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# Hackathon 2023

### Vendors

AWS (OQC): Machine Learning, Simulation

AWS (Rigetti): Machine Learning, Optimisation

AWS (QuEra): Optimisation

D-Wave: Optimisation

ORCA Computing: Optimisation, Machine Learning

Emulation: D-Wave: Optimisation

Emulation: AWS: Machine Learning, Optimisation, Simulation

Quantinuum: Simulation

IBMQ: Simulation, Optimisation, Machine Learning

Emulation IBMQ: Simulation, Optimisation, Machine Learning

Classiq (IonQ): Simulation

AWS(IonQ): Optimisation

Emulation: Classiq (IonQ): Simulation

### Project 1:

Practical equivariant embeddings for DNA sequencing over the current NISQ devices

* Machine learning
* Zaiku Group Ltd.
* Healthcare
* AWS (OQC)
* AWS (Rigetti)
* Emulation: AWS

The team identified the reverse-complement symmetry of DNA sequences and defined an angle-based embedding with two features per qubit, in which the symmetry was represented on the Hilbert space via conjugation by a tensor product of Pauli-X gates. They created a synthetic dataset of eight sequences in length and defined via their representation an equivariant circuit to detect the string ‘AT’ within a sequence - an equivariant version of a small, typical variational ansatz. They compared this model’s performance to an analogous non-equivariant model on a simulated device. Time did not permit training on a real device but the angle-based solution would have been suitable for NISQ devices.

Outcome

The equivariant model appeared to reach a lower cost than the non-equivariant counterpart given the same amount of training, which was a nice conclusion.

Time limitations meant that the team could not practise a training/validation/test data split for benchmarking. Further, the hybrid nature of training loops meant that performing the task on a real device would have taken too long. These loose ends would be a natural starting point for further investigation, along with applications of the method to real-world datasets. It would also be interesting to compare the two quantum models to a classical approach to the same task.

References

J. J. Meyer, M. Mularski, E. Gil-Fuster, A. A. Mele, F. Arzani, A. Wilms, and J. Eisert, “Exploiting symmetry in variational quantum machine learning,” arXiv:2205.06217, 2022.

N. Innan and M. Al-Zafar Khan, “Classical-to-Quantum Sequence Encoding in Genomics,” arXiv:2304.10786, 2023.

### Project 2

The travelling salesman problem – route optimisation in healthcare

* Optimisation
* NHS
* Healthcare
* AWS (QuEra)
* D-Wave
* Emulation: AWS

Routing and scheduling optimisation is a constant exercise when seeking cost reduction and improvement of service times in the healthcare operational environment. In addition to the transportation of patients via ambulance, NHS services also require the transportation of time-sensitive material to multiple locations. The computation of optimal routes is of value and a common classical problem. An algorithm in computer science is said to be “efficient” if it executes in polynomial time or less. Owing to the nature of routing and scheduling problems as NP-complete, the application of quantum computing for problem solving in a healthcare setting is an exciting proposition. Routing and scheduling optimisation problems are commonplace, and innovative ways to tackle these problems may offer advantages not yet realised via classical methods.

Solution

To make the problem tractable, the team used a hybrid method that combines classical compute for clustering (k-means-constrained) with quantum annealing. The clustering technique focuses on finding non-overlapping clusters, constraining the search space, and making the solution viable for existing hardware and at scale.

The team used the D-Wave solver to implement the quantum annealing. Their objective function is defined in

Simulated annealing in a classical setting is prone to being trapped in local minima. Finding the global minimum using classical compute is computationally intensive and takes time. Quantum annealing takes advantage of low-energy states in quantum physics to find the low-energy states of a problem, and the solutions provided by D-wave are designed for these types of problems. Once the team encoded their problem onto an initial Hamiltonian, mapping eigenstates to energies, they sought an optimal solution.

Outcome

Several clustering methods were attempted, and k-means-constrained proved most useful. Hospitals were clustered before using D-Wave to provide solutions for the optimal route based on the shortest path between clusters. The team had a limited number of qubits to use but were still capable of finding solutions for up to five health centres.

References

S., Jain, 2021. Solving the traveling salesman problem on the d-wave quantum computer. Frontiers in Physics, p.646.

Quantum chemistry; Electronic structure problem

Dynamics can be simulated using Hamiltonian simulation (typically Trotter methods) [18] Clinton, L., Bausch, J., and Cubitt, T. “Hamiltonian simulation algorithms for near-term quantum hardware.” Nat. Commun. 12 (2021), 4989. arXiv:2003.06886.

and have been demonstrated for an 8 × 1 lattice on 16 superconducting qubits [46] Arute, F., Arya, K., Babbush, R., et al. “Observation of separated dynamics of charge and spin in the Fermi–Hubbard model.” arXiv:2010.07965 (2020).

### Project 3

Explore the use of quantum computing for unit commitment to balance the electricity grid

* Optimisation
* National Grid ESO
* Energy
* ORCA Computing
* D-Wave
* Emulation: D-Wave

The Unit Commitment (UC) problem is a fundamental problem in the electric power industry. The objective of UC is to determine an optimal schedule for each generating unit to meet the demand for power with the minimum cost.

Given its mixed-integer programming (MIP) nature, UC solution speeds could potentially be greatly enhanced with quantum computing.

Solution

We took a simplified version of UC to the hackathon that made it a combinatorial problem in which all the optimisation variables were binary, representing whether a generator was online or offline. Modelled constraints were positive margins and minimum up/down times for generators.

Objective function – minimise costs to operate the system:



Subject to:



We worked with ORCA Computing and D-Wave to solve this problem using quantum hardware and simulators.

Outcome

The team explored the possibility of formulating UC as a quadratic unconstrained binary optimisation (QUBO). Additionally, we used D-Wave’s hybrid solver to implement the constrained problem. This way, the team succeeded in solving a toy case of four generators and four time periods.

We found that:

* Formulating a QUBO problem for a simplified version of UC wasn’t straightforward and the limited time available made it more challenging. We can only speculate how much harder it would be for the full Security-Constrained UC problem
* Solving constrained optimisation problems using quantum platforms allows specifying ‘a-priory’ Langrage multipliers for the constraints. This means that it’s difficult to assess the optimality of a solution and the general applicability of an implementation without a reference solution
* While quantum computing shows great potential to solve complex optimisation problems in other sectors, there’s an outstanding gap before it can be directly applicable to power system operation. We’d be keen to continue exploring how to bridge this gap.

### Project 4

Quantum computing for nuclear fusion engineering and design with the finite element method

* Simulation
* UKAEA
* Energy
* AWS (OQC)
* Quantinuum
* Emulation: AWS

The design of nuclear fusion reactors requires accurate simulations of complex phenomena to optimise design parameters and reduce the need for costly physical prototypes. Unfortunately, the computational cost of some of these complex simulations limits their applicability and benefits. The improved computational performance promised by quantum computers will be of great benefit for shortening engineering design cycles and improving the accuracy of designs.

Solution

Finite Element Analysis (FEA) is a numerical simulation technique used for fusion reactor design that solves the complex dynamics of the fusion domain using a linearised set of equations. This is equivalent to solving the equation Ax=b, where the inverse of the matrix A is used to determine the vector x given a set of initialised values of b. The Harrow-Hassidim-Loyd (HHL) algorithm was deployed to solve the equation Ax=b, as an early demonstrator of a quantum solver for linear equations. The algorithm requires a large circuit depth, due to the initialisation operations required to store the value of the vector b. Gate operations were then conducted to apply the inverse matrix A on the qubit value of vector b to solve for vector x. To solve for a single qubit circuit line, seven qubits were used as control and scratch qubits. This was implemented on the eight-qubit Lucy quantum processor provided by Oxford Quantum Circuits.

Outcome

The experiment demonstrates that it is possible to solve linear matrix operations. However, these were based on classical binary input values, and representing large vectors with a large matrix space at the binary level will require large amounts of qubits and quantum information to represent the binary data and respective quantum transformation. Therefore, it is proposed to improve the encoding of classical high-level data to quantum qubit data to improve the computational expense and complex quantum algorithms with large depths of circuits and possible larger entanglement requirements. Also, to implement one logical qubit requires approximately seven physical qubits, which will significantly increase the number of physical qubits required if error corrects are to be considered.

FEA is a widely used numerical simulation technique, and therefore this algorithm has applicability in all complex engineering sectors such as aerospace, automotive, construction and so forth. In future exploration it would be interesting to merge quantum numerical simulation techniques in neural network loss functions with optimisations to improve the training for Physics Informed Neural Networks (PINNS).

### Project 5

1-D Monte Carlo particle transport

* Simulation
* Jacobs
* Energy
* Quantinuum
* IBMQ
* Emulation: IBMQ

Mathematical modelling of the transport of subatomic particles in matter, such as neutrons, plays an important role in the operation of radioactive facilities. The Monte Carlo (MC) approach to simulating radiation transport provides accurate results but is computationally expensive. Quantum computing may have a role in speeding up MC simulations.

Solution

The MC method consists of sampling from specified statistical distributions to determine the collision type, direction and distance travelled by the particle. Quantum sampling may be more advantageous to classical sampling due to accuracy and speed improvements. An alternative method involved encoding the probability distribution of particle penetration as a biased quantum coin, with the probability of penetration estimated via a circuit for quantum amplitude estimation (QAE). The H1 Emulator provided by Quantinuum was used to implement these circuits, with sampling of uniform distribution achieved via circuits with a depth of one and four gates. Sampling of exponential distribution was done via a state preparation box, leading to a deeper circuit. The circuit for QAE consists of more quantum gates, corresponding to greater depth if non-optimised, and is ideal for fault-tolerant systems, while quantum sampling may be better suited for NISQ devices.

Outcome

The solutions obtained via quantum sampling showed a large variation from the analytical solutions. Error correction techniques were not implemented, which could account for the difference in expected and obtained results. The use case was also a simple example with only two energy levels and limited neutron interactions (capture, scatter, leak). Future extensions could consider higher dimensions, more energy levels, as well as fission interactions. The alternative method using QAE was not fully explored, and could be better investigated in the future.

### Project 6

Near-term quantum linear solver algorithms

* Simulation
* Rolls Royce
* Aerospace
* Classiq (IonQ)
* IBMQ
* Emulation: Classiq (IonQ)

Rolls Royce designs and manufactures power systems for applications such as aviation and marine propulsion. For the simulation and modelling of modern power systems, engineers utilise Computational Fluid Dynamics and Finite Element Method algorithms. These reduce to the computationally intensive task of matrix inversion for solving systems of differential equations, which can bottleneck even supercomputing throughputs. Quantum computing’s dense matrix algebra indicates a potential advance for this use case.

Solution

Examples of the problem present as small instances of linear systems of equations, which may be formulated as Ax=b, presented with a matrix of equations A and a vector of constants b to solve for the vector x. Examples from sizes of 2x2 to 16x16 matrices were solved for this use case. Two different algorithms were studied to approach this, a Coherent Variational Quantum Linear Solver (CVQLS) that could be easily implemented on NISQ hardware and the Quantum Singular Value Transformation (QSVT), which is more intended for fault-tolerant systems. These were predominantly developed in Classiq to optimally compile a circuit with minimal execution time, with some bits being done in Pennylane and exported via QASM file to Classiq.



Outcome

The team performed runs of the CVQLS on the 16-qubit IBM Guadalupe device using Classiq and IBM Quantum, and on a 20-algorithmic qubit IonQ Aria device as well as the IonQ Harmony device using Classiq. Limited by the circuit size, the team was able to reach results for linear systems of up to 4x4 using the hardware devices, while simulation reached up to 16x16 matrix sizes. Besides normally not being a NISQ algorithm, the QSVT encountered issues in its hardware implementation as Pennylane’s newly introduced QSVT module did not compile to QASM code, and this will be a necessary step towards implementing the QSVT in hardware. Further implementations of quantum linear solvers are expected to be developed by Rolls Royce and partners for the future development of hydrogen-based systems.

References

<https://pennylane.ai/qml/demos/tutorial_coherent_vqls>

https://pennylane.ai/qml/demos/tutorial\_apply\_qsvt/

### Project 7

Skills constrained capacitated vehicle routing problem with time window (SC-CVRP-TW)

* Optimisation
* Unisys
* Logistics
* IBMQ
* D-Wave
* Emulation: IBMQ

A specific version of the Vehicle Routing Problem (VRP) is the Vehicle Routing Problem with Time Window and Skill Set constraints (VRP-TWSS). This involves calculating optimal routes for a fleet of vehicles where each vehicle has a particular set of skills, and each destination has a required skill and time window.

Providing a successful resolution to the optimisation of vehicle routing problems will:

Current classical solutions to these problems do not scale to the level faced by many of our customers, even with High Performance Computing (HPC).

Solution

No quantum circuit was developed as the solution was developed on D-Wave’s quantum annealer. Instead, the mathematical model was implemented directly using the Constrained Quadratic Model (CQM) in D-Wave’s Ocean Software Development Kit (SDK).

The solution was based on the mathematical model defined in L. Han’s paper.[1] In the time available, no consistent solution was returned by D-Wave. Different solutions were considered optimal by the quantum annealer on different runs of the code. This may very well result from the high density of constraints, a problem Unisys have encountered before and outlined in our whitepaper.[2]

Outcome

During the hackathon, the team very quickly (within a few hours) encountered hardware limitations using the IBMQ platform. The team’s use case was solving a small vehicle routing problem (32 nodes and 5 vehicles, or n32-k5) with time-window and skill-set constraints. Even without the time-window and skill constraints embedded in the model, the IBMQ platform did not yield results after running the model, even with a smaller model consisting of 8 nodes and 3 vehicles (n8-k3). By comparison, running the same model on the High-performance parallel linear optimisation Software (HIGHS) classical solver installed on an Orange Pi 5 returned results within minutes. Using a quantum annealer from D-Wave, results were also obtained within minutes.

References

[1] L. Han, “Metaheuristic Algorithms For The Vehicle Routing Problem With Time Window And Skill Set Constraints”, Dec 2016. Available: Han-Lu-MSc-IENG-Dec-2016.pdf (dal.ca)

[2] S. Sinno, T. Gross, A. Mott, A. Sahoo, D. Honnalli, S. Thruvavakkath, B. Bhalgamiya et al., “Performance of Commercial Quantum Annealing Solvers for the Capacitated Vehicle Routing Problem,”, Sep 2023. Available: 2309.05564.pdf (arxiv.org)

### Project 8

Price prediction over different time horizons

* Machine learning
* Nomura International Plc.
* Finance
* IBMQ
* ORCA Computing
* Emulation: IBMQ

The team was provided with a problem to predict the time series of financial data. The data are well known to be noisy with very low signal-to-noise ratio, and also have complex memory structure. The aim was to create a supervised machine-learning model that makes use of quantum resources.

Solution

The main approach to the problem was to utilise a quantum-enhanced Long Short-Term Memory (LSTM) model. The LSTM model is a neural network-based model that separately models the long and short memory, along with the process of forgetting the past. The process contains several parallel neural networks that are trained as part of the calibration. We replaced the neural networks with quantum equivalents and trained the model with IBMQ resources. The model showed promising results within the reach of currently available hardware (16-qubit processor), while we utilised a simulator for most of the analysis.

Outcome

The result was very encouraging and showed potential for how existing quantum hardware can be used to enhance existing algorithms or as a hybrid combination of classical and quantum parts. The project opened more questions to pursue in the future, such as the optimal combination, and which one dominates any existing setup, but it suggests that some form of enhancement is within reach in the short term.

### Project 9

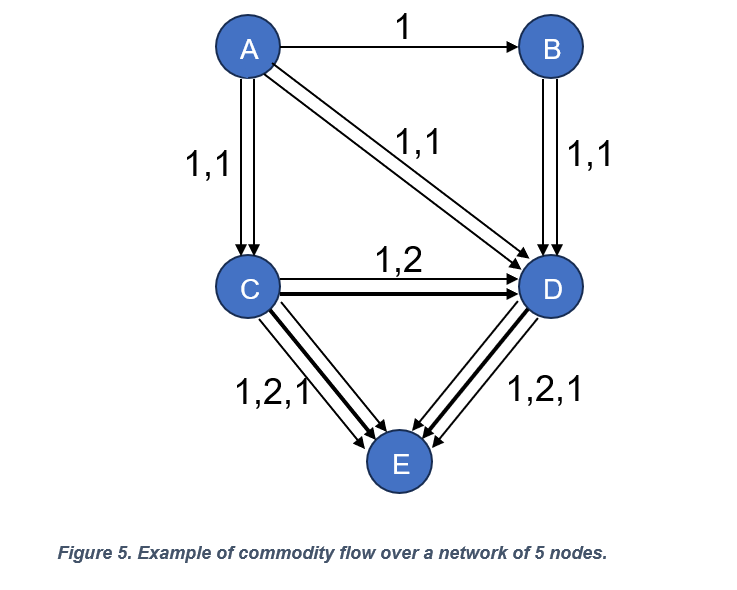
Generating efficient and resilient routes for unicast and multicast traffic

* Optimisation
* BT
* Telecommunications
* D-Wave
* AWS (Rigetti)
* Emulation: D-Wave

Allocating routes for transmitting data across telecommunication networks can become computationally hard under certain conditions, such as when the network is very congested, with different demands when the data traffic allocation on each channel is broken into a small number of options (integer flow). This can occur, for example, when assigning optical channels at layer 1, and where it is required to provide resilience by planning two independent routes for each demand that is completely independent of the first route. Further complications can include requirements for multicast (one source to many sinks) traffic and constraints such as the maximum latency of a route.

Solution

The team identified that data traffic flow is a variation of the standard commodity flow satisfaction problem. The team used a Quadratic Unconstrained Binary Optimisation (QUBO) representation of the routing and demand satisfaction model, and this was run on a D-Wave quantum annealing system with 5000 qubits. A number of approaches were investigated to represent this problem using the QUBO form. For single-commodity flow problems (both unicast routes and multicast trees), the team settled on a flow continuity model that used Kirchoff’s current laws at each node. Qubits represented the links of the network. The capacity of each link could be constrained using the choice of encoding the amount of flow in the link by using a binary expansion of the total capacity of each link (such that no configuration of weights could exceed the maximum capacity). This was efficient, creating a number of weighted qubits of order log C for each edge. The encoding of single-commodity flow required approximately E log2 C qubits (where E is the number of links in the original network, and C is the average capacity). However, for highly connected networks, additional qubits would be needed to overcome native Quantum Processing Unit (QPU) connectivity constraints. For the more realistic multicommodity flow problem (planning routes for different types of data), it was necessary to create multiple copies of the original qubit representation of the different commodity flows on the network coupled to represent the shared capacity constraints, with slack variables because the capacity represented an upper limit.



Outcome

The team showed that it was possible to encode a large number of different variations of the efficient routing problem. Smaller problems up to network sizes of 10 nodes were solved using the D-Wave native QPU (5000 qubits). Larger problems were run on the D-Wave Leap hybrid solver. Repeated anneals usually returned some correct solutions (with the lowest energy in the sample set), but the QUBO formulation had some technical issues that could affect the quality of the solution. Changing the weighting between the linearly independent terms (representing different constraints) often affected the probability of returning a valid solution in any given run. This was true both for the D-Wave native QPU and the hybrid solver.

The fact that very complex routing problems could be represented quite efficiently in numbers of qubits in a QUBO was very promising. However, the fact that the ground state optimum (and correct) solutions were not found a high percentage of the time was a limitation. This was not unexpected given that the annealer has some noise, and the encoding of the problem had not given any consideration to error mitigation, plus we expect larger problems to have smaller energy gaps between the ground state solution, and excited states. Whether an encoding on the current D-Wave annealer could mitigate errors (for example, by coupling qubits in redundant groups to represent single logical QUBO variables) and whether this would be efficient would be interesting to explore. The effect of varying the weightings of the different linearly independent constraint terms on the quality of the solution set was also something that needs to be explored and understood further. Ground state solutions were found, however, which are promising, especially in light of the potential to improve the annealing performance with emerging developments in quantum annealer hardware and methods. Continued increase in quantum annealer QPU size will also be helpful.

This use case was further developed by the hackathon team, leading to a paper entitled ‘Optical Routing with Binary Optimisation and Quantum Annealing’ where the details of this problem are explored in more depth and future work building from that conducted at the hackathon is reported.

References

E. Davies et al., “Optical Routing with Binary Optimisation and Quantum Annealing,” arXiv, 2402.07600v1, 2024

### Project 10

Vaccination centre location

* Optimisation
* Applied
* Quantum Computing
* Healthcare
* AWS (IonQ)
* D-Wave
* Emulation: AWS

Optimising the location of vaccination centres during a pandemic is an important means of reducing the pandemic’s impact. Optimal locations will help to maximise vaccination rates in the population, thereby reducing the chances of the vaccinated individuals catching the disease and also helping reduce the rate of spread, benefiting the whole population. The real-world problem objective is to maximise vaccination take-up by considering travel times (to be minimised), clinic capacity, population size and demographics, and the proportion of the population already vaccinated. Here, we consider the simplified problem of minimising population to vaccine centre travel times. At large scale, such problems cannot be optimally solved using classical means.

Solution

The problem can be considered as a weighted-set cover problem and formulated as a QUBO, which can be translated into Ising form for running on a quantum computer.[1] The objective function, which is to be minimised, encodes the total distance from the population centres, N, (nodes) to the vaccination centre(s), V, (also nodes) and includes certain problem constraints encoded using the Lagrange multiplier method, such as the requirement that each population centre is only served by one vaccination centre.

Two NISQ-era hybrid algorithms were used: QAOA (Quantum Approximate Optimisation Algorithm) and VQE (Variational Quantum Eigensolver), each of which seeks to optimise a parameterised circuit.[2, 3] An example circuit to run the VQE parameterised algorithm is shown above. Two simulators were used: Amazon Braket SDK for VQE and IBM Qiskit for QAOA.



Outcome

Two small-scale instances of the problem were considered: (A) N=4, V=2 and (B) N=3, V=2, with instance (A) run using QAOA and instance (B) using VQE. Each was run using up to 20 random initial choices for the circuit parameters and was successful in very significantly improving the probability of finding the optimal configuration (the ground state) by comparison with the initial problem starting state – for example, the VQE approach was able to achieve an 89% probability of finding the ground state with the best set of initial parameters.

An important unresolved question is how the approach scales with problem size and in particular, if the time to solution on a quantum processor for a real-world problem instance can be achieved (i.e. sufficiently short), which would make this approach practically valuable.

If improved versions of this method and associated hardware developments can be achieved, this approach could be applied to a wide variety of valuable applications in healthcare and other sectors.

References

A. Lucas, “Ising formulations of many NP problems,” arXiv, 1302.5843v3, 2013.

E. Farhi, J. Goldstone and S. Gutmann “A Quantum Approximate Optimization Algorithm,” arXiv, 1411.4028v1, 2014.

A. Peruzzo et al., “A variational eigenvalue solver on a photonic quantum processor,” Nature Communications, vol. 5, no. 4213, 2014.

Variational Quantum Algorithms (Delzel Page 258)

Factoring: Variational methods for factoring have been proposed which exploit a mapping between the factoring problem and that of finding the ground state of an Ising Hamiltonian [44] Anschuetz, E., Olson, J., Aspuru-Guzik, A., and Cao, Y. “Variational quantum factoring.” In: Quantum Technology and Optimization Problems (2019), 74–85. arXiv:1808.08927 . The authors use the QAOA ansatz and heuristically find that p = O(n) rounds of the ansatz can lead to a good solution overlap for small system sizes.

Combinatorial optimization: In the Quantum Approximate Optimization Algorithm (QAOA), combinatorial problems on bitstrings can be encoded in the Pauli-Z basis with Hamiltonian HP [30].Farhi, E., Goldstone, J., and Gutmann, S. “A Quantum Approximate Optimization Algorithm.” arXiv:1411.4028 (2014). By finding the state that minimizes ⟨ϕ(θ)|HP |ϕ(θ)⟩, where |ϕ(θ)⟩ = U(θ)|0⟩, the optimal bit-string can be extracted by sampling the optimized state in the computational basis. A widely studied ansatz for this problem is the Quantum Alternating Operator Ansatz (which bears the same acronym as the algorithm), inspired by Trotterized adiabatic evolution [31]. The ansatz takes the form U(γ, β) = Qp l=1 e−iβlHMe−iγlHP where HM is a specific “mixing” Hamiltonian. This ansatz is known to be computationally universal (when p → ∞) for certain classes of Hamiltonians [32, 33]. Moreover, under reasonable complexity-theoretic assumptions, it is known that sampling from the output of the QAOA at p = 1 is classically hard [34]. On the other hand, there is evidence that shallow (small p) QAOA does not perform well [35, 36, 37, 38], leading to intuition that p may need to grow with problem size to produce better approximate solutions than what can be easily found classically. Alternatively, there is some evidence that an exponential number of samples from shallow QAOA circuits may yield polynomial speedups over classical methods for finding exactly optimal solutions [39, 40], see the page on beyond-quadratic speedups for combinatorial optimization.

# Analysis of Focus Areas

1. **Common Problem Types**

|  |  |  |  |
| --- | --- | --- | --- |
| **Category** | **Projects** | **Best Hardware** | **Best Emulators** |
| **Optimization** | Traveling Salesman, Vehicle Routing, Vaccination Location | D-Wave, AWS (Rigetti/IonQ) | D-Wave Ocean, AWS Braket |
| **Simulation** | Nuclear Fusion, Monte Carlo, Linear Solvers | Quantinuum, AWS (OQC), IBMQ | IBM Qiskit, AWS Braket |
| **Machine Learning** | DNA Sequencing, Price Prediction | IBMQ, AWS (OQC) | IBM Qiskit, Classiq (IonQ) |

2. **Algorithms**:

* **Optimization Algorithms**:
  + Quadratic Unconstrained Binary Optimization (QUBO) Effective for combinatorial problems like routing.
  + Quantum Approximate Optimization Algorithm (QAOA) Suited for parameterized quantum circuits and optimization challenges.
  + Variational Quantum Eigensolver (VQE) : Useful for variational approaches in hybrid quantum-classical setups.
* **Simulation Algorithms**:
  + Harrow-Hassidim-Lloyd (HHL) for solving linear system of equations, vital for finite element analysis and matrix inversion.
  + Quantum Amplitude Estimation (QAE): Enhances Monte Carlo methods and sampling accuracy.
* **Machine Learning Techniques**:
  + Quantum-enhanced Long Short-Term Memory (LSTM) : Strengthens time-series prediction.
  + Variational Quantum Factoring: Useful for machine learning-based optimization

3. Key Quantum Systems and Emulators:

* **Hardware:**
  + D-Wave (specialized in QUBO and annealing)
  + IBM Quantum (IBMQ) (gate-model system) Proven track record for ML applications
  + AWS Quantum Solutions (Rigetti, IonQ): Versatile for QAOA and hybrid approaches
  + AWS Quantum Solutions (OQC) Suitable for scalable simulation tasks, for quantum-enhanced learning
  + Quantinuum (gate-model systems): Supports dense matrix operations and fault-tolerant simulations
* **Emulators**:
  + IBM Qiskit: circuit prototyping and iterative refinement
  + D-Wave Ocean SDK for scalability and flexibility
  + AWS Braket SDK: circuit prototyping and iterative refinement
  + Classiq (IonQ) algorithm development and debugging.

# Background on Algorithms

## Quantum Amplitude Estimation (QAE)

A fundamental quantum algorithm that extends Grover's search algorithm to estimate the amplitude of a specific quantum state. Introduced by Gilles Brassard, Peter Høyer, Michele Mosca, and Alain Tapp in 2000, it plays a pivotal role in achieving quantum speedups for problems involving probability estimation, sampling, and integration. Below is an overview of its background and significance.

Quantum Amplitude Estimation remains a foundational component of quantum algorithms and hybrid quantum-classical frameworks. Advances in error correction, circuit optimization, and quantum hardware are expected to make QAE more practical in the coming years. Its importance in solving real-world problems, particularly in industries like finance, chemistry, and AI, underscores its central role in quantum computing's future.

In summary, QAE is a cornerstone algorithm that demonstrates the power of quantum computing to tackle probabilistic and sampling problems efficiently, making it a critical tool for future quantum applications.

**Problem Setting**

Quantum Amplitude Estimation addresses the following problem:

Given a unitary operator \( \mathcal{A} \) that prepares a quantum state:

\[

\mathcal{A} |0\rangle = \sqrt{a}|x\rangle + \sqrt{1-a}|x^\perp\rangle,

\]

where \( a \) is the amplitude associated with the state \( |x\rangle \), the goal is to estimate \( a \) to a specified degree of precision.

- \( a \): The amplitude of the "desired" state \( |x\rangle \).

- \( |x^\perp\rangle \): The orthogonal subspace containing other states.

This task is particularly important in quantum applications where probabilities or weights associated with quantum states are critical.

**Core Methodology**

The algorithm combines:

1. **Quantum Phase Estimation (QPE)**:

- Encodes the amplitude \( a \) as a phase that can be extracted and estimated.

2. **Grover Iterations**:

- Amplifies the amplitude of the desired state \( |x\rangle \) to make it easier to distinguish and measure.

QAE achieves this by using a controlled application of Grover's operator and phase estimation to iteratively refine the estimate of \( a \).

#### **Quantum Speedup**

Classically, estimating \( a \) using Monte Carlo sampling requires \( O(1/\epsilon^2) \) iterations to achieve an error of \( \epsilon \). Quantum Amplitude Estimation achieves the same accuracy with \( O(1/\epsilon) \) iterations, providing a quadratic speedup.

### **How QAE Works**

1. **State Preparation**:

- Prepare the quantum state \( \mathcal{A}|0\rangle \) using the given unitary \( \mathcal{A} \).

2. **Phase Estimation**:

- Apply Quantum Phase Estimation to extract the eigenphase associated with the Grover operator \( Q \). The phase is related to \( a \) and can be decoded to estimate the amplitude.

3. **Inverse Mapping**:

- Convert the estimated phase into the desired amplitude \( a \).

4. **Iterative Refinement**:

- Use multiple rounds of estimation with increasing precision to reduce the error.

**Importance of Quantum Amplitude Estimation**

1**. Broad Applicability**

QAE is a core algorithm used in quantum speedups for various computational tasks. Its versatility comes from its ability to efficiently estimate probabilities, which underpins many quantum algorithms.

2**. Applications**

- Monte Carlo Simulations:

- QAE accelerates the convergence of Monte Carlo methods, commonly used in finance (e.g., option pricing), risk analysis, and engineering simulations.

- **Integration Problems**:

- QAE improves the efficiency of numerical integration by estimating areas or volumes represented by quantum states.

- **Optimization and Machine Learning**:

- Used in hybrid quantum-classical algorithms for gradient estimation, Bayesian inference, and sampling-based optimization.

- **Quantum Chemistry**:

- Assists in estimating molecular properties such as ground-state energies or reaction rates.

- **Search Problems**:

- Extends Grover’s algorithm to probabilistic settings where the "desired state" is not deterministic.

3**. Quadratic Speedup**

The quadratic speedup offered by QAE significantly reduces the computational effort required for probabilistic tasks. For example, in Monte Carlo simulations, classical methods require \( O(1/\epsilon^2) \) samples, while QAE reduces this to \( O(1/\epsilon) \), making previously intractable problems solvable.

**Challenges and Practical Limitations**

1. **Implementation Complexity**:

- QAE requires precise control of quantum gates and deep quantum circuits, which can be challenging on noisy intermediate-scale quantum (NISQ) devices.

2. **Error Sensitivity**:

- The algorithm is sensitive to noise and decoherence, which can significantly affect the accuracy of amplitude estimation.

3. **State Preparation**:

- Efficiently preparing the state \( \mathcal{A}|0\rangle \) is non-trivial and problem-dependent, often requiring additional quantum resources.

4. **Resource Intensity**:

- QPE-based techniques involve deep circuits and multiple ancilla qubits, making it resource-intensive for current quantum hardware.

## Quantum Amplitude Estimation (QAE)

a fundamental quantum algorithm introduced by Gilles Brassard, Peter Høyer, Michele Mosca, and Alain Tapp in 2000. It builds on Grover’s search algorithm and Quantum Phase Estimation (QPE) to estimate the probability amplitude of a desired quantum state. QAE is significant because it provides a quadratic speedup over classical Monte Carlo methods for problems involving probability estimation, integration, and sampling.

Quantum Amplitude Estimation is a cornerstone algorithm that exemplifies the power of quantum computing to solve probabilistic problems efficiently. By providing a quadratic speedup over classical methods, QAE lays the foundation for transformative applications across science, engineering, and industry, highlighting the promise of quantum technology in solving real-world challenges.

**Background of QAE**

#### **The Problem QAE Solves**

QAE addresses the problem of estimating the amplitude \( a \) of a quantum state \( |x\rangle \), which is part of a superposition state prepared by a unitary operator \( \mathcal{A} \):

\[

\mathcal{A}|0\rangle = \sqrt{a}|x\rangle + \sqrt{1-a}|x^\perp\rangle,

\]

where:

- \( a \): The probability amplitude of the desired state \( |x\rangle \),

- \( |x^\perp\rangle \): The orthogonal component of the superposition.

The goal is to estimate \( a \) to a desired precision \( \epsilon \). Classically, this would require \( O(1/\epsilon^2) \) samples via Monte Carlo techniques. QAE achieves this in \( O(1/\epsilon) \), providing a **quadratic speedup.**

#### **Algorithm Overview**

The QAE algorithm combines:

1. **Quantum State Preparation**:

- The unitary operator \( \mathcal{A} \) prepares the desired quantum superposition state.

2. **Grover’s Search Amplification**:

- Grover’s operator \( Q \) amplifies the amplitude of the desired state \( |x\rangle \).

3. **Quantum Phase Estimation (QPE)**:

- QPE extracts phase information about the Grover operator, which is related to the amplitude \( a \).

By iteratively applying \( Q \) and measuring the resulting state, QAE estimates \( a \) with high precision.

### **Importance of QAE**

1**. Foundational Quantum Algorithm**

QAE is a building block for many quantum applications. Its ability to estimate probabilities and amplitudes efficiently makes it central to algorithms in:

- Quantum Monte Carlo simulations,

- Numerical integration,

- Optimization,

- Machine learning,

- Quantum chemistry.

2**. Quadratic Speedup**

- Classical Monte Carlo methods converge at \( O(1/\epsilon^2) \) for an accuracy \( \epsilon \).

- QAE achieves the same precision in \( O(1/\epsilon) \), significantly reducing the computational effort for large-scale problems.

3**. Applications**

QAE underpins various quantum algorithms, including:

- **Monte Carlo Simulations**: Accelerates pricing models in finance (e.g., option pricing) and risk analysis.

- **Integration Problems**: Enhances accuracy and speed of numerical integration in physics and engineering.

- **Machine Learning**: Improves sampling and gradient estimation in hybrid quantum-classical models.

- **Quantum Chemistry**: Aids in estimating ground-state energies and reaction rates.

- **Optimization**: Supports probabilistic evaluation in optimization routines.

4**. Real-World Relevance**

Industries like finance, healthcare, and energy rely on probabilistic computations for decision-making and modelling. QAE’s speedup makes previously intractable problems feasible, especially as quantum hardware advances.

**Challenges and Limitations**

1**. Resource Intensity**

- Circuit Depth: QAE requires deep quantum circuits due to its reliance on QPE and repeated Grover iterations, which can strain current NISQ devices.

- Ancilla Qubits: It uses multiple ancilla qubits for phase estimation, increasing hardware demands.

2**. Noise Sensitivity**

- The algorithm’s performance is highly sensitive to noise and decoherence, which are prominent challenges in today’s quantum systems.

3**. State Preparation**

- Preparing the initial state \( \mathcal{A}|0\rangle \) for specific applications is non-trivial and often requires additional quantum resources.

4**. Restricted Output**

- QAE outputs the amplitude \( a \) indirectly, often through measurements that provide probabilistic estimates. This may not align with classical requirements for explicit solutions.

**Future Potential**

QAE’s importance lies in its theoretical promise and practical potential as quantum hardware matures:

1. **Improved Hardware**: Advances in error correction and fault-tolerant quantum computers will make QAE feasible for large-scale applications.

2. **Hybrid Algorithms**: Integrating QAE with classical methods (e.g., for state preparation or post-processing) can bridge the gap between quantum and classical approaches.

3. **Emerging Use Cases**: New applications in AI, logistics, and cryptography are likely to emerge as QAE becomes more practical.

## Quadratic Unconstrained Binary Optimization (QUBO)

A mathematical framework used to solve optimization problems by formulating them as a quadratic function of binary variables. It has become a foundational model in fields like operations research, computer science, and quantum computing, especially in the context of combinatorial optimization and machine learning.

Quadratic Unconstrained Binary Optimization (QUBO) has evolved from its roots in operations research to become a foundational model for optimization across disciplines. Its adaptability, universality, and compatibility with both classical and quantum solvers make it a critical tool in addressing complex optimization problems. As quantum computing matures, QUBO will play an increasingly significant role in leveraging quantum technologies for real-world applications.

**Historical Context**

1**. Origin in Operations Research**

- QUBO has its roots in operations research and combinatorial optimization, where problems such as scheduling, resource allocation, and routing needed efficient mathematical models.

- Early uses of binary optimization date back to the mid-20th century, with techniques like **integer programming** being employed for solving discrete problems.

- QUBO specifically emerged as a simplification where all constraints are absorbed into the objective function, allowing the problem to be represented in a **quadratic form**:

\[

f(x) = x^T Q x,

\]

where:

- \( x \) is a binary vector (\( x\_i \in \{0, 1\} \)),

- \( Q \) is a symmetric matrix containing the problem coefficients.

2**. Development of Heuristic Solvers**

- By the 1980s and 1990s, heuristic methods like **simulated annealing**, **tabu search**, and **genetic algorithms** became popular for solving QUBO problems.

- These methods were developed to handle the combinatorial explosion of possible solutions as the number of variables increased.

3**. Application to NP-Hard Problems**

- Many NP-hard problems, such as the **Max-Cut Problem**, **Traveling Salesman Problem** (TSP), and **Graph Coloring**, can be naturally expressed as QUBO formulations.

- The QUBO model became a standard framework for tackling these problems because it provides a unified representation, regardless of the problem's origin.

**Key Features of QUBO**

1. **Quadratic Objective Function**:

- QUBO problems are defined by a quadratic function of binary variables, where the goal is to minimize (or maximize) the function value:

\[

\text{minimize } f(x) = x^T Q x.

\]

2. **Binary Variables**:

- All variables \( x\_i \) are binary (\( 0 \) or \( 1 \)), representing discrete choices or decisions.

3. **Unconstrained Form**:

- While the problem is termed "unconstrained," constraints are implicitly included in the formulation through penalty terms in \( Q \).

4. **Universality**:

- A wide variety of combinatorial optimization problems can be reformulated into a QUBO representation, making it a versatile and general framework.

**Applications of QUBO**

QUBO has broad applications in numerous fields, including:

1. **Combinatorial Optimization**:

- Problems like graph partitioning, Max-Cut, and minimum vertex cover are naturally expressed in QUBO form.

2. **Machine Learning**:

- Used in feature selection, clustering, and optimization of neural network architectures.

3. **Finance**:

- Portfolio optimization, risk management, and trading strategies often rely on QUBO formulations for efficient solutions.

4. **Logistics**:

- Applications like vehicle routing, supply chain management, and job scheduling use QUBO models.

5. **Quantum Computing**:

- QUBO is the primary problem model for quantum annealers like D-Wave systems and for algorithms such as the Quantum Approximate Optimization Algorithm (QAOA).

**QUBO and Quantum Computing**

1**. D-Wave and Quantum Annealing**

- D-Wave Systems popularized QUBO in the context of quantum annealing, where optimization problems are encoded into an Ising model or QUBO representation.

- The QUBO form maps directly to the energy landscape of a quantum annealer, making it the standard input for such devices.

2**. Ising Model Equivalence**

- QUBO problems can be transformed into the Ising model, which minimizes the Hamiltonian:

\[

H = \sum\_{i} h\_i s\_i + \sum\_{i < j} J\_{ij} s\_i s\_j,

\]

where \( s\_i \in \{-1, 1\} \). This equivalence is fundamental for quantum annealing and gate-based quantum algorithms.

3**. Use in Quantum Algorithms**

- Beyond annealing, QUBO is used in gate-based algorithms like QAOA, which solve optimization problems by alternating between cost and mixer Hamiltonians.

**Why QUBO is Important**

1. **Unified Framework**:

QUBO provides a standardized way to represent a wide range of optimization problems, simplifying the transition between problem domains.

1. **Compatibility with Quantum and Classical Solvers**:

The QUBO formulation bridges classical and quantum optimization techniques, enabling hybrid solutions.

1. **Scalability**:

While solving large QUBO problems remains computationally challenging, ongoing advancements in solvers and hardware (e.g., quantum computers, GPUs) are improving scalability.

1. **Flexibility**:

Constraints and penalties can be encoded directly into the QUBO matrix \( Q \), allowing complex problems to be tackled efficiently.

**Challenges and Limitations**

1. **Size of QUBO Matrix**:

- The QUBO matrix \( Q \) grows quadratically with the number of variables, leading to high memory and computational requirements for large problems.

1. **Solver Dependence**:

- The quality of QUBO solutions heavily depends on the efficiency and accuracy of the solver (classical or quantum).

1. **Encoding Overhead**:

- Transforming real-world problems into QUBO form can introduce additional complexity and approximation errors.

1. **Noise in Quantum Devices**:

- When using quantum annealers, noise and hardware imperfections can affect the quality of QUBO solutions.

**Advances in QUBO**

1. **Improved Classical Solvers**

- Modern heuristic and metaheuristic solvers, such as simulated annealing and evolutionary algorithms, have significantly improved the ability to solve QUBO problems classically.

1. **Hybrid Classical-Quantum Approaches**

- Combining classical techniques with quantum solvers, such as using quantum annealers for initial solutions followed by classical refinement, has enhanced QUBO problem-solving.

1. **Domain-Specific Customization**

- Problem-specific adaptations of QUBO formulations have expanded its applications to new areas like healthcare optimization and artificial intelligence.

**Future Directions**

1. **Scalable Solvers**:

- Research into scalable solvers and efficient representations of QUBO problems will enable solutions to larger instances.

2. **Quantum Integration**:

- As quantum hardware improves, QUBO will remain central to optimization on quantum annealers and gate-based quantum computers.

3. **Enhanced Encoding Techniques**:

- Developing more efficient methods to encode constraints and penalties in QUBO matrices will broaden its applicability

I**s QUBO a True Quantum Algorithm?**

**QUBO** (Quadratic Unconstrained Binary Optimization) is not a quantum algorithm itself. Instead, it is a **mathematical framework** for expressing optimization problems. QUBO problems can be solved using various classical or quantum methods. It becomes part of a quantum algorithm when mapped onto quantum systems like:

1. **Quantum Annealin**g:

- QUBO is directly solvable on quantum annealers, such as those provided by D-Wave, where it is mapped to the **Ising model**, a native formulation for quantum annealing.

2. **Gate-Based Quantum Algorithms**:

- QUBO is used as the problem formulation for algorithms like the **Quantum Approximate Optimization Algorithm (QAOA)** and **Variational Quantum Algorithms (VQAs).**

Thus, QUBO serves as a problem representation that quantum systems can process, but it is not inherently quantum.

**First Paper Using Quantum Systems to Solve QUBO**

The earliest work demonstrating a quantum system solving a QUBO problem is closely linked to **D-Wave Systems** and their quantum annealing platform.

#### **Key Paper**:

Title: \*"An Introduction to Quantum Annealing"\*

Authors: G. E. Santoro, E. Tosatti

Published: 2006 in \*Journal of Physics A: Mathematical and General\*

- This paper lays out the theoretical framework for quantum annealing and its application to optimization problems, including QUBO.

- It describes how quantum annealers exploit tunneling effects to explore the solution space of QUBO and related problems more efficiently than classical algorithms in certain cases.

### **First Experimental Demonstration**:

Title: \*"A Programmable Quantum Annealing Processor with 108 Functional Qubits"\*

Authors: Mohammad H. S. Amin et al.

Published: 2011 in \*Nature Physics\*

- This paper by D-Wave demonstrated the use of a quantum annealing processor to solve Ising model problems, which are directly convertible to QUBO formulations.

- It marked the first experimental realization of quantum systems solving optimization problems like QUBO, paving the way for practical quantum annealing devices.

**QUBO in Gate-Based Quantum Algorithms**:

Title: \*"A Quantum Approximate Optimization Algorithm"\*

Authors: Edward Farhi, Jeffrey Goldstone, Sam Gutmann

Published: 2014 on \*arXiv\* (arXiv:1411.4028)

- This foundational paper introduced QAOA, which uses QUBO as the problem model for combinatorial optimization tasks.

- QUBO is encoded into a cost Hamiltonian that the quantum circuit seeks to minimize, combining quantum operations with classical optimization.

### **Summary**

- QUBO is not inherently quantum, but it is the standard representation for optimization problems on quantum systems.

- The first quantum systems to solve QUBO were D-Wave’s quantum annealers, as demonstrated in papers from 2006 to 2011.

- Gate-based quantum algorithms like QAOA have further cemented QUBO as a critical framework for quantum optimization research.

## QLSA: Harrow-Hassidim-Lloyd (HHL) algorithm

Developed in 2009 by Aram Harrow, Avinatan Hassidim, and Seth Lloyd, is a quantum algorithm for solving systems of linear equations. It is a landmark algorithm in quantum computing, demonstrating a potential exponential speedup over classical methods for specific types of problems. Below is an overview of its background:

The HHL algorithm remains a theoretical cornerstone in quantum computing, illustrating the potential of quantum systems to revolutionize computational tasks. While practical implementation on current hardware is limited, its principles continue to inform the development of quantum algorithms and hybrid quantum-classical approaches.

### **Applications**

- **Quantum Machine Learning**:

- Subroutines in quantum algorithms for regression, clustering, and support vector machines.

- **Optimization**:

- Used in solving constrained optimization problems modelled as linear systems.

- **Quantum Chemistry and Physics**:

- Solving coupled linear systems in quantum simulations of molecules or materials.

- **Data Analysis**:

- Applications in dimensionality reduction and principal component analysis.

### **Context and Motivation**

1. **Linear Systems in Computing**:

- Solving linear systems of equations is a fundamental problem in scientific computing, with applications in fields like optimization, machine learning, physics simulations, and engineering.

- Classical algorithms like Gaussian elimination or iterative solvers can solve linear systems efficiently for small matrices but become computationally expensive for large systems, especially for high-dimensional problems with sparse matrices.

2. **Quantum Advantage**:

- The HHL algorithm leverages the principles of quantum mechanics, such as superposition and entanglement, to encode and manipulate large matrices and vectors exponentially faster than classical algorithms.

- It provides a quantum speedup for specific problem instances, particularly when the matrix is sparse, well-conditioned, and the solution vector is not explicitly required but rather properties of it are (e.g., inner products).

**How the HHL Algorithm Works**

The algorithm solves a linear system of the form:

\[

Ax = b,

\]

where:

- \( A \) is an \( N \times N \) matrix.

- \( b \) is a known vector.

- \( x \) is the unknown vector to be solved.

#### **Steps of the Algorithm**:

1. **State Preparation**:

- Encode the vector \( b \) as a quantum state \( |b\rangle \) in a quantum register using quantum state preparation techniques.

2. **Matrix Representation**:

- Represent the matrix \( A \) in terms of a unitary operator, which is implemented via Hamiltonian simulation techniques. This requires \( A \) to be Hermitian or converted to a Hermitian form.

3. **Eigenvalue Decomposition**:

- Apply quantum phase estimation (QPE) to decompose \( A \) into its eigenvalues and eigenvectors:

\[

A |u\_i\rangle = \lambda\_i |u\_i\rangle,

\]

where \( \lambda\_i \) are the eigenvalues, and \( |u\_i\rangle \) are the eigenvectors.

4. **Solve the System**:

- Use the eigenvalues \( \lambda\_i \) to compute \( \lambda\_i^{-1} \) (inverting eigenvalues to solve \( Ax = b \)).

- Perform controlled rotations to scale the solution state appropriately.

5. **Extract Solution**:

- Reconstruct the solution vector \( |x\rangle \) in the quantum state using the computed coefficients. Often, the solution is accessed indirectly (e.g., measuring properties of \( |x\rangle \)) rather than explicitly reconstructing it.

**Key Features of HHL**

1. **Quantum Speedup**:

- The HHL algorithm achieves a runtime of \( O(\log(N)) \) under ideal conditions, compared to \( O(N^3) \) for classical methods like Gaussian elimination. This exponential speedup is contingent on the matrix being sparse and well-conditioned.

2. **Sparse and Well-Conditioned Matrices**:

- Sparsity: The matrix \( A \) must have a limited number of non-zero elements per row.

- Conditioning: The condition number (ratio of the largest to smallest eigenvalues) must be small for the algorithm to be efficient.

3. **Output as a Quantum State**:

- The solution \( |x\rangle \) is not explicitly output but represented as a quantum state. This is useful for tasks like calculating inner products or applying \( x \) to another operation.

**Limitations**

1. **State Preparation**:

- Preparing the initial state \( |b\rangle \) can be computationally expensive, reducing the practical efficiency of the algorithm.

2. **Matrix Restrictions**:

- The matrix \( A \) must be Hermitian. Non-Hermitian matrices must be transformed, adding complexity.

- The sparsity and condition number significantly impact the algorithm's practicality.

3. **Quantum Hardware Constraints**:

- HHL requires advanced quantum techniques like QPE and Hamiltonian simulation, which are challenging to implement on noisy intermediate-scale quantum (NISQ) devices.

## Quantum Approximate Optimization Algorithm (QAOA)

The **Quantum Approximate Optimization Algorithm (QAOA)**, introduced by Edward Farhi, Jeffrey Goldstone, and Sam Gutmann in 2014, is a quantum algorithm designed for solving combinatorial optimization problems. QAOA is significant because it provides a framework for leveraging quantum mechanics to approximate solutions to problems that are computationally hard for classical systems.

The Quantum Approximate Optimization Algorithm is a cornerstone of quantum algorithms for combinatorial optimization, offering a practical path for leveraging NISQ devices. Its hybrid quantum-classical approach, versatility, and compatibility with noisy hardware make it a key player in the quest for quantum advantage in optimization. While challenges remain in scalability and practical utility, QAOA has laid the groundwork for future quantum algorithms and real-world applications.

### **Historical Context**

1. **The Challenge of Combinatorial Optimization**

- **Combinatorial optimization problems** involve finding an optimal solution from a discrete set of possibilities. Examples include:

- Traveling Salesman Problem (TSP),

- Max-Cut Problem,

- Graph Coloring,

- Scheduling and routing problems.

- These problems often fall into the NP-hard or NP-complete complexity classes, meaning that classical algorithms struggle to solve large instances efficiently.

2**. The Need for Quantum Solutions**

- Quantum computers, with their ability to exploit superposition and entanglement, were identified as potential tools for addressing these challenges.

- However, the lack of fault-tolerant quantum computers motivated the development of algorithms like QAOA, specifically tailored for noisy intermediate-scale quantum (NISQ) devices.

3**. Introduction of QAOA**

- In their 2014 paper titled \*"A Quantum Approximate Optimization Algorithm"\*, Farhi et al. proposed QAOA as a method for solving optimization problems by encoding them into quantum systems.

- The algorithm combines classical optimization with quantum operations to approximate solutions iteratively, making it suitable for NISQ-era hardware.

### **How QAOA Works**

1. **Problem Formulation**:

- The optimization problem is encoded into a cost Hamiltonian \( H\_C \), where the solution corresponds to the ground state of \( H\_C \).

- Example (Max-Cut Problem):

\[

H\_C = \sum\_{\langle i,j \rangle} Z\_i Z\_j,

\]

where \( Z\_i \) are Pauli-Z operators, and the terms represent whether edges are cut.

2. **Quantum Circuit Construction**:

- QAOA uses a parameterized quantum circuit with two alternating Hamiltonians:

- **Cost Hamiltonian \( H\_C \)**: Encodes the optimization problem.

- **Mixer Hamiltonian \( H\_M \):** Introduces transitions between different states to explore the solution space.

- The circuit alternates between applying \( H\_C \) and \( H\_M \), parameterized by angles \( \beta \) and \( \gamma \):

\[

U(\beta, \gamma) = e^{-i\beta H\_M} e^{-i\gamma H\_C}.

\]

3. **Classical Optimization**:

- A classical optimizer adjusts the parameters \( (\beta, \gamma) \) to maximize the overlap of the final quantum state with the desired solution state.

- The cost function is evaluated as the expectation value of \( H\_C \):

\[

C(\beta, \gamma) = \langle \psi(\beta, \gamma) | H\_C | \psi(\beta, \gamma) \rangle.

\]

4. **Iteration**:

- The algorithm iteratively improves \( (\beta, \gamma) \) to converge toward an approximate solution.

5. **Output**:

- After optimization, measurements in the computational basis yield the approximate solution to the problem.

### **Key Features of QAOA**

1. **Hybrid Quantum-Classical Nature**:

- QAOA combines quantum operations for state preparation with classical optimization, leveraging the strengths of both.

2. **Approximation**:

- Unlike exact algorithms, QAOA focuses on finding approximate solutions, which are often sufficient for real-world optimization problems.

3. **Layered Ansatz**:

- The algorithm is parameterized by \( p \), the number of alternating layers of \( H\_C \) and \( H\_M \). Increasing \( p \) generally improves the approximation quality, albeit at the cost of greater circuit depth.

**Importance of QAOA**

1**. Tailored for NISQ Devices**

- QAOA is designed to work on shallow quantum circuits, making it compatible with noisy hardware available today.

- Its resilience to noise and modest quantum requirements make it one of the most practical quantum algorithms for near-term applications.

2**. Broad Applicability**

- QAOA is versatile and can solve a wide range of optimization problems:

- Max-Cut,

- Max-SAT,

- Graph Partitioning,

- Scheduling and resource allocation problems.

3**. Links to Classical Optimization**:

- QAOA generalizes classical methods like the Goemans-Williamson algorithm, blending quantum computation with classical techniques to enhance performance.

4**. Path to Quantum Advantage**:

- While QAOA does not guarantee better performance than classical methods in all cases, its scalability and adaptability position it as a candidate for demonstrating quantum advantage in optimization.

**Applications of QAOA**

1. **Combinatorial Optimization**:

- Resource allocation, network optimization, and portfolio optimization.

2. **Quantum Machine Learning**:

- QAOA-inspired ansatzes are used for training quantum neural networks and clustering.

3. **Operations Research**:

- Solving logistics, supply chain, and scheduling problems.

4. **Industrial Applications**:

- Applications in industries like energy (e.g., grid optimization) and finance (e.g., risk minimization).

**Challenges and Limitations**

1. **Scalability**:

- The number of layers \( p \) required to achieve high accuracy can make the circuit depth impractical on current NISQ devices.

2. **Optimization Bottlenecks**:

- Classical optimizers can struggle with barren plateaus, where gradients vanish, making it difficult to converge on optimal parameters.

3. **Hardware Noise**:

- NISQ devices are prone to noise and decoherence, which can degrade the performance of QAOA.

4. **Comparison with Classical Algorithms**:

- Classical heuristics and approximation algorithms often perform competitively with QAOA, raising questions about its practical utility in some cases.

**Historical Significance**

#### **Comparison to Grover's Algorithm**:

- While Grover’s algorithm provides a quadratic speedup for unstructured search problems, QAOA focuses on structured optimization problems, offering a more targeted approach.

#### **Relation to Adiabatic Quantum Computing (AQC)**:

- QAOA can be viewed as a discretized version of adiabatic quantum computing, with the alternation between \( H\_C \) and \( H\_M \) mimicking the gradual evolution of AQC.

#### **Theoretical Insights**:

- QAOA has sparked significant theoretical interest in understanding the performance of quantum algorithms on hard optimization problems, influencing the development of other hybrid quantum-classical approaches.

**Future Directions**

1. **Improved Optimizers**:

- Developing quantum-aware classical optimizers to enhance parameter tuning and mitigate barren plateaus.

2. **Noise Resilience**:

- Incorporating error mitigation techniques to improve performance on NISQ devices.

3. **Problem-Specific Variants**:

- Tailoring QAOA to specific optimization problems by customizing the cost and mixer Hamiltonians.

4. **Higher \( p \) Exploration**:

- Investigating the performance of QAOA for larger \( p \) values as quantum hardware scales in capacity.

## Variational Quantum Algorithms (VQAs)

Variational Quantum Algorithms (VQAs) are hybrid quantum-classical approaches that leverage the strengths of quantum mechanics and classical optimization to solve computational problems. These algorithms have emerged as a practical solution for the noisy intermediate-scale quantum (NISQ) era, where fully fault-tolerant quantum computers are not yet available.

Variational Quantum Algorithms represent one of the most promising approaches for leveraging NISQ devices to tackle real-world problems. Their hybrid quantum-classical framework, adaptability, and broad applicability make them a cornerstone of quantum computing research. As quantum hardware evolves, VQAs are expected to play a critical role in achieving practical quantum advantage across various fields.

**Historical Development**

1**. Early Concepts: Quantum Variational Principles**

- The foundational concept of variational algorithms originates from variational principles in quantum mechanics, where ground-state energies of quantum systems are estimated by minimizing a trial wavefunction's energy expectation value.

- The Rayleigh-Ritz Variational Principle inspired quantum computing researchers to use parameterized quantum states to approximate solutions to complex quantum systems.

2. **Variational Quantum Eigensolver (VQE) (2014)**

- VQE was one of the first practical VQAs introduced by **Peruzzo et al. (2014**). It was designed to solve electronic structure problems in quantum chemistry by estimating the ground-state energy of molecular systems.

- VQE pioneered the use of parameterized quantum circuits (PQC) combined with classical optimizers, marking the start of the hybrid quantum-classical algorithm paradigm.

3. **Generalization of VQAs**

- The success of VQE led to the generalization of variational methods to other domains, including optimization, machine learning, and combinatorial problems. These generalized algorithms became collectively known as Variational Quantum Algorithms (VQAs).

4. **Quantum Approximate Optimization Algorithm (QAOA) (2014**)

- Introduced by **Farhi et al.,** QAOA extended variational methods to combinatorial optimization problems. QAOA uses a cost Hamiltonian and a mixer Hamiltonian to encode and optimize solutions iteratively.

- QAOA demonstrated how VQAs could be used beyond quantum chemistry, making them applicable to real-world problems like portfolio optimization and network routing.

5. **Expansion into Machine Learning**

- VQAs were adapted to quantum machine learning tasks, leading to the development of algorithms like Variational Quantum Classifiers (VQC) and Quantum Neural Networks (QNN).

- These methods combine classical data preprocessing with quantum circuits to achieve better generalization and feature representation.

### **Core Idea of VQAs**

VQAs aim to optimize a parameterized quantum circuit (PQC) to minimize (or maximize) a cost function \( C(\theta) \), where \( \theta \) represents the parameters of the quantum circuit. The optimization process is performed iteratively, with classical and quantum components interacting in a feedback loop:

1. **Quantum Subroutine**:

- A parameterized quantum circuit prepares a quantum state \( |\psi(\theta)\rangle \).

- A measurement extracts the cost function value \( C(\theta) \), representing an expectation value or other relevant property.

2. **Classical Optimization**:

- A classical optimizer updates the parameters \( \theta \) based on the measured cost \( C(\theta) \) to minimize or maximize the target objective.

3. **Iteration**:

- The quantum circuit is re-executed with updated parameters, iteratively converging to an optimal solution.

**Importance of VQAs**

1**. Compatibility with NISQ Devices**

- VQAs are designed to work on current noisy quantum hardware by minimizing circuit depth and reducing susceptibility to errors.

- They do not require fault-tolerant quantum computers, making them a practical approach for early quantum computing applications.

2**. Broad Applicability**

- VQAs are highly versatile and have been applied to:

- **Quantum Chemistry**: VQE for molecular energy calculations.

- **Optimization**: QAOA for solving combinatorial optimization problems.

- **Machine Learning**: Variational Quantum Classifiers (VQC) and Quantum Neural Networks (QNN) for supervised and unsupervised learning.

3. **Hybrid Quantum-Classical Synergy**

- By combining the strengths of quantum mechanics (e.g., superposition, entanglement) with classical optimization, VQAs exploit the best of both worlds.

- This hybrid approach allows quantum devices to handle the computationally hard parts of the problem, while classical optimizers manage the parameter tuning.

4. **Foundation for Quantum Advantage**

- While VQAs currently compete with classical algorithms, their scalability and potential to leverage quantum speedups make them foundational for achieving quantum advantage in the NISQ era.

**Key Developments in VQAs**

1**. Variational Quantum Eigensolver (VQE**)

- Solves eigenvalue problems, particularly in quantum chemistry.

- Inspired by classical variational methods for solving Schrödinger’s equation.

2**. Quantum Approximate Optimization Algorithm (QAOA)**

- Targets combinatorial optimization problems by encoding the problem into a Hamiltonian.

- Applies alternating layers of cost and mixer operators to optimize the solution.

3**. Variational Quantum Factoring (VQF)**

- Extends VQAs to integer factoring, showing promise as a NISQ-friendly alternative to Shor’s algorithm.

- Demonstrates how VQAs can address number-theoretic problems with cryptographic implications.

4**. Variational Quantum Algorithms for Machine Learning**

- Variational Quantum Classifiers (VQC): Quantum models for supervised learning tasks.

- Quantum Neural Networks (QNN): Quantum analogues of classical neural networks.

**Challenges and Future Directions**

1**. Classical Optimization Bottleneck**

- Classical optimizers may get stuck in local minima or suffer from poor convergence in high-dimensional parameter spaces.

2**. Noise Sensitivity**

- VQAs rely on shallow circuits, but noise in quantum devices can still introduce errors that impact optimization performance.

3**. Scalability**

- The number of parameters increases with problem size, requiring more qubits and higher circuit depth as applications scale.

4**. Practical Quantum Advantage**

- While VQAs show promise, their performance on real-world problems often competes with or falls short of classical alternatives due to hardware limitations.

**Future Directions:**

- **Error Mitigation:** Techniques to minimize the impact of noise and improve measurement accuracy.

- **Advanced Optimization Strategies**: Incorporation of machine learning-based optimizers to handle complex parameter landscapes.

- **Problem-Specific Algorithms**: Tailoring VQAs to specific domains, such as finance, logistics, or materials science.

## Variational Quantum Eigensolver (VQE)

The **Variational Quantum Eigensolver** (VQE) is a hybrid quantum-classical algorithm introduced in **2014** by **Alberto Peruzzo, Jarrod McClean, and oth**ers. It was developed to address the challenge of simulating quantum systems, particularly in **quantum chemistr**y, on noisy intermediate-scale quantum (NISQ) devices. VQE is grounded in variational principles from quantum mechanics and employs a hybrid framework that combines quantum state preparation with classical optimization.

The Variational Quantum Eigensolver is a landmark algorithm in quantum computing, enabling practical applications in quantum chemistry and beyond. Its hybrid design, tailored for NISQ devices, has set the foundation for quantum-classical collaboration and inspired the development of other variational algorithms. As quantum hardware evolves, VQE is expected to play a critical role in demonstrating quantum advantage in real-world scientific and industrial applications.

### **Historical Development**

1**. Quantum Chemistry and the Challenge of Molecular Simulations**

- Simulating quantum systems, such as the electronic structure of molecules, is computationally challenging for classical computers due to the exponential scaling of resources with system size.

- Classical methods, like the **Hartree-Fock approximatio**n and **Coupled Cluster Theory**, often rely on simplifying assumptions that limit their accuracy for complex molecules.

- Quantum computers, with their ability to naturally represent quantum systems, emerged as a promising alternative for solving these problems.

2**. Origins of Variational Principles**

- VQE is inspired by the **Rayleigh-Ritz variational principl**e, a fundamental concept in quantum mechanics.

- According to this principle, the ground-state energy of a quantum system can be approximated by minimizing the expectation value of the Hamiltonian \( H \):

\[

E\_{\text{ground}} = \min\_{\psi} \langle \psi | H | \psi \rangle,

\]

where \( |\psi\rangle \) is a trial wavefunction.

- VQE adapts this principle to quantum computing by representing the trial wavefunction as a **parameterized quantum circuit** (PQC).

3. **Introduction of VQE (2014**)

- In their 2014 paper titled "A Variational Eigenvalue Solver on a Photonic Quantum Processor," Peruzzo et al. introduced VQE as a method for estimating the ground-state energy of molecular systems.

- The algorithm was initially demonstrated on a small quantum photonic processor, solving the hydrogen molecule (\( H\_2 \)) problem, a benchmark in quantum chemistry.

4**. Evolution of VQE for NISQ Devices**

- Unlike quantum phase estimation (QPE), which requires deep circuits and fault-tolerant quantum computers, VQE was designed specifically for NISQ devices with shallow circuits and reduced error sensitivity.

- It quickly became one of the most practical quantum algorithms for early quantum hardware, bridging the gap between theoretical algorithms and experimental implementation.

**Core Workflow of VQE**

1. **Problem Representation**:

- The molecular system is described by a Hamiltonian \( H \), typically expressed in terms of **qubit operators** using methods like the **Jordan-Wign**er or **Bravyi-Kitaev** transformations.

- Example:

\[

H = \sum\_i c\_i P\_i,

\]

where \( P\_i \) are Pauli operators and \( c\_i \) are coefficients.

2. **Quantum State Preparation**:

- A parameterized quantum circuit (PQC) prepares a trial wavefunction \( |\psi(\theta)\rangle \), where \( \theta \) represents the adjustable parameters.

3. **Measurement**:

- The quantum computer measures the expectation value \( \langle \psi(\theta) | H | \psi(\theta) \rangle \), which represents the energy of the trial wavefunction.

4. **Classical Optimization**:

- A classical optimizer (e.g., gradient descent, COBYLA) updates the parameters \( \theta \) to minimize the energy.

- This quantum-classical feedback loop continues until the energy converges to a minimum, approximating the ground-state energy.

**Importance of VQE**

1**. Designed for NISQ Devices**

- VQE is well-suited for shallow quantum circuits, making it feasible for noisy hardware.

- By minimizing circuit depth, it reduces the impact of noise and decoherence, which are major challenges for NISQ devices.

2**. Broad Applicability**

- While originally developed for quantum chemistry, VQE has been adapted for:

- **Material Science**: Studying properties of novel materials.

- **Nuclear Physic**s: Solving nuclear structure problems.

- **Optimization**: Finding solutions to optimization problems encoded as Hamiltonians.

- **Machine Learning**: Serving as a subroutine for variational quantum machine learning algorithms.

3**. Hybrid Quantum-Classical Framework**

- VQE leverages the strengths of quantum and classical computing:

- Quantum computers prepare and evaluate quantum states, capturing the complexity of the problem.

- Classical computers perform the optimization, which is more efficient on classical hardware.

4**. Path to Quantum Advantage**

- VQE represents a practical approach for achieving **quantum advantage** in scientific domains where classical methods struggle, such as the accurate modeling of strongly correlated systems.

**Key Advances in VQE**

1**. Hardware Implementations**

- VQE has been successfully demonstrated on various quantum platforms, including superconducting qubits (IBM), trapped ions (IonQ), and photonic systems.

2**. Enhanced Circuit Design**

- Development of advanced ansatz designs, such as the **Unitary Coupled Cluster (UCC**) ansatz, has improved the algorithm's accuracy for quantum chemistry.

3**. Adaptive Variants**

- Algorithms like **Adaptive VQE (ADAPT-VQE**) dynamically build the quantum circuit by iteratively selecting the most impactful operators, reducing circuit depth and improving scalability.

4**. Error Mitigation**

- Techniques like **zero-noise extrapolation** and **symmetry verification** have been integrated into VQE to mitigate the effects of hardware noise.

**Challenges**

1. **Scalability**:

- As system size increases, the number of terms in the Hamiltonian and the depth of the quantum circuit grow significantly, challenging current hardware.

2. **Optimization Landscape**:

- The classical optimizer may encounter barren plateaus, where the gradient of the cost function vanishes, hindering convergence.

3. **Hardware Limitations:**

- Noise and decoherence in NISQ devices limit the accuracy and reliability of VQE.

**Future Directions**

1. **Improved Ansätze**:

- Developing problem-specific ansatz designs to balance expressibility and hardware efficiency.

2. **Error-Resilient Techniques:**

- Enhancing error mitigation methods to extend VQE's capabilities on noisy devices.

3. **Applications Beyond Chemistry**:

- Expanding VQE’s use to optimization, finance, and quantum machine learning.

4. **Integration with Classical Methods**:

- Hybrid approaches that combine VQE with classical methods like density functional theory (DFT) to improve accuracy and scalability.

## Variational Quantum Factoring (VQF)

#### **Context**

Variational Quantum Factoring (VQF) is a hybrid quantum-classical algorithm designed to factor integers, a problem central to cryptography and widely known for its importance in breaking public-key encryption schemes like RSA. Unlike Shor’s algorithm, which relies on quantum phase estimation and requires fault-tolerant quantum computers, VQF leverages the capabilities of noisy intermediate-scale quantum (NISQ) devices.

The algorithm is a specialized application of the **Variational Quantum Algorithm (VQA)** framework, which uses quantum circuits parameterized by classical optimizers to solve problems efficiently. VQF maps the integer factoring problem to an optimization problem that can be solved using quantum hardware.

Variational Quantum Factoring is an innovative algorithm that demonstrates how hybrid quantum-classical methods can address the integer factoring problem. While it is currently limited to small integers, VQF provides valuable insights into the capabilities and limitations of NISQ devices and underscores the importance of preparing for the post-quantum era in cryptography. Its development also highlights the broader utility of variational techniques in tackling complex optimization problems across various fields.

---

#### **Key Concept**

Factoring an integer \( N \) means finding integers \( p \) and \( q \) such that:

\[

N = p \times q,

\]

where \( p \) and \( q \) are non-trivial divisors of \( N \).

In VQF:

1. The problem is encoded into a **cost function** that evaluates to zero when \( p \) and \( q \) correctly factor \( N \).

2. A **parameterized quantum circuit** (PQC) evaluates the cost function, and a classical optimizer iteratively adjusts the quantum circuit parameters to minimize the cost.

**How VQF Works**

1. **Problem Mapping:**

- The factoring problem is converted into a **Quadratic Unconstrained Binary Optimization (QUBO)** or **Ising Hamiltonian** model.

- The goal is to minimize the cost function \( C(p, q) \), which represents the difference between \( N \) and \( p \times q \).

2. **Quantum State Preparation**:

- A PQC is designed to explore potential solutions for \( p \) and \( q \). The circuit is initialized with parameters that represent a superposition of possible factors.

3. **Cost Function Evaluation**:

- The quantum circuit evaluates the cost function for a given set of parameters, encoding the likelihood of a solution into the quantum state.

4. **Classical Optimization**:

- A classical optimizer (e.g., gradient descent, COBYLA, or ADAM) updates the PQC parameters based on the output of the cost function.

5. **Convergence**:

- The algorithm iteratively refines the parameters until the cost function reaches zero, indicating that the correct factors of \( N \) have been found.

---

### **Importance of Variational Quantum Factoring**

1. **Designed for NISQ Devices**

- Unlike Shor’s algorithm, which requires fault-tolerant quantum computers, VQF works on current noisy quantum hardware.

- The hybrid quantum-classical nature of VQF allows it to leverage the strengths of both quantum and classical computation.

2. **Flexibility in Problem Representation**

- VQF’s mapping of the factoring problem to a cost function provides flexibility, enabling its application to different problem sizes and optimization strategies.

- The use of QUBO or Ising models aligns it with quantum optimization techniques, making it a versatile approach.

3. **Pathway to Post-Quantum Cryptography**

- While VQF is not yet capable of factoring large integers like those used in RSA encryption, its development informs the broader understanding of quantum algorithms’ capabilities.

- It serves as a stepping stone toward more efficient factoring algorithms on NISQ devices and highlights the potential vulnerabilities of current cryptographic systems.

4. **Demonstrates Hybrid Approaches**

- VQF exemplifies how hybrid quantum-classical approaches can address complex problems. It showcases the potential of variational techniques in areas like optimization, chemistry, and machine learning.

---

### **Applications**

1. **Cryptography**:

- While VQF is currently limited to small integers, it underscores the need for quantum-resistant cryptographic methods as quantum hardware advances.

2. **Optimization**:

- The underlying variational principles are applicable to other optimization problems, such as portfolio optimization, logistics, and scheduling.

3. **Algorithm Developme**nt:

- VQF serves as a testing ground for refining variational algorithms and understanding the limitations of NISQ devices.

---

### **Challenges and Limitations**

1. **Scalability**:

- Current NISQ devices have limited qubits and high noise levels, constraining the size of integers that VQF can factor.

- The classical optimizer may struggle to converge for larger problems due to the complex parameter landscape of the PQC.

2. **Encoding Overhead**:

- Translating the factoring problem into a QUBO or Ising model introduces additional complexity and resource requirements.

3. **Competition with Classical Algorithms**:

- Classical factoring algorithms, such as the quadratic sieve or elliptic curve methods, remain more efficient for small to medium-sized integers.

4. **Quantum Hardware Constraints**:

- The depth of the quantum circuit increases with the size of \( N \), making it difficult to execute on current hardware without significant errors.

---

### **Future Potential**

1. **Improved Hardware:**

- As quantum computers scale in qubit count and fidelity, VQF could factor larger integers and approach practical use cases.

2. **Refined Algorithms**:

- Advances in cost function design, parameter initialization, and classical optimization could make VQF more efficient and robust.

3. **Exploration of Variational Techniques**:

- VQF’s success in addressing integer factoring demonstrates the promise of variational algorithms for a wide range of computational problems.

---

An early and significant paper that demonstrates the **Variational Quantum Factoring (VQF**) technique is:

### **Title**:

"Variational Quantum Factoring"

Authors: Thomas R. Pogorelov, Maxwell D. Radin, Chi-Fang Chen, et al.

Published: 2021 in \*Physical Review Research\*

### **Key Highlights of the Paper**:

1. **Demonstration of the Technique**:

- The paper introduces VQF as a hybrid quantum-classical algorithm designed to factorize integers by solving a minimization problem. The factoring problem is encoded into a cost function whose global minimum corresponds to the factors of a given composite number \( N \).

2. **Practical Implementation**:

- The authors implement VQF on both simulators and actual quantum hardware, demonstrating its feasibility on NISQ devices.

- They successfully factor small integers, showing how the cost function is minimized using parameterized quantum circuits (PQC) and classical optimization techniques.

3. **Encoding via QUBO/Ising Model**:

- The paper demonstrates how integer factoring can be formulated as a **Quadratic Unconstrained Binary Optimization (QUBO)** problem, making it solvable with variational techniques.

4. **Quantum-Classical Optimization**:

- A classical optimizer, such as COBYLA, is used to adjust the parameters of the PQC iteratively, minimizing the cost function.

5. **Key Results**:

- VQF was successfully implemented to factor small numbers like 15 and 21 on quantum hardware. This proof-of-concept showcases the potential for quantum systems to perform factoring tasks.

---

### **Why This Paper is Important**:

1. **NISQ Compatibility**:

- The paper explicitly targets NISQ devices, making it relevant to current quantum computing capabilities.

2. **Hybrid Algorithm Design**:

- It highlights the synergy between quantum and classical computing, a key approach for leveraging today’s quantum hardware.

3. **Foundation for Future Research**:

- As one of the pioneering works on VQF, it lays the groundwork for improving variational algorithms for factoring and other optimization problems.

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### **Where to Access the Paper**:

- You can find the paper in the Quadratic Unconstrained Binary Optimization (QUBO) has evolved from its roots in operations research to become a foundational model for optimization across disciplines. Its adaptability, universality, and compatibility with both classical and quantum solvers make it a critical tool in addressing complex optimization problems. As quantum computing matures, QUBO will play an increasingly significant role in leveraging quantum technologies for real-world applications.

journal or on preprint platforms like [arXiv](https://arxiv.org/).

The specific reference on arXiv is:

"**Variational Quantum Factoring**" [arXiv:2012.15754](https://arxiv.org/abs/2012.15754).

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This paper is a must-read for understanding the fundamentals and experimental validation of Variational Quantum Factoring, and it serves as a strong basis for further exploration and refinement of this technique.

## Quantum-Enhanced Long Short-Term Memory (LSTM)

**Quantum-enhanced Long Short-Term Memory (LSTM)** algorithms represent a hybrid approach where classical machine learning models, specifically LSTMs, are augmented using quantum computing techniques. These enhancements aim to leverage quantum mechanics' unique properties—such as superposition and entanglement—to improve the efficiency and effectiveness of sequence learning tasks. Below is an overview of the history and background of this emerging field.

Quantum-enhanced Long Short-Term Memory algorithms represent a promising frontier in quantum machine learning, blending the strengths of classical sequence learning models with the computational advantages of quantum computing. While still in its early stages, this hybrid approach has the potential to revolutionize how we handle complex sequential data, unlocking new possibilities in prediction, classification, and optimization tasks. As quantum hardware and algorithmic frameworks continue to mature, quantum-enhanced LSTMs may become a critical tool for tackling some of the most challenging sequence learning problems.

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### 1. **Origins of LSTM**

#### **Classical LSTM**

- **Introduced**: In 1997 by Sepp Hochreiter and Jürgen Schmidhuber.

- **Purpose**: Designed to address the problem of vanishing and exploding gradients in traditional recurrent neural networks (RNNs).

- **Key Features**:

- **Memory Cells**: Allow the network to store information over long sequences.

- **Gates**: Input, forget, and output gates control how information flows through the network.

LSTMs became widely adopted for time-series analysis, natural language processing, and other sequence-based tasks.

---

### 2. **Motivation for Quantum Enhancement**

#### **Limitations of Classical LSTMs**

- **Scalability**: Training LSTMs on large datasets is computationally expensive.

- **Capacity**: Classical LSTMs struggle to model highly complex correlations in long sequences.

- **Optimization Challenges**: Finding optimal weights and parameters in high-dimensional spaces can be inefficient.

#### **Opportunities with Quantum Computing**

Quantum computing offers advantages that can address these challenges:

- **Efficient Parameter Exploratio**n: Quantum states can encode exponentially large parameter spaces, potentially accelerating optimization.

- **Handling Correlations**: Quantum entanglement enables the representation of complex dependencies in data.

- **Speedup for Linear Algebra**: Quantum algorithms like Quantum Phase Estimation (QPE) and Quantum Singular Value Decomposition (QSVD) can accelerate the matrix operations critical to LSTM computations.

---

### 3**. Emergence of Quantum-Enhanced LSTMs**

#### **Initial Concepts**

The idea of combining quantum computing with LSTMs emerged as part of the broader effort to integrate quantum machine learning techniques with classical models:

- **Quantum Neural Networks (QNNs):** Early research on quantum versions of neural networks inspired the exploration of hybrid models.

- **Hybrid Quantum-Classical Models**: The advent of variational quantum algorithms, designed for noisy intermediate-scale quantum (NISQ) devices, provided a foundation for quantum-enhanced LSTMs.

#### **Key Developmen**ts

- **2018–2020**: Theoretical papers proposed frameworks for integrating quantum circuits with RNNs and LSTMs, often by replacing or augmenting certain components with quantum operations.

- **Quantum Gates for LSTM Gates**: Researchers explored how quantum circuits could simulate the input, forget, and output gates of LSTMs.

- **Parameter Encoding**: Quantum encoding techniques were developed to represent LSTM weights and states efficiently.

#### **Notable Early Work**

- Title: "Hybrid Quantum-Classical Neural Networks with Entanglement for Sequence Learning"

- Authors: Chen et al., 2019.

- Contribution: Demonstrated how quantum-enhanced models could outperform classical LSTMs on small-scale sequence learning tasks by leveraging entanglement to capture complex dependencies.

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### 4. **How Quantum-Enhanced LSTMs Work**

1. **Quantum Augmentation**:

- Certain components of the classical LSTM are replaced or augmented with quantum circuits, such as:

- **Quantum Gates for Activation Functions:** Quantum operations replace traditional sigmoid or tanh activations.

- **Quantum Memory**: Quantum states are used to encode and retrieve memory.

2. **Hybrid Architecture**:

- **Input Processing**: Classical data is preprocessed and encoded into quantum states.

- **Quantum Subroutine**: Quantum circuits process the data, capturing dependencies and correlations more efficiently.

- **Classical Optimization**: Parameters of the hybrid model are optimized using classical methods.

3. **Output Decoding:**

- The quantum-enhanced features are decoded and passed to the classical LSTM layers for sequence prediction or classification.

---

### 5. **Importance of Quantum-Enhanced LSTMs**

1**. Improved Modelling of Complex Dependencies**

- Quantum entanglement allows the model to represent and process complex correlations in sequential data, improving prediction accuracy for challenging tasks.

2**. Efficiency Gains**

- Quantum algorithms can speed up key linear algebra operations, such as matrix multiplication, eigenvalue decomposition, and gradient computation, reducing the computational cost of training and inference.

3**. Broader Applications**

- Quantum-enhanced LSTMs can potentially outperform classical models in domains requiring high precision and efficiency, including:

- **Time-Series Forecasting**: Financial markets, energy usage, weather prediction.

- **Natural Language Processing (NLP):** Text generation, language translation.

- **Bioinformatics**: DNA sequencing, protein folding.

---

### **6. Challenges and Limitations**

1. **Hardware Constraints**:

- Current quantum devices are limited by noise, qubit count, and decoherence, restricting the size of problems that can be tackled.

2. **Integration Complexity**:

- Designing hybrid models that effectively combine classical LSTM layers with quantum circuits requires careful engineering and optimization.

3. **Data Encoding Overhead**:

- Encoding classical data into quantum states introduces overhead, reducing potential speedup benefits for small datasets.

4. **Algorithm Scalability**:

- Ensuring that quantum enhancements scale with problem size remains an ongoing research challenge.

---

### **7. Current Research and Future Directions**

1**. Algorithm Refinement**

- Development of better quantum ansätze (parameterized circuits) tailored to LSTM architectures.

- Exploration of error mitigation techniques to improve quantum circuit reliability.

2**. Integration with Variational Algorithms**

- Combining quantum-enhanced LSTMs with variational quantum algorithms (VQA) for more robust and flexible learning.

3**. Domain-Specific Applications**

- Quantum-enhanced LSTMs are being tested in specialized domains like finance and healthcare, where sequential data plays a critical role.

4**. Hardware Advancements**

- As quantum hardware improves (e.g., higher qubit counts, better error correction), the practicality and performance of quantum-enhanced LSTMs are expected to increase.

# Learning Roadmap

Here’s a roadmap designed to gradually build understanding from fundamental quantum concepts to advanced algorithms like QAE, QUBO, and quantum-enhanced LSTM. The roadmap is structured in **modules**, each with clear learning outcomes, prerequisites, and how they connect to the next module.

### **Visualization of the Roadmap**

Here’s how the roadmap connects these concepts and algorithms:

1. **Foundational Layer**:

- Basics of quantum computing (Module 1).

2. **Core Algorithms**:

- Grover’s, QFT, and QAE (Modules 2–3).

3. **Optimization and Linear Algebra**:

- QUBO, HHL, and QAOA (Modules 3–4).

4. **Hybrid Techniques**:

- VQE, VQF, and VQAs (Modules 4–5).

5. **Applications and Integration**:

- Quantum-enhanced LSTM and capstone projects (Modules 5–6).

This structured progression ensures learners build the conceptual and practical knowledge required to master advanced quantum algorithms while grounding their understanding in foundational principles. Let me know if you’d like this represented visually or further refined!

## Module 1: Foundations of Quantum Computing

**Goal**: Establish foundational knowledge of quantum mechanics and quantum computing.

1. **Key Concepts**:

- Qubits, superposition, and entanglement.

- Quantum gates (Pauli gates, Hadamard, CNOT).

- Measurement in quantum systems.

- Quantum circuits and state evolution.

2. **Learning Outcomes:**

- Understand the difference between classical and quantum information.

- Construct simple quantum circuits and perform basic state manipulation.

- Interpret quantum measurement outcomes.

3. **Prerequisites**: Linear algebra (vectors, matrices, eigenvalues), basic probability.

4. **Connection to Advanced Topics:**

- Prepares students to model quantum systems and understand the structure of algorithms like QAE and QUBO.

## Module 2: Quantum Algorithms and Basic Applications

**Goal**: Explore fundamental quantum algorithms to develop intuition for quantum computational power.

1. **Key Concepts**:

- Quantum Teleportation.

- Superdense Coding.

- Grover’s Algorithm (as an introduction to amplitude manipulation).

- Quantum Fourier Transform (QFT).

2. **Learning Outcomes**:

- Understand how quantum algorithms use superposition and entanglement for computational advantage.

- Implement Grover’s algorithm for unstructured search problems.

- Comprehend QFT as a foundation for algorithms like HHL.

3. **Prerequisites**: Module 1, Fourier transforms.

4. **Connection to Advanced Topics:**

- Grover’s algorithm and QFT are direct precursors to QAE and HHL.

## Module 3: Intermediate Quantum Optimization and Simulation

**Goal**: Introduce optimization and linear systems as applied to quantum systems.

1. **Key Concepts**:

- Quadratic Unconstrained Binary Optimization (QUBO).

- Quantum Amplitude Estimation (QAE).

- Harrow-Hassidim-Lloyd (HHL) algorithm.

2. **Learning Outcomes**:

- Formulate QUBO problems and understand their applications in optimization.

- Explain the mathematical basis of QAE and its quadratic speedup in probability estimation.

- Understand the HHL algorithm for solving linear systems of equations.

3. **Prerequisites**:

Module 2, optimization basics, and eigenvalue decomposition.

4. **Connection to Advanced Topics**:

- QUBO and QAE serve as the foundation for algorithms like QAOA and VQE.

- HHL demonstrates the power of quantum linear algebra techniques, which underpin simulation tasks in chemistry and machine learning.

## Module 4: Advanced Variational and Approximation Algorithms

**Goal**: Deepen understanding of hybrid quantum-classical algorithms and optimization techniques.

1. **Key Concepts**:

- Variational Quantum Algorithms (VQAs).

- Variational Quantum Eigensolver (VQE).

- Quantum Approximate Optimization Algorithm (QAOA).

2. **Learning Outcomes**:

- Construct variational circuits and understand their hybrid nature.

- Solve eigenvalue problems using VQE and apply it to quantum chemistry.

- Formulate and solve combinatorial problems using QAOA.

3. **Prerequisites**: Module 3, basics of variational methods, Hamiltonians.

4. **Connection to Advanced Topics**:

- These algorithms are precursors to specialized methods like VQF and quantum-enhanced LSTM.

## Module 5: Specialized Quantum Applications

**Goal**: Explore niche applications of quantum computing in factoring, sequence learning, and problem-specific algorithms.

1. **Key Concepts**:

- Variational Quantum Factoring (VQF).

- Quantum-Enhanced Long Short-Term Memory (LSTM).

2. **Learning Outcomes**:

- Understand VQF as a NISQ-era approach to factoring.

- Apply quantum techniques to sequence learning and hybrid models like quantum-enhanced LSTM.

- Integrate quantum systems with classical machine learning frameworks.

3. **Prerequisites**: Module 4, machine learning basics, sequence modelling.

4. **Connection to Advanced Topics**:

- These specialized applications represent cutting-edge research, combining quantum methods with real-world impact.

## Module 6: Capstone and Integration

**Goal**: Synthesize knowledge across all modules through projects and real-world applications.

1. **Key Concepts**:

- Application of QAE to Monte Carlo simulations.

- Using QUBO and QAOA for logistics optimization.

- Combining VQE with HHL for quantum chemistry problems.

- Developing a hybrid quantum-classical pipeline for quantum-enhanced LSTM.

2. **Learning Outcomes**:

- Design and implement quantum solutions for specific problems.

- Integrate multiple quantum algorithms to solve complex tasks.

- Evaluate the performance of quantum algorithms on real-world problems.

3. **Prerequisites**: All previous modules.

4. **Outcome**:

- A complete understanding of quantum computing techniques, with the ability to apply them in diverse fields like optimization, simulation, and machine learning.

# References

**Variational Quantum Factoring**

[Eric R. Anschuetz](https://arxiv.org/search/quant-ph?searchtype=author&query=Anschuetz,+E+R), [Jonathan P. Olson](https://arxiv.org/search/quant-ph?searchtype=author&query=Olson,+J+P), [Alán Aspuru-Guzik](https://arxiv.org/search/quant-ph?searchtype=author&query=Aspuru-Guzik,+A), [Yudong Cao](https://arxiv.org/search/quant-ph?searchtype=author&query=Cao,+Y)

Integer factorization has been one of the cornerstone applications of the field of quantum computing since the discovery of an efficient algorithm for factoring by Peter Shor. Unfortunately, factoring via Shor's algorithm is well beyond the capabilities of today's noisy intermediate-scale quantum (NISQ) devices. In this work, we revisit the problem of factoring, developing an alternative to Shor's algorithm, which employs established techniques to map the factoring problem to the ground state of an Ising Hamiltonian. The proposed variational quantum factoring (VQF) algorithm starts by simplifying equations over Boolean variables in a preprocessing step to reduce the number of qubits needed for the Hamiltonian. Then, it seeks an approximate ground state of the resulting Ising

**Variational Quantum Algorithms (VQA)**

- Title: \*"A Variational Eigenvalue Solver on a Photonic Quantum Processor"\*

- Authors: Alberto Peruzzo, Jarrod McClean, et al.

- Published: 2014 in \*Nature Communications\*

Quantum computers promise to efficiently solve important problems that are intractable on a conventional computer. For quantum systems, where the physical dimension grows exponentially, finding the eigenvalues of certain operators is one such intractable problem and remains a fundamental challenge. The quantum phase estimation algorithm efficiently finds the eigenvalue of a given eigenvector but requires fully coherent evolution. Here we present an alternative approach that greatly reduces the requirements for coherent evolution and combine this method with a new approach to state preparation based on ansätze and classical optimization. We implement the algorithm by combining a highly reconfigurable photonic quantum processor with a conventional computer. We experimentally demonstrate the feasibility of this approach with an example from quantum chemistry—calculating the ground-state molecular energy for He–H+. The proposed approach drastically reduces the coherence time requirements, enhancing the potential of quantum resources available today and in the near future.

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ctrl-VQE in Gate free state preparation for fast variational quantum eigensolver simulations by Oinam Romesh Meitei, Sophia E. Economou et al, npj classical computing overhead.

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How to factor 2048 bit RSA integers in 8 hours using 20 million noisy qubits by Craig Gidney and Martin Ekerå, 2019 (25 pages).

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**Quantum Approximate Optimization Algorithm (QAOA)**

- Title: \*"A Quantum Approximate Optimization Algorithm"\*

- Authors: Edward Farhi, Jeffrey Goldstone, Sam Gutmann

- Published: 2014

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