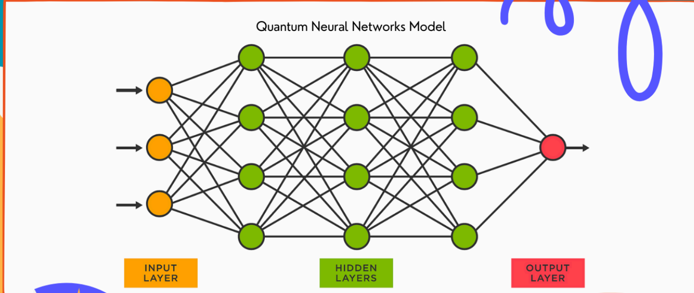
This project aims to apply Quantum Machine Learning (QML) techniques to predict Spotify user preferences. Leveraging quantum computing can potentially enhance the efficiency and accuracy of machine learning models in handling large and complex Spotify music and users datasets.

03. DATASET

Dataset : In this project, a dataset comprising 1200 songs mapped to users' personal traits was utilized. The file includes features of Spotify tracks along with corresponding labels that indicate user preferences

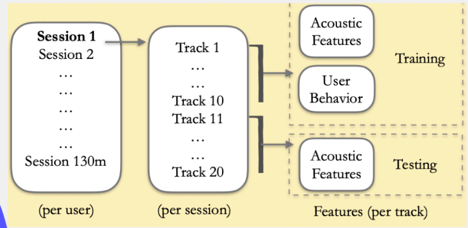
04. PRE-PROCESSING

Data Preparation : Features from the dataset are standardized and reduced in dimensionality using PCA. The features are scaled to fit the range (-π, π) for compatibility with quantum circuits.



05. QUANTUM ML ALGORITHMS

The code uses a hybrid quantum-classical machine learning approach, specifically leveraging quantum circuits within a neural network framework. This involves the following components:
Quantum Circuits: Each data sample is encoded into a quantum circuit.
Parameterized Quantum Circuits (PQCs): These circuits have trainable parameters that can be optimized during the training process.
Quantum Layers in TensorFlow Quantum: The quantum circuits are integrated into a TensorFlow Keras model using TensorFlow Quantum, which allows quantum circuits to be used as layers in a neural network.



06. PROCESS BREAKDOWN

Quantum Circuit Encoding: Each song's features are converted into a quantum circuit, where each feature controls the rotation of a qubit.

Quantum Model Training: The encoded circuits are fed into a Parametric Quantum Circuit (PQC) integrated within a neural network framework. Through training with labeled data, the model acquires the ability to differentiate between songs suitable for recommendation and those that are not.

Prediction: The same preprocessing and encoding procedures are applied to new or test songs. Subsequently, the trained quantum model predicts the recommendation score for each song based on its learned parameters.

Recommendation: The predicted scores undergo analysis. Songs receiving high positive scores are deemed strong recommendations, which can then be suggested to the user based on their preferences and listening history.

07. RESULTS/CONCLUSION

The prediction model outputs a range of values for each input data point, spanning from negative to positive. These continuous values in the output array represent the model's recommendations for the test data:

- **Positive Values:** Values approaching 1 suggest strong recommendations.
- **Negative Values:** Values nearer to -1 imply weak or no recommendation.

To provide actionable recommendations, the model can filter predictions using a threshold (e.g., considering only predictions above 0.8 as strong recommendations).

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Introduction to Quantum Research for Girls (IQRG 2024)

ThinkingBeyond • Girls in Quantum

UNDERSTANDING QUANTUM TELEPORTATION

Mentor: Mr. Mohammed Alabdullah
Members: Natália Lopes da Silva
Juliana Valencia Lozano

1 INTRODUCTION

This research poster explores Quantum Teleportation (QT), its applications, and its secure implementation.

Quantum Teleportation, a process in which a quantum state is transferred from one location to another without traveling through the intervening space, relies on two fundamental phenomena: Quantum Entanglement and Bell State Measurement.

- Quantum entanglement occurs when two or more quantum particles become interconnected, and the measurement of one particle's properties instantly affects the other (if one particle has spin 'up', the other instantly has spin 'down').
- Bell States are quantum states where two particles are maximally entangled. They are created by applying the Hadamard (H) gate and the CNOT gate, resulting in exactly four distinct Bell States.

$$|\Phi^+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \qquad |\Psi^+\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}$$

$$|\Phi^-\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}} \qquad |\Psi^-\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}$$

2 E91 PROTOCOL

In the E91 protocol for security in quantum communication, multiple entangled particles are generated at a source and then distributed to Alice and Bob. Both of them measure the spin of their particles in three different directions (Alice in directions 0, π/8, π/4, and Bob in directions −π/8, 0, π/8). Then, they communicate the measurement bases used for the qubits and categorize the results into two groups, A and B:

- Group A (the states do not match) - a Bell Inequality Test is performed to detect any interception.
- Group B (the states do match) - the data is used to build a secure key by encoding the qubits (0 for down and 1 for up).

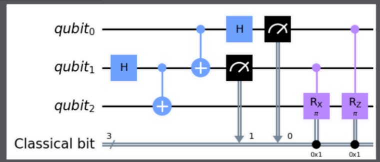
If no interception is found in the group A data, then the data from group B is used to create a secure key. If interception is detected, the protocol is repeated.

3 QUANTUM NETWORK

In 2016, China achieved quantum teleportation by connecting two laboratories located 30 kilometers apart using optical fibers. Scientists created pairs of entangled photons in laboratory A and successfully transmitted them through the optical fibers to laboratory B.

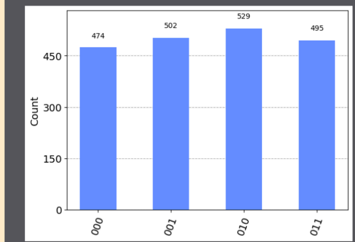
This demonstrated the security of quantum teleportation for communication over long distances, which is crucial for the development of quantum internet networks, promising the advancement in secure information.

4 MODELING QT



- Alice is the sender and her qubits are qubits 0 and 1.
- Qubit 0 is the qubit state that will be teleported.
- Bob is the receiver and his qubit is qubit 2.
- Qubits 1 and 2 (one from Alice and the other from Bob) are entangled by H and CNOT gates.
- Qubit 0 (state to teleport) and 1 are entangled by CNOT and H gates (identity).
- Alice measures qubits 0 and 1, and sends the results to Bob (owner of qubit 2).
- Based on the measurement results from Alice, Bob applies the unitary transformation (X and Z gates).
- If the measurement result is 00, no additional operation is needed.

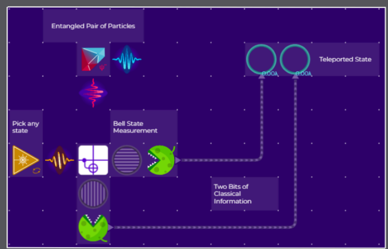
5 GRAPHICAL RESULTS



In the final measurement of quantum teleportation, there are only four possible states (Bell States). Each of these states should have a 25% probability of occurring.

Nevertheless, errors can occur and affect the accuracy of real-life communication due to factors such as hardware limitations and the challenges of maintaining coherence.

6 QUANTUM FLYTRAP



In this model of the Quantum Flytrap, an interactive game on quantum models, it offers a representation of a quantum teleportation circuit.

This model shows Alice's and Bob's entangled pair of particles, as well as Alice's qubit 0 (orange element) that will be teleported to Bob.

7 CONCLUSION

Unlike the teleportation depicted in movies such as Star Trek, quantum teleportation does not involve the physical transfer of objects. Instead, it is based on transferring quantum information between entangled particles.

Quantum Teleportation advances the fields of quantum computing, cryptography, and networking. Moreover, when performed with optical fibers, even over kilometers apart, it demonstrated that teleportation allows the secure transmission of quantum information.

8 REFERENCES

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Acess it to see our QT code!

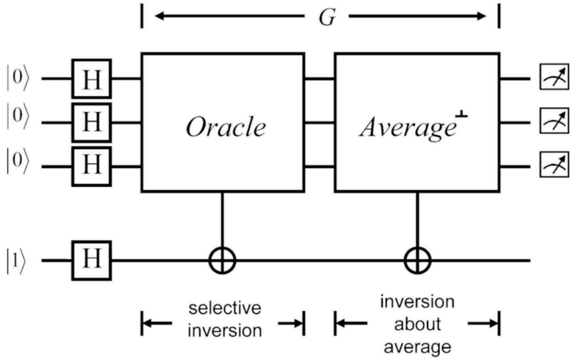
Quantum computers excel at solving certain problems **exponentially** faster than classical computers. Grover's algorithm exemplifies this potential, offering efficient search capabilities for unstructured databases. This research project explores Grover's algorithm's **advantages** over classical search methods, introducing quantum computing basics and the principles underlying the algorithm. It delves into the mathematical formulation and time complexity analysis, demonstrating a **quadratic speedup** compared to classical search algorithms. This breakthrough highlights the transformative potential of quantum computing in tackling complex computational challenges.

2.Algorithm Steps

1. Initial state: $|s\rangle = H^{\otimes n}|0\rangle^{\otimes n} = \frac{1}{\sqrt{N}}\sum_{x=0}^{N-1}|x\rangle$
2. Oracle: $O|x\rangle = -|x\rangle$ if x is a solution, $|x\rangle$ otherwise
3. Diffusion: $D = 2|s\rangle\langle s| - I$
4. Iteration: $G = D \cdot O$
5. Final state: $|\psi_f\rangle = G^r|s\rangle, \quad r \approx \frac{\pi}{4}\sqrt{\frac{N}{M}}$

3.Comparison

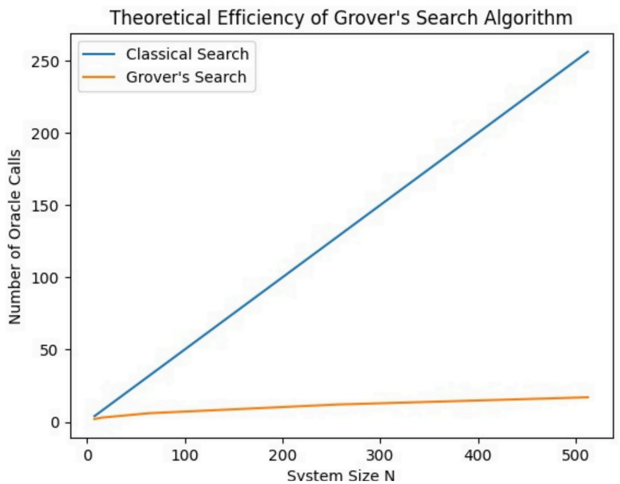
Grover's algorithm offers a quantum approach to searching unstructured databases, achieving a **quadratic speedup** over classical methods. It finds items in approximately √N steps, compared to N steps classically, by using superposition and interference. The algorithm iteratively applies **Oracle and Diffusion operators** to amplify the target state. While not a universal solution, it demonstrates quantum computing's potential to outperform classical systems in specific tasks, particularly unstructured searches. This breakthrough opens doors for applications in various fields and catalyzes further quantum algorithm development.



Grovers Algorithm

ThinkingBeyond | Girls In Quantum
Judy Ayman, Manal Hakeem
Under the supervision of Vanessa D.

Comparison graph



1. **Drug Discovery**: Accelerating the search for potential compounds in vast chemical libraries, significantly impacting the development of new medications.
2. **Supply Chain Optimization**: Streamlining the search for optimal routes and logistics solutions in complex supply chain networks, potentially saving time and resources.
3. **Database Search**: Quickly finding specific records in large unstructured databases.
4. **Cryptography**: Speeding up the brute-force search for cryptographic keys, which is relevant for cracking cryptographic systems and testing their security.
5. **Optimization Problems**: Enhancing the efficiency of solving various optimization problems by searching through potential solutions more rapidly.

5.Conclusion

Grover's algorithm is a quantum computing **breakthrough** that demonstrates the potential to outperform classical approaches in certain tasks. By leveraging superposition and interference, it achieves a quadratic speedup in searching **unstructured databases**. Grover's algorithm has practical implications across various industries and serves as a catalyst for further research and innovation in quantum algorithms, promising to tackle complex problems with unprecedented efficiency and shape the future of computation.

Code

Citations

SPOTIFY MUSIC RECOMMENDATION

Based on Personality Traits

Mentor: Prof. Dr. Gerhard Hellstern
Students: Irina Trivić

1.INTRODUCTION

Today, Spotify has one of the most advanced recommendation algorithms present on the market. It gathers data from the experience of all users (Collaborative Filtering) and from analyzing raw-audio and textual data extracted from the tracks themselves (Content-based Filtering and Natural Language Processing).

Instead of using classical Machine Learning, the aim of this research project was to make a recommendation system using a Quantum Neural Network. The motivation behind this was to test the quantum advantage - exponentially larger memory capacity, faster learning, better performance with a decreased number of qurons, higher information processing speed.

2.METHODOLOGY

The main objective of this project was to create a QNN for Spotify's music recommendations that is based on personality traits. We implemented a dataset which connected certain characteristics obtained through the Big Five personality test to respective song traits Spotify considered. This personality test was chosen due to its simplicity (compared to other considered options), popul.arity and availability of reqired data.

The algorithm was written using the Python programming language. Prior to writing the code, necessary modules were installed. This included general-use libraries, such as NumPy for mathematical operations, Pandas formanipulating dataframes and Scikit-Learn for utilizing ML-specific functions. Qiskit, a module specialized for running quantum computing algorithms (or, more precisely, for simulating quantum circuits) on classical computers, was also used.

First, the number of processed components was reduced using a PCA algorithm. The mechanism behind the PCA algorithm is explained on the Figure 1 in simple terms.

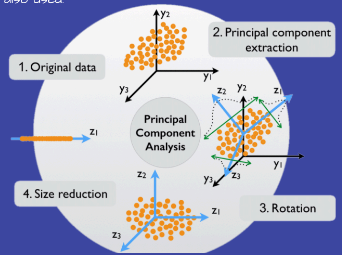


Figure 1: PCA algorithm diagram (Bellemans, A. , Aversano, G., Coussement, A., Parente, A. 2018. Feature extraction from principal component analysis based reduced-order models using orthogonal rotation)

The next step was encoding data into the quantum state. This was done through the angular encoding method, by using the Ry-gates.

To achive quantum parallelism, the qubits were put into the state of superposition.. This was done by applying an H-gate to the qubits. Theoretically, this was supossed to enable us to acquire the ability to perform multiple calculations at once.

After all operations on the qubits have been performed, measurements have been conducted and results obtained.

3.RESULTS

It is important to state that the code from which our results were obtained had many points that could have been optimized. As such, they were not a reliable source of information by themselves, but were interpreted in comparison to several other relevant studies conducted on this topic.

Nevertheless, despite all faults of the code, it was obvious to conclude that there is, in facct, no sight of the theoretically predicted quantum advantage.

One of the posibble implications of these results is that the QNN needed more training. The encoding method that was utilized might also be malfunctioning.

4.DISCUSSION

There are many aspects in which the algorithm might be improved. These possibilities include: finding a more optimal dataset (perhaps even creating a dataset of our own), giving the QNN more training (possibly increase the training dataset), optimizing improving the function that encodes classical data to quantum states. Also, finding a more sophisticated feature selection technique might bring considerable benefits.

Despite the theoretical predictions, there is yet no trace of the quantum advantage. For now, the supremacy of quantum computing has been spotted only in specific problems, such as complex simulations of particles in the quantum realm, for example. At least for now, there are no indications of Quantum Machine Learning algorithms being better than their respective classical couters.

5.CONCLUSION

The main purpose of this project was to implement a Quantum Neural Network that would return song recommendations as output when given a certain personality type as input. The results we obtained were in allegiance with other relevant work done in the field.

Oin futur, one of the posibble further steps could include giving the QNN more training, as well as finding better feature selection procedures.

REFERENCES

Spotify Recommendation System using Quantum Machine Learning

by Eva Shah
Mentor: Gerhard Hellstern

References:

SCAN THIS TO SEE MY REFERNCES!

SCAN THIS TO ACCESS MY CODE!

Overview:

The purpose of this research project is to build a recommendation system for Spotify songs using a Quantum Support Vector Machine (QSVM) and compare its accuracy to that of classical Support Vector Machine (SVM) to come to a conclusion as to which one is best suited for this task.

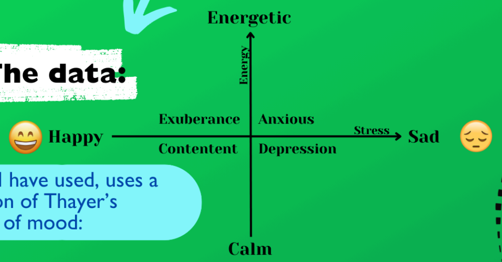
The classical SVMs used for comparison are:

- A polynomial SVM
- A linear SVM
- A radial basis function (RBF) SVM
- A sigmoid SVM

The data:

1

The dataset that I have used, uses a generalised version of Thayer's traditional model of mood:



2

It includes the 4 basic moods: Happy, Sad, Calm, Energetic
By analysis of mood and personality, where the big 5 personality traits are:
Openness to Experience: Imagination, creativity, and curiosity.
Conscientiousness: Organization, dependability, and discipline.
Extraversion: Sociability, assertiveness, and excitement-seeking.
Agreeableness: Trust, altruism, and cooperation.
Neuroticism: Tendency towards emotional instability and negative emotions.

3

I noted that the mood 'sad' corresponds to higher neuroticism and lower extroversion, the mood 'happy' corresponds to higher extroversion and agreeableness, the mood 'energetic' corresponds to higher extroversion and openness, the mood 'calm' corresponds to higher agreeableness, conscientiousness and lower neuroticism.

Therefore:
Sad music: Preferred by individuals high in neuroticism.
Happy music: Preferred by individuals high in extraversion and agreeableness.
Energetic music: Preferred by individuals high in extraversion and openness.
Calm music: Preferred by individuals high in agreeableness and conscientiousness

The model:

4

The QSVM uses classiq's construct_qsvm_model, synthesize and execute functions to create the QSVM. The QSVM uses a Second-order Pauli-Z evolution encoding circuit. The model uses a quantum kernel that employs a specific quantum feature map:

$$\phi(\mathbf{x}) = \exp(i\alpha\mathbf{x}^T P\mathbf{x})$$

where: $P = \sigma_z \otimes \sigma_z$(Pauli ZZ matrix). The kernel is calculated as:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$$

capturing the inner product of the quantum states transformed by $\phi(\mathbf{x}_i)$ and $\phi(\mathbf{x}_j)$.

5

Unlike classical kernels (e.g., linear, polynomial, Gaussian), this quantum kernel operates in the quantum Hilbert space, leveraging quantum states and operations.
Therefore the Pauli ZZ quantum kernel is tailored for quantum SVM applications, where it harnesses quantum computational principles to potentially enhance the classification of emotional states based on music data.

6

A recommendation function then retrieves and suggests songs that were classified under the chosen emotional category by the QSVM, providing personalized music selections based on user preferences. This approach enhances music exploration by automating tailored recommendations through quantum-enhanced classification techniques.

Analysis:

7

Compared the accuracy rate with a polynomial, linear, radial basis function & sigmoid classical SVM. The classical SVMs got the respective accuracy rates:
linear kernel classification test score: 0.67 = 67%
poly kernel classification test score: 0.74 = 74%
rbf kernel classification test score: 0.77 = 77%
sigmoid kernel classification test score: 0.53 = 53%
Whereas the QSVM got a 96% accuracy rate.
Although the accuracy rate of the QSVM is higher, it did take 5 minutes and 31 seconds to compute, whereas the classical SVMs took 74.8 milliseconds to finish classifying the data. Therefore, we can say that the QSVM has some kind of a quantum advantage (if one is not bothered by the difference in computing time) for classifying the songs into the different emotions, due to which there will also be a quantum advantage for recommending songs to a user.

Quantum Computing Concepts with Qubit Manipulation

Carin Samer
Aya Ahmed
(2A)

Abstract

From simple wooden devices to digital electronic computers,to supercomputers, physics and computation have always been intertwined due to the use of physical systems in encoding information. Recently, the focus has shifted towards utilizing the quantum aspects of physical systems to perform computations. This approach offers significant benefits, despite the challenges that are still present.

Google's Quantum Computer "Sycamore"

Introduction

When the first world quantum computer, Sycamore, was found, Google claimed its ability to compute faster than the fastest supercomputer, summit, by approximately 10000 years! Quantum computing is a research area that extends the set of physical laws classical computers operate on by accessing the quantum aspects of a physical world, opening up new ways of processing information. The need for a quantum computer stems from the inability of classical computers to solve "complex problems" as transistors can no more continue doubling and minimizing coupling with Moore's law.

Methodology of Working of a Quantum Computer

q[0]

1 Quantum Bits

Quantum bits (qubits) lie at the heart of quantum computing, promising ***exponential computational power*** compared to classical bits, with a two-state (or two-level) quantum-mechanical system. Unlike bits, qubits can be superposed until measured which gives the quantum computers the exponential computational power.

2 Quantum Gates

Fundamental operations to manipulate qubits, they can be unitary as Pauli gates and represented by ***unitary matrices*** or ***non unitary*** as measurement. Applying them corresponds physically to applying microwave signals or others to control qubit state.

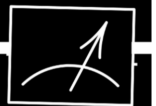
q[1]

3 Qubit Manipulation

Qubit manipulation involves precise control over their quantum states, enabling operations such as superposition, entanglement, and gate transformations. Researchers explore techniques like laser pulses, microwave fields, and magnetic resonance to manipulate qubits. These advancements pave the way for quantum algorithms, quantum error correction, and quantum supremacy.

4 The Bloch Sphere

The significance of the Bloch sphere lies in obtaining presice visualization of a qubit state and spotting errors ,where the two north and south poles of the block represent the zero and one states and every other point of the sphere corresponds to a superposition state.



q[2]

5 Mathematical Underpinnings of Quantum Computing

Mathematically, qubit is assumed to be a vector in Hilbert space having a general state: $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, where $|\alpha|^2 + |\beta|^2 = 1$ which is known as ***Borne's Rule*** ***, which does not change by applying any unitary gate to a qubit*** as shown:

$$H^{\otimes 2}\left(\begin{bmatrix}1\\0\end{bmatrix} \otimes \begin{bmatrix}1\\0\end{bmatrix}\right) = \frac{1}{2}\begin{bmatrix}1 & 1 & 1 & 1\\1 & -1 & 1 & -1\\1 & 1 & -1 & -1\\1 & -1 & -1 & 1\end{bmatrix}\begin{bmatrix}1\\0\\0\\0\end{bmatrix} = \frac{1}{2}\begin{bmatrix}1\\1\\1\\1\end{bmatrix}$$

Applying H gate on 2 qubits set to "0"

6 Conclusion

Despite the technical challenges as quantum noise, the future of quantum computing holds significant promise and potential across various fields and with continued research, trans formative advances in quantum computing capabilities over the coming decades will occur.

c[3]

Tools and Experiments

Using the IBM Quantum Composer , Qiskit and Pennylane, several experiments that consolidates the discussed concepts were conducted.

Scan for experiments!

Scan for references!

Developing a Predictive Model Using QML for Forecasting Best-Selling Mobile Phones

Boutheine Teyeb and Sara Barthel de Weydenthal

Quantum model

The quantum model encodes mobile phone features into quantum states using angle embeddings and processes them through a variational quantum circuit with entangling layers. This circuit, parameterized by trainable weights, captures complex patterns in the data. Measurements of the quantum states are then passed to a classical neural network layer to make predictions, leveraging quantum computing's advanced data representation capabilities.

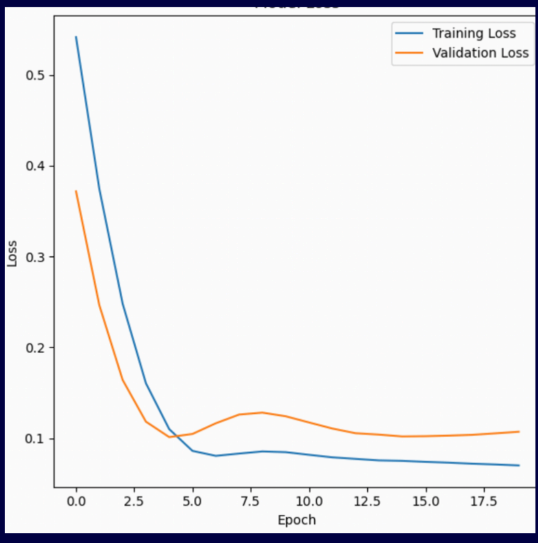
Abstract

This project uses Quantum Machine Learning (QML) to improve prediction accuracy by analyzing data from specifications, user reviews, and market trends.

QML leverages quantum computing to create a superior predictive model, uncovering hidden patterns and non-linear correlations in complex data, thereby offering better market insights and predictions.

Classical model

The classical regression model predicts mobile phone sales by applying a linear combination of input features, including one-hot encoded manufacturer data. Each feature is weighted, and the model includes a bias term. During training, weights are optimized to minimize the prediction error using gradient descent, enhancing the model's accuracy.



Method

1. Data Collection: Used Kaggle's dataset on best-selling mobile phones, including specifications, user reviews, and sales data.
2. Quantum Feature Mapping: Encoded data features into quantum states to capture complex relationships.
3. Model Development: Created a hybrid classical-quantum model with TensorFlow and PennyLane, integrating a variational quantum circuit into a classical neural network.
4. Training and Evaluation: Split data into training and testing sets, normalized it, and trained the model using Mean Squared Error (MSE) for evaluation.