

# Instance Space Analysis on Quantum Algorithms

Vivek Katal

02/03/2023

# Introduction

# Background

- Developing a framework to robustly evaluate quantum algorithms using Instance Space Analysis
- Explore the tools needed to develop Quantum Algorithms:
  - Adiabatic Quantum Algorithms (year 1)
  - Universal Gate Based Quantum Algorithms (year 2)
  - Explore various optimization problems, initialization techniques and instance classes (year 3)

# Agenda

- Optimization Problems

# Agenda

- Optimization Problems
- Quantum Algorithms

# Agenda

- Optimization Problems
- Quantum Algorithms
- Methodology

# Agenda

- Optimization Problems
- Quantum Algorithms
- Methodology
- Results

# Agenda

- Optimization Problems
- Quantum Algorithms
- Methodology
- Results
- Next Steps



# Agenda

- Optimization Problems
- Quantum Algorithms
- Methodology
- Results
- Next Steps
- Research Plan

# Optimisation Problems

- MAXCUT (will explore today)
- Other studied problems:
  - Traveling Salesperson Problem (TSP) and Vehicle Routing (VRP)
  - 3SAT - Exact Cover

# Quantum Algorithms

- **Adiabatic Quantum Computing**

# Quantum Algorithms

- **Adiabatic Quantum Computing**
  - AQC is a specific type of quantum computing that uses adiabatic evolution to solve optimization problems [1].

# Quantum Algorithms

- **Adiabatic Quantum Computing**
  - AQC is a specific type of quantum computing that uses adiabatic evolution to solve optimization problems [1].
  - AQC relies on the natural evolution of the quantum system, avoiding the need for precise control over individual quantum gates [2].

# Quantum Algorithms

- **Adiabatic Quantum Computing**
  - AQC is a specific type of quantum computing that uses adiabatic evolution to solve optimization problems [1].
  - AQC relies on the natural evolution of the quantum system, avoiding the need for precise control over individual quantum gates [2].
- **Gate Based Quantum Computing**

# Quantum Algorithms

- **Adiabatic Quantum Computing**
  - AQC is a specific type of quantum computing that uses adiabatic evolution to solve optimization problems [1].
  - AQC relies on the natural evolution of the quantum system, avoiding the need for precise control over individual quantum gates [2].
- **Gate Based Quantum Computing**
  - Uses a series of quantum gates to manipulate the quantum system and perform specific computations [3].

# Quantum Algorithms

- **Adiabatic Quantum Computing**

- AQC is a specific type of quantum computing that uses adiabatic evolution to solve optimization problems [1].
- AQC relies on the natural evolution of the quantum system, avoiding the need for precise control over individual quantum gates [2].

- **Gate Based Quantum Computing**

- Uses a series of quantum gates to manipulate the quantum system and perform specific computations [3].
- Requires precise control over individual quantum gates, which can be challenging to implement [4].



# Quantum Algorithms

- **Adiabatic Quantum Computing**

- AQC is a specific type of quantum computing that uses adiabatic evolution to solve optimization problems [1].
- AQC relies on the natural evolution of the quantum system, avoiding the need for precise control over individual quantum gates [2].

- **Gate Based Quantum Computing**

- Uses a series of quantum gates to manipulate the quantum system and perform specific computations [3].
- Requires precise control over individual quantum gates, which can be challenging to implement [4].
- Potential for faster performance, as it can use advanced techniques such as error correction and quantum parallelism [3].

# MAXCUT

# MAXCUT

- Given a graph  $G = (V, E)$  with vertices  $V$  and edges  $E$ .

# MAXCUT

- Given a graph  $G = (V, E)$  with vertices  $V$  and edges  $E$ .
- Each edge  $(i, j) \in E$  has a weight  $w(i, j)$ .

# MAXCUT

- Given a graph  $G = (V, E)$  with vertices  $V$  and edges  $E$ .
- Each edge  $(i, j) \in E$  has a weight  $w(i, j)$ .
- Partition the vertices into two disjoint sets  $S$  and  $T$ , such that  $S \cup T = V$  and  $S \cap T = \emptyset$ .

# MAXCUT

- Given a graph  $G = (V, E)$  with vertices  $V$  and edges  $E$ .
- Each edge  $(i, j) \in E$  has a weight  $w(i, j)$ .
- Partition the vertices into two disjoint sets  $S$  and  $T$ , such that  $S \cup T = V$  and  $S \cap T = \emptyset$ .
  - Assign a binary variable  $x_{i,t}$  to represent which the city visited at time step  $t$

# MAXCUT

- Given a graph  $G = (V, E)$  with vertices  $V$  and edges  $E$ .
- Each edge  $(i, j) \in E$  has a weight  $w(i, j)$ .
- Partition the vertices into two disjoint sets  $S$  and  $T$ , such that  $S \cup T = V$  and  $S \cap T = \emptyset$ .
  - Assign a binary variable  $x_{i,t}$  to represent which the city visited at time step  $t$
  - Our goal is to find a partition that maximizes the MAXCUT value:

# MAXCUT

- Given a graph  $G = (V, E)$  with vertices  $V$  and edges  $E$ .
- Each edge  $(i, j) \in E$  has a weight  $w(i, j)$ .
- Partition the vertices into two disjoint sets  $S$  and  $T$ , such that  $S \cup T = V$  and  $S \cap T = \emptyset$ .
  - Assign a binary variable  $x_{i,t}$  to represent which the city visited at time step  $t$
  - Our goal is to find a partition that maximizes the MAXCUT value:
  -

$$C(\mathbf{x}) = \sum_{i,j} w_{i,j} x_i(1 - x_j)$$



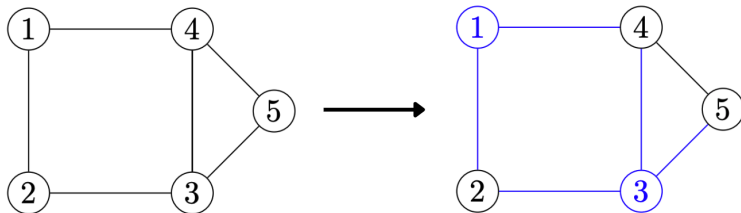
# MAXCUT

- Given a graph  $G = (V, E)$  with vertices  $V$  and edges  $E$ .
- Each edge  $(i, j) \in E$  has a weight  $w(i, j)$ .
- Partition the vertices into two disjoint sets  $S$  and  $T$ , such that  $S \cup T = V$  and  $S \cap T = \emptyset$ .
  - Assign a binary variable  $x_{i,t}$  to represent which the city visited at time step  $t$
  - Our goal is to find a partition that maximizes the MAXCUT value:
  -

$$C(\mathbf{x}) = \sum_{i,j} w_{i,j} x_i(1 - x_j)$$

- This problem is NP-hard [5]

# MAXCUT Formulation



**Solution:** Two partitions are  $S = \{1, 2\}$  and  $T = \{2, 4, 5\}$ . The size of the cut is 5.

# Classical Limitations of MAXCUT

- NP-hard to achieve better approximation ratio than [6]:

# Classical Limitations of MAXCUT

- NP-hard to achieve better approximation ratio than [6]:

# Classical Limitations of MAXCUT

- NP-hard to achieve better approximation ratio than [6]:

$$\alpha \sim 0.941$$

- Best known classical approximation achieved using *Goemans-Williamson* algorithm [7]

# Classical Limitations of MAXCUT

- NP-hard to achieve better approximation ratio than [6]:

$$\alpha \sim 0.941$$

- Best known classical approximation achieved using *Goemans-Williamson* algorithm [7]

# Classical Limitations of MAXCUT

- NP-hard to achieve better approximation ratio than [6]:

$$\alpha \sim 0.941$$

- Best known classical approximation achieved using *Goemans-Williamson* algorithm [7]

$$\alpha \sim 0.878$$

# Mapping MAXCUT to QUBO

- To solve this problem on a Quantum Computer we need to map it to a QUBO.







## Mapping MAXCUT to QUBO

- To solve this problem on a Quantum Computer we need to map it to a QUBO.
- $c_i = \sum_{j=1}^n W_{ij}$ ,  $Q_{ij} = -W_{ij}$

$$C(x) = \sum_{i,j=1}^n x_i Q_{ij} x_j + \sum_i c_i x_i = x^T Q x + c^T x$$

- We can assign a qubit to each decision variable, make the following substitution  $x_i = \frac{(I-Z_i)}{2}$ . This gives us the resulting encoding for a problem Hamiltonian  $H_c$  that can be encoded onto a quantum circuit.

## Mapping MAXCUT to QUBO

- To solve this problem on a Quantum Computer we need to map it to a QUBO.
- $c_i = \sum_{j=1}^n W_{ij}$ ,  $Q_{ij} = -W_{ij}$

$$C(x) = \sum_{i,j=1}^n x_i Q_{ij} x_j + \sum_i c_i x_i = x^T Q x + c^T x$$

- We can assign a qubit to each decision variable, make the following substitution  $x_i = \frac{(I-Z_i)}{2}$ . This gives us the resulting encoding for a problem Hamiltonian  $H_c$  that can be encoded onto a quantum circuit.

## Mapping MAXCUT to QUBO

- To solve this problem on a Quantum Computer we need to map it to a QUBO.
- $c_i = \sum_{j=1}^n W_{ij}$ ,  $Q_{ij} = -W_{ij}$

$$C(x) = \sum_{i,j=1}^n x_i Q_{ij} x_j + \sum_i c_i x_i = x^T Q x + c^T x$$

- We can assign a qubit to each decision variable, make a the following substitution  $x_i = \frac{(I-Z_i)}{2}$ . This gives us the resulting encoding for a problem Hamiltonian  $H_C$  that can be encoded onto a quantum circuit.

$$H_C = \sum_{i,j=1}^n \frac{1}{4} Q_{ij} Z_i Z_j - \sum_{i=1}^n \frac{1}{2} \left( c_i + \sum_{j=1}^n Q_{ij} \right) Z_i + \left( \sum_{i,j=1}^n \frac{Q_{ij}}{4} + \sum_{i=1}^n \frac{c_i}{2} \right)$$

# QAOA

- The QAOA algorithm is characterised by a unitary  $U(\beta, \gamma)$  to prepare a quantum state  $|\psi(\beta, \gamma)\rangle$

# QAOA

- The QAOA algorithm is characterised by a unitary  $U(\beta, \gamma)$  to prepare a quantum state  $|\psi(\beta, \gamma)\rangle$
- The goal of the algorithm is to find optimal parameters  $(\beta_{opt}, \gamma_{opt})$  such that the quantum state encodes the solution to the problem.

# QAOA

- The QAOA algorithm is characterised by a unitary  $U(\beta, \gamma)$  to prepare a quantum state  $|\psi(\beta, \gamma)\rangle$
- The goal of the algorithm is to find optimal parameters  $(\beta_{opt}, \gamma_{opt})$  such that the quantum state encodes the solution to the problem.
- The state is prepared by applying the unitary  $p$  times:



# QAOA

- The QAOA algorithm is characterised by a unitary  $U(\beta, \gamma)$  to prepare a quantum state  $|\psi(\beta, \gamma)\rangle$
- The goal of the algorithm is to find optimal parameters  $(\beta_{opt}, \gamma_{opt})$  such that the quantum state encodes the solution to the problem.
- The state is prepared by applying the unitary  $p$  times:

# QAOA

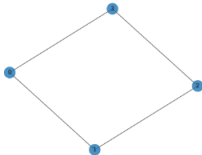
- The QAOA algorithm is characterised by a unitary  $U(\beta, \gamma)$  to prepare a quantum state  $|\psi(\beta, \gamma)\rangle$
- The goal of the algorithm is to find optimal parameters  $(\beta_{opt}, \gamma_{opt})$  such that the quantum state encodes the solution to the problem.
- The state is prepared by applying the unitary  $p$  times:

$$|\psi(\beta, \gamma)\rangle = \underbrace{U(\beta)U(\gamma) \cdots U(\beta)U(\gamma)}_{p \text{ times}} |\psi_0\rangle$$

- Where  $U(\beta) = e^{-i\beta H_b}$  and  $U(\gamma) = e^{-i\gamma H_c}$

# QAOA Algorithm

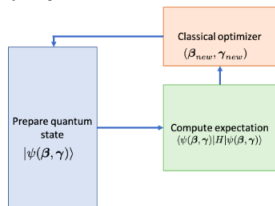
Instance



Formulation

QUBO  
Hamiltonian

Hybrid Algorithm



Quantum Circuit

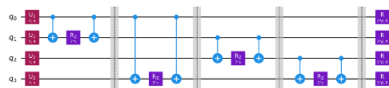
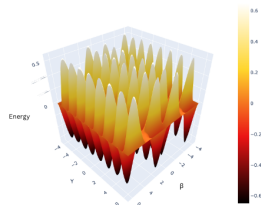
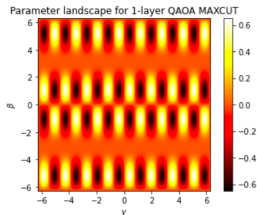
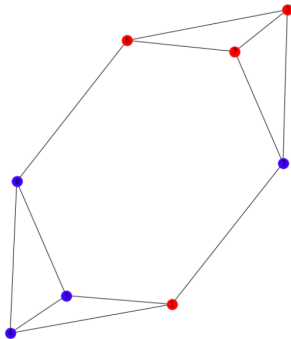


Figure 1: QAOA Strategy

# Landscape for $p = 1$

- With QAOA we observe periodicity in  $\gamma$  and  $\beta$

3-Regular Graph



## Applying ISA in the Quantum Context

# Quantum Algorithms and Variations Studied

- QAOA (experimenting with number of layers)

# Quantum Algorithms and Variations Studied

- QAOA (experimenting with number of layers)
  - $p = 1, \dots, 10$

# Quantum Algorithms and Variations Studied

- QAOA (experimenting with number of layers)
  - $p = 1, \dots, 10$
- QAOA (experimenting with parameter optimization methods)



# Quantum Algorithms and Variations Studied

- QAOA (experimenting with number of layers)
  - $p = 1, \dots, 10$
- QAOA (experimenting with parameter optimization methods)
  - COBYLA, SPSA, NELDER\_MEAD

# Quantum Algorithms and Variations Studied

- QAOA (experimenting with number of layers)
  - $p = 1, \dots, 10$
- QAOA (experimenting with parameter optimization methods)
  - COBYLA, SPSA, NELDER\_MEAD
- QAOA (experimenting Initialisation Techniques)

# Quantum Algorithms and Variations Studied

- QAOA (experimenting with number of layers)
  - $p = 1, \dots, 10$
- QAOA (experimenting with parameter optimization methods)
  - COBYLA, SPSA, NELDER\_MEAD
- QAOA (experimenting Initialisation Techniques)
  - Six methods (outlined further)

# Quantum Algorithms and Variations Studied

- QAOA (experimenting with number of layers)
  - $p = 1, \dots, 10$
- QAOA (experimenting with parameter optimization methods)
  - COBYLA, SPSA, NELDER\_MEAD
- QAOA (experimenting Initialisation Techniques)
  - Six methods (outlined further)
- Variational Quantum Algorithms (VQE-2 Local, F-VQE, QAOA Vanilla)

# Quantum Algorithms and Variations Studied

- QAOA (experimenting with number of layers)
  - $p = 1, \dots, 10$
- QAOA (experimenting with parameter optimization methods)
  - COBYLA, SPSA, NELDER\_MEAD
- QAOA (experimenting Initialisation Techniques)
  - Six methods (outlined further)
- Variational Quantum Algorithms (VQE-2 Local, F-VQE, QAOA Vanilla)
- **22** unique algorithm variations

# Quantum Algorithms and Variations Studied

- QAOA (experimenting with number of layers)
  - $p = 1, \dots, 10$
- QAOA (experimenting with parameter optimization methods)
  - COBYLA, SPSA, NELDER\_MEAD
- QAOA (experimenting Initialisation Techniques)
  - Six methods (outlined further)
- Variational Quantum Algorithms (VQE-2 Local, F-VQE, QAOA Vanilla)
- **22 unique algorithm variations**
- **Can we measure characteristics of instances that make specific algorithms more suited to solve certain graphs?**

## Current Literature

- Improvements in QAOA and VQE have largely been limited to exploring three types of graphs:

## Current Literature

- Improvements in QAOA and VQE have largely been limited to exploring three types of graphs:
- Filtering VQE (uses an additional filtering operator to improve convergence) [8]

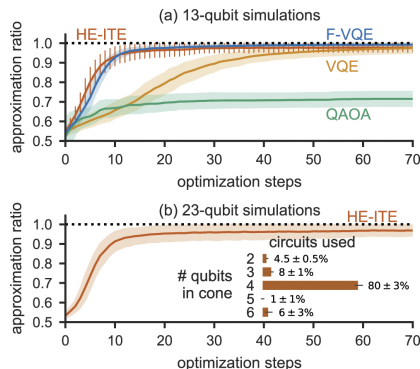


## Current Literature

- Improvements in QAOA and VQE have largely been limited to exploring three types of graphs:
- Filtering VQE (uses an additional filtering operator to improve convergence) [8]

# Current Literature

- Improvements in QAOA and VQE have largely been limited to exploring three types of graphs:
- Filtering VQE (uses an additional filtering operator to improve convergence) [8]



- Study only investigated using 3-regular graphs

# Current Literature

- Warm Starting QAOA [9] – seeding initial state

# Current Literature

- Warm Starting QAOA [9] – seeding initial state
  - Erdős–Rényi Graphs

# Current Literature

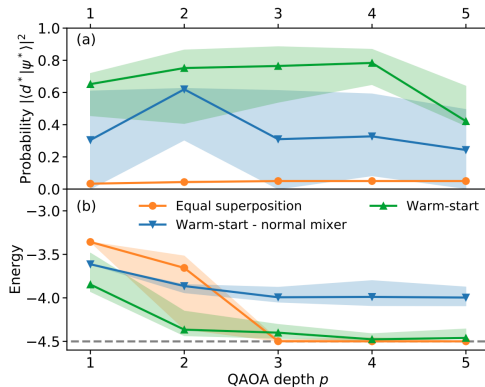
- Warm Starting QAOA [9] – seeding initial state
  - Erdős–Rényi Graphs
  - $k$ -regular graphs

# Current Literature

- Warm Starting QAOA [9] – seeding initial state
  - Erdős–Rényi Graphs
  - $k$ -regular graphs

# Current Literature

- Warm Starting QAOA [9] – seeding initial state
  - Erdős–Rényi Graphs
  - $k$ -regular graphs



## Current Literature

- Optimal QAOA parameters showing concentration over different problem instances [10], [11], [12]



## Current Literature

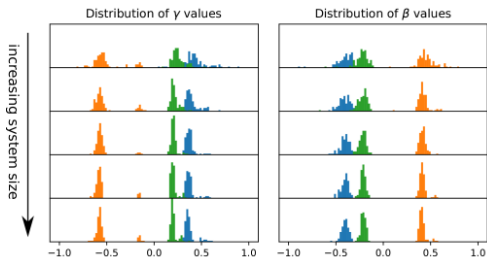
- Optimal QAOA parameters showing concentration over different problem instances [10], [11], [12]
- Study only investigated using 3-regular graphs

## Current Literature

- Optimal QAOA parameters showing concentration over different problem instances [10], [11], [12]
- Study only investigated using 3-regular graphs

# Current Literature

- Optimal QAOA parameters showing concentration over different problem instances [10], [11], [12]
- Study only investigated using 3-regular graphs



- **Do new developments in Quantum Algorithms in current literature extend for all classes of instances?**

# Instance Space Analysis

# Algorithm Selection

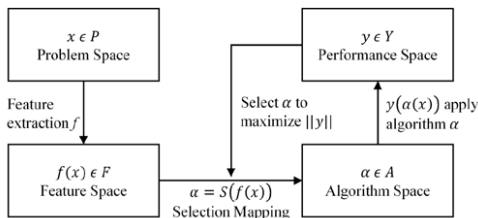
- Given a set of problem instances, predicting which algorithm is most likely to best perform was first explored by Rice [13].

# Algorithm Selection

- Given a set of problem instances, predicting which algorithm is most likely to best perform was first explored by Rice [13].

# Algorithm Selection

- Given a set of problem instances, predicting which algorithm is most likely to best perform was first explored by Rice [13].



- However, what we are interested in is probing the strengths and weaknesses of Quantum Algorithms for different instances of MAXCUT, TSP and 3SAT.

# Instance Space Methodology

- The instance space methodology presented in [14–16] extends Rice's framework.

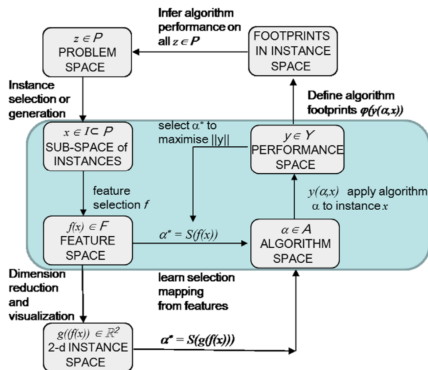


# Instance Space Methodology

- The instance space methodology presented in [14–16] extends Rice's framework.

# Instance Space Methodology

- The instance space methodology presented in [14–16] extends Rice's framework.



# Metadata: Instances

- The problem space  $\mathcal{P}$  consists of all possible graph instances

# Metadata: Instances

- The problem space  $\mathcal{P}$  consists of all possible graph instances
- The instance space  $\mathcal{I} \subset \mathcal{P}$  comprises of **867** MAXCUT instances.

# Metadata: Instances

- The problem space  $\mathcal{P}$  consists of all possible graph instances
- The instance space  $\mathcal{I} \subset \mathcal{P}$  comprises of **867** MAXCUT instances.
  - Regular Graphs

# Metadata: Instances

- The problem space  $\mathcal{P}$  consists of all possible graph instances
- The instance space  $\mathcal{I} \subset \mathcal{P}$  comprises of **867** MAXCUT instances.
  - Regular Graphs
  - Uniform Random Graphs

# Metadata: Instances

- The problem space  $\mathcal{P}$  consists of all possible graph instances
- The instance space  $\mathcal{I} \subset \mathcal{P}$  comprises of **867** MAXCUT instances.
  - Regular Graphs
  - Uniform Random Graphs
  - Watts-Strogatz Small World

# Metadata: Instances

- The problem space  $\mathcal{P}$  consists of all possible graph instances
- The instance space  $\mathcal{I} \subset \mathcal{P}$  comprises of **867** MAXCUT instances.
  - Regular Graphs
  - Uniform Random Graphs
  - Watts-Strogatz Small World
  - Nearly Complete Bipartite Graphs



# Metadata: Instances

- The problem space  $\mathcal{P}$  consists of all possible graph instances
- The instance space  $\mathcal{I} \subset \mathcal{P}$  comprises of **867** MAXCUT instances.
  - Regular Graphs
  - Uniform Random Graphs
  - Watts-Strogatz Small World
  - Nearly Complete Bipartite Graphs
  - Power Law Tree Graphs

# Metadata: Instances

- The problem space  $\mathcal{P}$  consists of all possible graph instances
- The instance space  $\mathcal{I} \subset \mathcal{P}$  comprises of **867** MAXCUT instances.
  - Regular Graphs
  - Uniform Random Graphs
  - Watts-Strogatz Small World
  - Nearly Complete Bipartite Graphs
  - Power Law Tree Graphs
  - Nearly Complete Bipartite Graphs

# Metadata: Instances

- The problem space  $\mathcal{P}$  consists of all possible graph instances
- The instance space  $\mathcal{I} \subset \mathcal{P}$  comprises of **867** MAXCUT instances.
  - Regular Graphs
  - Uniform Random Graphs
  - Watts-Strogatz Small World
  - Nearly Complete Bipartite Graphs
  - Power Law Tree Graphs
  - Nearly Complete Bipartite Graphs
  - Geometric Graphs

# Metadata: Features

- The feature space  $\mathcal{F}$  consists of 21 different instance features generated 21 features were considered

| Graph Based Features                  | Boolean Features                     |
|---------------------------------------|--------------------------------------|
| Average Distance                      | Bipartite                            |
| Clique Number                         | Connected                            |
| Algebraic Connectivity                | Acyclic                              |
| Diameter                              | Eulerian                             |
| Edge Connectivity                     | Regularity                           |
| Vertex Connectivity                   | Planar                               |
| Maximum Node Degree                   | <b>Laplacian (Spectral Features)</b> |
| Minimum Node Degree                   | Largest Eigenvalue                   |
| Cardinality of minimal dominating set | Laplacian Second Largest Eigenvalue  |
| Number of Components                  | Smallest Eigenvalue                  |
| Number of vertices                    |                                      |
| Radius                                |                                      |

# Algorithm Portfolio

- We produce the following different instance space analyses:

# Algorithm Portfolio

- We produce the following different instance space analyses:
  - QAOA, increasing layers  $p = 1, \dots, 10$

# Algorithm Portfolio

- We produce the following different instance space analyses:
  - QAOA, increasing layers  $p = 1, \dots, 10$
  - QAOA, optimiser routines COBYLA, NELDER\_MEAD, SLSQP

# Algorithm Portfolio

- We produce the following different instance space analyses:
  - QAOA, increasing layers  $p = 1, \dots, 10$
  - QAOA, optimiser routines COBYLA, NELDER\_MEAD, SLSQP
  - Initialisation Technique of the ground state



# Algorithm Portfolio

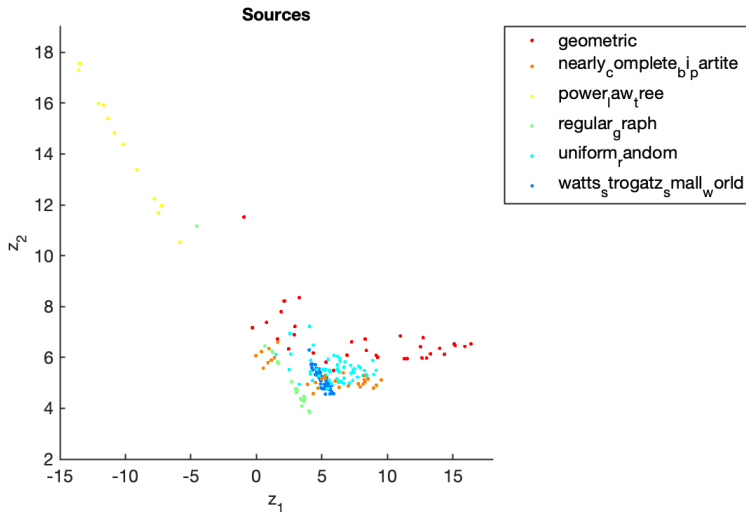
- We produce the following different instance space analyses:
  - QAOA, increasing layers  $p = 1, \dots, 10$
  - QAOA, optimiser routines COBYLA, NELDER\_MEAD, SLSQP
  - Initialisation Technique of the ground state
  - Various variational techniques (VQE, F-VQE, QAOA)

# Algorithm Portfolio

- We produce the following different instance space analyses:
  - QAOA, increasing layers  $p = 1, \dots, 10$
  - QAOA, optimiser routines COBYLA, NELDER\_MEAD, SLSQP
  - Initialisation Technique of the ground state
  - Various variational techniques (VQE, F-VQE, QAOA)
- The performance metric  $y \in \mathcal{Y}$  is energy gap ( $E_{\text{gap}} = \frac{\langle \psi | H | \psi \rangle}{\langle \psi_g | H | \psi_g \rangle}$ )

# Results

# ISA



# Feature Distribution

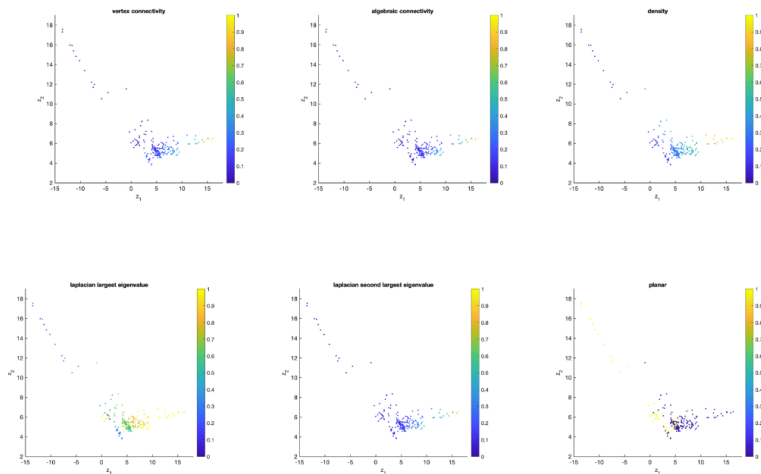
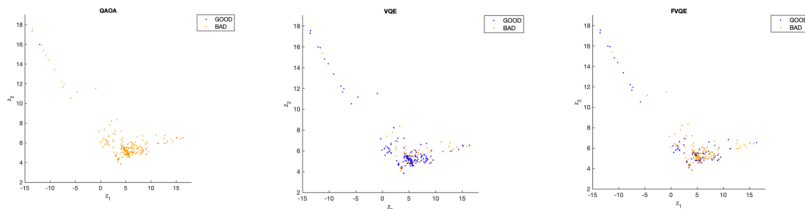


Figure 3: Features

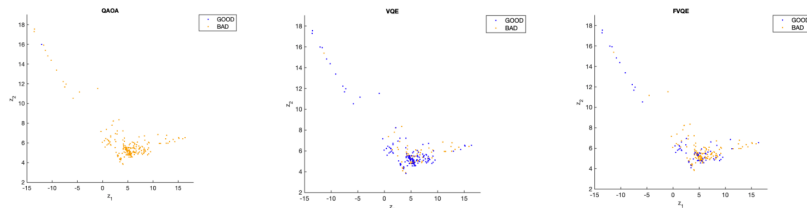
# Performance Distribution



## Vanilla QAOA, increasing layers

- These experiments are still currently running on SPARTAN

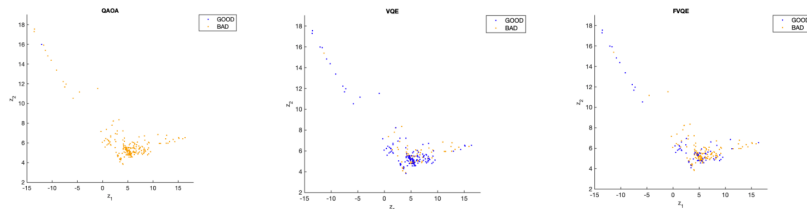
# Performance Distribution



## Vanilla QAOA, increasing layers

- These experiments are still currently running on SPARTAN
- Run a vanilla QAOA instance for layers  $p = 1, \dots, 10$

# Performance Distribution

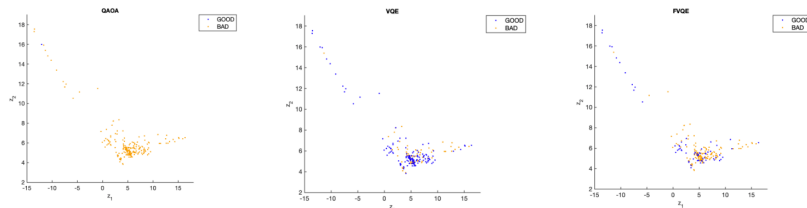


## Vanilla QAOA, increasing layers

- These experiments are still currently running on SPARTAN
- Run a vanilla QAOA instance for layers  $p = 1, \dots, 10$ 
  - 5 restarts



# Performance Distribution



## Vanilla QAOA, increasing layers

- These experiments are still currently running on SPARTAN
- Run a vanilla QAOA instance for layers  $p = 1, \dots, 10$ 
  - 5 restarts
  - 200 13 node MAXCUT instances of each source

# Vanilla QAOA with Classical Optimisation Techniques (SPSA, COBYLA, NELDER\_MEAD)

- Run a vanilla QAOA instance for layers  $p = 7$  (optimal result for previous)

# Vanilla QAOA with Classical Optimisation Techniques (SPSA, COBYLA, NELDER\_MEAD)

- Run a vanilla QAOA instance for layers  $p = 7$  (optimal result for previous)
  - 5 restarts

# Vanilla QAOA with Classical Optimisation Techniques (SPSA, COBYLA, NELDER\_MEAD)

- Run a vanilla QAOA instance for layers  $p = 7$  (optimal result for previous)
  - 5 restarts
  - 200 13 node MAXCUT instances of each source

# Initialisation Techniques of the ground state (QAOA)

- Run a vanilla QAOA instance for layers  $p = 7$  and a classical optimizer of COBYLA
- Trotterized Quantum Annealing (TQA) [17]
- Random Initialisation
- Perturb from previous layer
- Ramped up Initialisation,
- Optimise  $\gamma$  and  $\beta$  in the Fourier Space (FT)

# Thesis Outline

-Thesis Structure - Introduction - Solving Optimisation Problems using a Quantum Computer - Quantum Algorithms Studied - Instance Space Analysis - ISA: MAXCUT - ISA: TSP - ISA: 3SAT - Conclusion

## Discuss thesis outline

- Here is a link to the thesis outline

# Next Steps

- Complete Instance Space Analysis on existing algorithms and additional adaptations (2 months)



## Next Steps

- Complete Instance Space Analysis on existing algorithms and additional adaptations (2 months)
- Formalize findings into a paper (currently in progress - 1 month)

## Next Steps

- Complete Instance Space Analysis on existing algorithms and additional adaptations (2 months)
- Formalize findings into a paper (currently in progress - 1 month)
- Completing and submitting thesis (3 months)

## Appendix

## Other Optimisation Problems Explored

# Other Optimisation Problems Explored

- TSP

# Other Optimisation Problems Explored

- TSP
- 3SAT

# The Traveling Salesman Problem (TSP)

# The Traveling Salesman Problem (TSP)

- The Traveling Salesman Problem (TSP) is a well-known combinatorial optimization problem that involves finding the shortest possible route that visits a given set of cities exactly once and returns to the starting city.



# The Traveling Salesman Problem (TSP)

- The Traveling Salesman Problem (TSP) is a well-known combinatorial optimization problem that involves finding the shortest possible route that visits a given set of cities exactly once and returns to the starting city.
- Let  $C = c_1, c_2, \dots, c_n$  be a set of cities, where  $c_i$  is the  $i$ -th city.

# The Traveling Salesman Problem (TSP)

- The Traveling Salesman Problem (TSP) is a well-known combinatorial optimization problem that involves finding the shortest possible route that visits a given set of cities exactly once and returns to the starting city.
- Let  $C = c_1, c_2, \dots, c_n$  be a set of cities, where  $c_i$  is the  $i$ -th city.
- Let  $d(c_i, c_j)$  be a function that calculates the distance between cities  $c_i$  and  $c_j$ .

# The Traveling Salesman Problem (TSP)

- The Traveling Salesman Problem (TSP) is a well-known combinatorial optimization problem that involves finding the shortest possible route that visits a given set of cities exactly once and returns to the starting city.
- Let  $C = c_1, c_2, \dots, c_n$  be a set of cities, where  $c_i$  is the  $i$ -th city.
- Let  $d(c_i, c_j)$  be a function that calculates the distance between cities  $c_i$  and  $c_j$ .
- The Traveling Salesman Problem (TSP) is to find a Hamiltonian cycle  $\pi = \pi_1, \pi_2, \dots, \pi_n$  of minimum total length.

# The Traveling Salesman Problem (TSP)

- The Traveling Salesman Problem (TSP) is a well-known combinatorial optimization problem that involves finding the shortest possible route that visits a given set of cities exactly once and returns to the starting city.
- Let  $C = c_1, c_2, \dots, c_n$  be a set of cities, where  $c_i$  is the  $i$ -th city.
- Let  $d(c_i, c_j)$  be a function that calculates the distance between cities  $c_i$  and  $c_j$ .
- The Traveling Salesman Problem (TSP) is to find a Hamiltonian cycle  $\pi = \pi_1, \pi_2, \dots, \pi_n$  of minimum total length.
- The cycle  $\pi$  must visit each city in the set  $C$  exactly once and  $\pi_{n+1} = \pi_1$ .

# The Traveling Salesman Problem (TSP)

- The Traveling Salesman Problem (TSP) is a well-known combinatorial optimization problem that involves finding the shortest possible route that visits a given set of cities exactly once and returns to the starting city.
- Let  $C = c_1, c_2, \dots, c_n$  be a set of cities, where  $c_i$  is the  $i$ -th city.
- Let  $d(c_i, c_j)$  be a function that calculates the distance between cities  $c_i$  and  $c_j$ .
- The Traveling Salesman Problem (TSP) is to find a Hamiltonian cycle  $\pi = \pi_1, \pi_2, \dots, \pi_n$  of minimum total length.
- The cycle  $\pi$  must visit each city in the set  $C$  exactly once and  $\pi_{n+1} = \pi_1$ .
- The TSP can be defined mathematically as:

# The Traveling Salesman Problem (TSP)

- The Traveling Salesman Problem (TSP) is a well-known combinatorial optimization problem that involves finding the shortest possible route that visits a given set of cities exactly once and returns to the starting city.
- Let  $C = c_1, c_2, \dots, c_n$  be a set of cities, where  $c_i$  is the  $i$ -th city.
- Let  $d(c_i, c_j)$  be a function that calculates the distance between cities  $c_i$  and  $c_j$ .
- The Traveling Salesman Problem (TSP) is to find a Hamiltonian cycle  $\pi = \pi_1, \pi_2, \dots, \pi_n$  of minimum total length.
- The cycle  $\pi$  must visit each city in the set  $C$  exactly once and  $\pi_{n+1} = \pi_1$ .
- The TSP can be defined mathematically as:
- 

$$\min_{\pi} \sum_{i=1}^n d(c_{\pi_i}, c_{\pi_{i+1}})$$

# TSP Example

# TSP mapping to QUBO

- Represent cities as binary variables:



# TSP mapping to QUBO

- Represent cities as binary variables:
  - Assign a binary variable  $x_{i,t}$  to represent which the city visited at timestep  $t$

# TSP mapping to QUBO

- Represent cities as binary variables:
  - Assign a binary variable  $x_{i,t}$  to represent which the city visited at timestep  $t$
  - We can now represent the cost as a function of the decision variables:

# TSP mapping to QUBO

- Represent cities as binary variables:
  - Assign a binary variable  $x_{i,t}$  to represent which the city visited at timestep  $t$
  - We can now represent the cost as a function of the decision variables:
  -

$$\text{Cost} = \sum_t \sum_{i,j \in C} d(i,j) x_{i,t} x_{j,t+1}$$

# TSP mapping to QUBO

- Represent cities as binary variables:
  - Assign a binary variable  $x_{i,t}$  to represent which the city visited at timestep  $t$
  - We can now represent the cost as a function of the decision variables:
  -

$$\text{Cost} = \sum_t \sum_{i,j \in C} d(i,j) x_{i,t} x_{j,t+1}$$

- **Constraints:**

# TSP mapping to QUBO

- Represent cities as binary variables:
  - Assign a binary variable  $x_{i,t}$  to represent which the city visited at timestep  $t$
  - We can now represent the cost as a function of the decision variables:
  -

$$\text{Cost} = \sum_t \sum_{i,j \in C} d(i,j) x_{i,t} x_{j,t+1}$$

- **Constraints:**
  - Each city must be visited:  $\sum_{j=1}^n x_{ij} = 1$  for all  $i \in 1, 2, \dots, n$ .

# TSP mapping to QUBO

- Represent cities as binary variables:
  - Assign a binary variable  $x_{i,t}$  to represent which the city visited at timestep  $t$
  - We can now represent the cost as a function of the decision variables:
  -

$$\text{Cost} = \sum_t \sum_{i,j \in C} d(i,j) x_{i,t} x_{j,t+1}$$

- **Constraints:**
  - Each city must be visited:  $\sum_{j=1}^n x_{ij} = 1$  for all  $i \in 1, 2, \dots, n$ .
  - Each city must be reached from exactly one city:  $\sum_{i=1}^n x_{ij} = 1$  for all  $j \in 1, 2, \dots, n$ .

# TSP mapping to QUBO

- Represent cities as binary variables:
  - Assign a binary variable  $x_{i,t}$  to represent which the city visited at timestep  $t$
  - We can now represent the cost as a function of the decision variables:
  -

$$\text{Cost} = \sum_t \sum_{i,j \in C} d(i,j) x_{i,t} x_{j,t+1}$$

- **Constraints:**
  - Each city must be visited:  $\sum_{j=1}^n x_{ij} = 1$  for all  $i \in 1, 2, \dots, n$ .
  - Each city must be reached from exactly one city:  $\sum_{i=1}^n x_{ij} = 1$  for all  $j \in 1, 2, \dots, n$ .
  - No two cities can be visited at the same time:  $x_{ij} + x_{ji} \leq 1$  for all  $i, j \in 1, 2, \dots, n$ .

# TSP mapping to QUBO

- Represent cities as binary variables:
  - Assign a binary variable  $x_{i,t}$  to represent which the city visited at timestep  $t$
  - We can now represent the cost as a function of the decision variables:
  -

$$\text{Cost} = \sum_t \sum_{i,j \in C} d(i,j) x_{i,t} x_{j,t+1}$$

- **Constraints:**
  - Each city must be visited:  $\sum_{j=1}^n x_{ij} = 1$  for all  $i \in 1, 2, \dots, n$ .
  - Each city must be reached from exactly one city:  $\sum_{i=1}^n x_{ij} = 1$  for all  $j \in 1, 2, \dots, n$ .
  - No two cities can be visited at the same time:  $x_{ij} + x_{ji} \leq 1$  for all  $i, j \in 1, 2, \dots, n$ .
  - To convert this problem to a QUBO express constraints as penalty terms in the objective function.



## TSP mapping to QUBO

- First constraint can be expressed as  $P_1 \left( \sum_{j=1}^n x_{ij} - 1 \right)^2$ , where  $P_1$  is a large positive constant.

# TSP mapping to QUBO

- First constraint can be expressed as  $P_1 \left( \sum_{j=1}^n x_{ij} - 1 \right)^2$ , where  $P_1$  is a large positive constant.
- Similarly, the other constraints can be expressed as penalty terms in the objective function.

## TSP mapping to QUBO

- First constraint can be expressed as  $P_1 \left( \sum_{j=1}^n x_{ij} - 1 \right)^2$ , where  $P_1$  is a large positive constant.
- Similarly, the other constraints can be expressed as penalty terms in the objective function.
- The final objective function becomes a QUBO of the form:  

$$P_1 \left( \sum_{j=1}^n x_{ij} - 1 \right)^2 + P_2 \left( \sum_{i=1}^n x_{ij} - 1 \right)^2 + \sum_{i=1}^n \sum_{j=1}^n P_3 (x_{ij} + x_{ji} - 1)^2 + \sum_{i=1}^n \sum_{j=1}^n d_{ij} x_{ij}.$$

## TSP mapping to QUBO

- First constraint can be expressed as  $P_1 \left( \sum_{j=1}^n x_{ij} - 1 \right)^2$ , where  $P_1$  is a large positive constant.
- Similarly, the other constraints can be expressed as penalty terms in the objective function.
- The final objective function becomes a QUBO of the form:  

$$P_1 \left( \sum_{j=1}^n x_{ij} - 1 \right)^2 + P_2 \left( \sum_{i=1}^n x_{ij} - 1 \right)^2 + \sum_{i=1}^n \sum_{j=1}^n P_3 (x_{ij} + x_{ji} - 1)^2 + \sum_{i=1}^n \sum_{j=1}^n d_{ij} x_{ij}.$$
- To simplify, we can also have  $A = P_1 = P_2 = P_3$

## TSP mapping to QUBO

- First constraint can be expressed as  $P_1 \left( \sum_{j=1}^n x_{ij} - 1 \right)^2$ , where  $P_1$  is a large positive constant.
- Similarly, the other constraints can be expressed as penalty terms in the objective function.
- The final objective function becomes a QUBO of the form:  

$$P_1 \left( \sum_{j=1}^n x_{ij} - 1 \right)^2 + P_2 \left( \sum_{i=1}^n x_{ij} - 1 \right)^2 + \sum_{i=1}^n \sum_{j=1}^n P_3 (x_{ij} + x_{ji} - 1)^2 + \sum_{i=1}^n \sum_{j=1}^n d_{ij} x_{ij}.$$
- To simplify, we can also have  $A = P_1 = P_2 = P_3$
- This QUBO can then solved by a quantum algorithm

# TSP mapping to QUBO

Assign a qubit to each decision variable, make a the following substitution

$$x_{l,t} = \frac{(1 - Z_{l,t})}{2}.$$

# Extending TSP to VRP

- If we have  $N$  vehicles. Implement spectral clustering create  $N$  cluster.

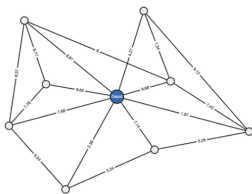
# Extending TSP to VRP

- If we have  $N$  vehicles. Implement spectral clustering create  $N$  cluster.
- Solve each cluster independently.

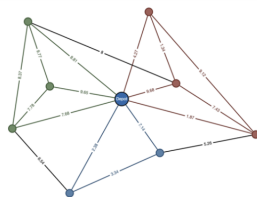


# Extending TSP to VRP

- If we have  $N$  vehicles. Implement spectral clustering create  $N$  cluster.
- Solve each cluster independently.



clustering



## 3SAT - Exact Cover

## 3SAT (Exact Cover)

- The satisfiability problem, abbreviated SAT, is a classic example of an NP-complete problem [18]

## 3SAT (Exact Cover)

- The satisfiability problem, abbreviated SAT, is a classic example of an NP-complete problem [18]
- The basic SAT formulation can be described as follows: Given a boolean formula (AND  $\wedge$ , OR  $\vee$ , NOT  $\neg$ ) over  $n$  variables ( $z_1, z_2, \dots, z_n$ ). Can one set  $z_i$ 's in a manner such that the Boolean formula is true?

## 3SAT (Exact Cover)

- The satisfiability problem, abbreviated SAT, is a classic example of an NP-complete problem [18]
- The basic SAT formulation can be described as follows: Given a boolean formula (AND  $\wedge$ , OR  $\vee$ , NOT  $\neg$ ) over  $n$  variables  $(z_1, z_2, \dots, z_n)$ . Can one set  $z_i$ 's in a manner such that the Boolean formula is true?
- A clause is an expression which the variables must satisfy. For example  $z_1 \wedge z_2 \implies z_1 = z_2 = 1$

## 3SAT (Exact Cover Example)

- Consider a 4-bit number with two clauses:

## 3SAT (Exact Cover Example)

- Consider a 4-bit number with two clauses:
  - $z_1 \wedge z_2 \wedge z_3$

## 3SAT (Exact Cover Example)

- Consider a 4-bit number with two clauses:
  - $z_1 \wedge z_2 \wedge z_3$
  - $z_1 \wedge z_3 \wedge z_4$



## 3SAT (Exact Cover Example)

- Consider a 4-bit number with two clauses:
  - $z_1 \wedge z_2 \wedge z_3$
  - $z_1 \wedge z_3 \wedge z_4$
- Here we have 16 possible assignments, namely:

## 3SAT (Exact Cover Example)

- Consider a 4-bit number with two clauses:
  - $z_1 \wedge z_2 \wedge z_3$
  - $z_1 \wedge z_3 \wedge z_4$
- Here we have 16 possible assignments, namely:
- 

$$\mathcal{Z} = \{ 0000, 0001, 0010, 0011, 0100, 0101, 0110, 0111, \\ 1000, 1001, 1010, 1011, 1100, 1101, 1110, 1111 \}$$

## 3SAT (Exact Cover Example)

- Consider a 4-bit number with two clauses:
  - $z_1 \wedge z_2 \wedge z_3$
  - $z_1 \wedge z_3 \wedge z_4$
- Here we have 16 possible assignments, namely:
- 

$$\mathcal{Z} = \{ 0000, 0001, 0010, 0011, 0100, 0101, 0110, 0111, \\ 1000, 1001, 1010, 1011, 1100, 1101, 1110, 1111 \}$$

- However, our **satisfying assignment** is only  $\vec{z} = 1111$

## 3SAT (Exact Cover Example)

- Consider a 4-bit number with two clauses:
  - $z_1 \wedge z_2 \wedge z_3$
  - $z_1 \wedge z_3 \wedge z_4$
- Here we have 16 possible assignments, namely:
- 

$$\mathcal{Z} = \{ 0000, 0001, 0010, 0011, 0100, 0101, 0110, 0111, \\ 1000, 1001, 1010, 1011, 1100, 1101, 1110, 1111 \}$$

- However, our **satisfying assignment** is only  $\vec{z} = 1111$
- We call a 3SAT problem with one satisfying assignment an instance of USA

## 3SAT (Exact Cover Example)

- Consider a 4-bit number with two clauses:
  - $z_1 \wedge z_2 \wedge z_3$
  - $z_1 \wedge z_3 \wedge z_4$
- Here we have 16 possible assignments, namely:
- 

$$\mathcal{Z} = \{ 0000, 0001, 0010, 0011, 0100, 0101, 0110, 0111, \\ 1000, 1001, 1010, 1011, 1100, 1101, 1110, 1111 \}$$

- However, our **satisfying assignment** is only  $\vec{z} = 1111$
- We call a 3SAT problem with one satisfying assignment an instance of USA
- Exact Cover implies that clauses are “exclusive” and in the form of  $z_i + z_j + z_k = 1$

# Mapping 3SAT to a Hamiltonian

- How do we construct  $H_B$  and  $H_P$  so that we can solve our optimisation problem?

# Mapping 3SAT to a Hamiltonian

- How do we construct  $H_B$  and  $H_P$  so that we can solve our optimisation problem?
- Farhi et al.[1] describe this construction in considerable detail.

# Mapping 3SAT to a Hamiltonian

- How do we construct  $H_B$  and  $H_P$  so that we can solve our optimisation problem?
- Farhi et al.[1] describe this construction in considerable detail.
- We then evolve our system with the following interpolation:



# Mapping 3SAT to a Hamiltonian

- How do we construct  $H_B$  and  $H_P$  so that we can solve our optimisation problem?
- Farhi et al.[1] describe this construction in considerable detail.
- We then evolve our system with the following interpolation:
- 

$$H(t) = [1 - \lambda(t)] H_B + \lambda(t) H_P, \quad \lambda(t) = \frac{t}{T}$$

# Mapping 3SAT to a Hamiltonian

- How do we construct  $H_B$  and  $H_P$  so that we can solve our optimisation problem?
- Farhi et al.[1] describe this construction in considerable detail.
- We then evolve our system with the following interpolation:
- 

$$H(t) = [1 - \lambda(t)] H_B + \lambda(t) H_P, \quad \lambda(t) = \frac{t}{T}$$

- Finally, complete measurement and our solution is our final state  $|\psi(t = T)\rangle$

## References I

1. Farhi E, Goldstone J, Gutmann S, et al. (2001) A quantum adiabatic evolution algorithm applied to random instances of an NP-complete problem. *Science* 292: 472–475.
2. Preskill J (2018) Quantum computing in the NISQ era and beyond. *Quantum* 2: 79.
3. Raussendorf R, Briegel HJ (2001) A one-way quantum computer. *Phys Rev Lett* 86: 5188–5191.
4. Childs AM, Goldstone J (2004) Spatial search by quantum walk. *Phys Rev A* 70: 022314.
5. Karp RM (1972) Reducibility among combinatorial problems., In: Miller RE, Thatcher JW (Eds.), *Complexity of computer computations*, Plenum Press, New York, 85–103.
6. Håstad J (2001) Some optimal inapproximability results. *J ACM* 48: 798–859.

## References II

7. Goemans MX, Williamson DP (1995) Improved approximation algorithms for maximum cut and satisfiability problems using semidefinite programming. *J ACM* 42: 1115–1145.
8. Amaro D, Modica C, Rosenkranz M, et al. (2022) Filtering variational quantum algorithms for combinatorial optimization. *Quantum Science and Technology* 7: 015021.
9. Egger DJ, Mareček J, Woerner S (2021) Warm-starting quantum optimization. *Quantum* 5: 479.
10. Farhi E, Goldstone J, Gutmann S, et al. (2022) The quantum approximate optimization algorithm and the sherrington-kirkpatrick model at infinite size. *Quantum* 6: 759.
11. Akshay V, Rabinovich D, Campos E, et al. (2021) Parameter concentration in quantum approximate optimization.

## References III

12. Streif M, Leib M (2019) Training the quantum approximate optimization algorithm without access to a quantum processing unit.
13. Rice JR et al. (1976) The algorithm selection problem. *Advances in computers* 15: 5.
14. Smith-Miles K, Bowly S (2015) Generating new test instances by evolving in instance space. *Computers & Operations Research* 63: 102–113.
15. Smith-Miles K, Lopes L (2012) Measuring instance difficulty for combinatorial optimization problems. *Computers & Operations Research* 39: 875–889.
16. Smith-Miles K, Baatar D, Wreford B, et al. (2014) Towards objective measures of algorithm performance across instance space. *Computers & Operations Research* 45: 12–24.

## References IV

17. Sack SH, Serbyn M (2021) Quantum annealing initialization of the quantum approximate optimization algorithm. *Quantum* 5: 491.
18. Cook SA (1971) The complexity of theorem-proving procedures, *Proceedings of the third annual ACM symposium on theory of computing*, ACM, 151–158.