



UNIVERSITY OF WESTERN AUSTRALIA

# A Quantum Solution to Graph Similarity Problems

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This thesis is presented for the degree of  
**Masters of Physics (Quantum Technology and Computing)**

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# Declaration

This is to certify that:

1. This thesis comprises of my original work.
2. Due acknowledgment has been made in the text to all other materials used.
3. This thesis consists of about 60 pages inclusive of tables and figures but exclusive of references and appendices.

I authorise the Head of the Department of Physics to make a copy of this thesis to any person judged to have an acceptable reason for access to the information, i.e, for research, study or instruction.

Student Name: Dylan O'Donoghue ID: 23158061

Signature

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Date

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Supervisor: Professor Jingbo Wang

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Date

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# **Summary of Student Achievement**

The graph similarity problem is an area of research that QUISA has engaged with

Learnt quantum computation

QAOA, QWOA, and NVQWOA

High-performance computing

Wrote code to parallelise the NVQWOA using QuOp

Investigated graph similarity using NVQWOA

Contributed to the ASCA Quantum Optimisation group

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# **Abstract**

Brief summary.....

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# Chapter 1

## Introduction

Physics, as a discipline in the modern world, is fundamentally concerned with understanding the parts of reality that are unknown. Much of modern research can be broadly framed within three frontiers, each defined by what knowledge remains elusive. One frontier is the very large; the scale of astrophysics and cosmology, characterised by measures of size, energy, and duration that are larger than the human scale. We build telescopes and detectors to search for evidence for theoretical models. Another frontier is the very small; the scale of quantum fields and fundamental particles, characterised by measures of size, energy, and duration that are smaller than the human scale. We build colliders, resonant cavities, and precise experiments to search for evidence for theoretical models.

An emerging frontier of physics research is the intractable; systems whose behaviour is not characterised by distance or scale, but by overwhelming complexity. Many physical systems well-described by the tools of physics remain unsolved, such as the behaviour of many-body quantum systems in materials, chemistry, and biology, or the solutions to large combinatorial optimisation problems in logistics, machine learning, and networks. Addressing problems in this domain requires new approaches: we design new algorithms and software and build quantum computers to push beyond classical computational limits. This is the context that motivates the development of quantum computing.

Quantum computing is a rapidly evolving field that leverages the principles of quantum mechanics to address problems that are intractable for classical computation. By utilising the unique properties of quantum bits (qubits), such as superposition and entanglement, quantum computers can perform computational tasks that classical systems cannot mimic. Realising the potential of this technology requires specialised quantum algorithms that restructure how problems are encoded and solved. Advances in hardware, algorithms, and applications are driving a growing interest in quantum computing across a wide range of scientific and technological domains.

One domain where quantum algorithms may offer significant advantages is graph theory. Graphs are fundamental models for complex systems and underpin many applications, such as search engines, social networks, logistics, transportation, and communication. In many such contexts, it is essential to quantify the similarity between graphs. For example, detecting changes in interaction patterns over time, analysing structural differences between graphs. TODO: FINISH AND CITE In all these cases, the similarity between two graphs with similar sets of nodes is assessed, and the detection of changes in the patterns of connectivity is important. For graphs that may match approximately, it is useful to obtain a measure of similarity.

Graph similarity measures are quantitative calculations based on comparisons made between the structure of network graphs. Different measures of graph similarity will produce a variety of results because of differences in how the structures of the graphs are analysed. There are many measures of graph similarity, including Maximum Common Subgraph, Graph Edit Distance, Frobenius Distance, and Edge Overlap. TODO: CITE THIS These measures are successful in indicating the degree to which two graphs are similar, and are used in practical tasks involving graph analysis.

However, graph similarity measures require a vertex-to-vertex matching between the two graphs, which is computationally expensive to determine. In particular, determining the optimal matching between two unlabelled graphs is an NP-hard problem, meaning that there is no known algorithm can exactly solve all instances

in polynomial-time. As a result, various heuristic and approximation techniques have been developed to tackle the graph similarity problem.

A recently introduced quantum algorithm, the non-variational quantum walk-based optimisation algorithm (NVQWOA), was designed to solve hard combinatorial optimisation problems [1, 2]. NVQWOA amplifies the probability of measuring high-quality solutions to a problem through an iterative process of phase-separation and mixing via a continuous-time quantum walk (CTQW) on a graph associated with the problem's structure. In the original work, it was shown through classical simulation that NVQWOA found globally optimal solutions on problems such as weighted maxcut,  $k$ -means clustering, quadratic assignment, and the capacitated facility location problem within a small number of iterations.

We seek to determine whether the NVQWOA will perform equally well on the problem of calculating graph similarity as it performed on its first problems. We approach this through classical simulation of the NVQWOA on a range of instances of the graph similarity problem, analysing its behaviour, scalability, and potential as a quantum algorithm for this important class of problems.

# Chapter 2

## Literature Review

### 2.1 Combinatorial Optimisation Problems

Combinatorial optimisation problems consist of a discrete set of feasible solutions, which can be represented as a set  $S$ , with finite order  $N = |S|$ . Each of the  $N$  solutions  $\mathbf{x} \in S$  can be represented as a vector of  $n$  variables  $\mathbf{x} = (x_1, x_2, \dots, x_n)$ , where  $x_j \in \{0, 1, \dots, k - 1\}$  are called the *decision variables*. The solution space  $S$  may contain all possible solutions of this form (of which there are  $N = k^n$ ) or  $S$  may be restricted to solutions which satisfy some constraint (such as in the case of permutation-based problems where  $k = n$  and  $N = n!$ ). Each solution has an associated objective value (or cost), given by a objective function (or cost function)  $f : S \rightarrow \mathbb{R}$ , which gives a measure of the quality of any solution. The goal of the optimisation problem is to find the *optimal solution*  $\mathbf{x}^*$  that maximises (or minimises) the objective (or cost) function:

$$\mathbf{x}^* = \arg \min_{\mathbf{x} \in S} f(\mathbf{x}) \text{ or } \mathbf{x}^* = \arg \max_{\mathbf{x} \in S} f(\mathbf{x})$$

The structure of the objective function is determined by the problem definition. The problem definition consists of a series of criteria which are defined on a subset of the variables in  $\mathbf{x}$ , and the objective function conveys the extent to which a solution satisfies the criteria.

Combinatorial optimisation problems are often NP-hard, meaning that no known polynomial-time algorithm can exactly solve all instances of the problem. Examples of NP-hard combinatorial optimisation problems include the travelling salesman problem and the knapsack problem.

The main challenge in solving these problems is that they often require a near-exhaustive search of the solution space, which usually grows exponentially or super-exponentially with problem size. An example of this super-exponential growth will be present in the graph similarity problem in section 2.2.

Research in combinatorial optimisation algorithms showing exponential speedup includes:

- Exact algorithms that find optimal solutions for special problem instances with certain properties. TODO: CITATIONS
- Approximate algorithms that find solutions which are near the optimal solutions for general problem instances.

Approximate algorithms are the focus of this thesis. TODO: EXPAND

To quantify how close a solution  $\mathbf{x}_i$  is to the optimal solution, the approximation ratio  $A$  is used:

$$A_i = \frac{f(\mathbf{x}_i)}{f(\mathbf{x}^*)}$$

This value compares the objective value of a solution against the maximum possible objective value. A successful approximate combinatorial optimisation algorithm should find solutions which give approximation ratios close to 1.

## 2.2 Graph Similarity Problem

The graph similarity problem involves determining how similar two graphs are to each other. This can be useful in various applications, such as social network analysis, bioinformatics, and pattern recognition.

There is a need to distinguish between the graph similarity problem and the graph isomorphism problem.

A pair of graphs  $G_1$  and  $G_2$  are considered isomorphic ( $G_1 \cong G_2$ ) if and only if there exists a bijection between their vertex sets such that any two vertices in  $G_1$  are adjacent if and only if their corresponding vertices in  $G_2$  are also adjacent. In this definition, the graphs are understood to be undirected, non-labelled, non-weighted graphs. However, isomorphism may apply to all other notions of graph by adding requirements to preserve any additional structures.

The graph isomorphism problem is then the task of correctly creating that bijection (or equivalently, proving that one exists). Algorithms that solve this problem are trivially verifiable, as checking the correctness of the solution only involves checking that the vertex bijection correctly preserves the edges. Since the graph isomorphism problem can be posed as a ‘yes-no’ question on a set of inputs values, it is called a decision problem.

In contrast, the graph similarity problem is the problem of calculating how close a pair of graphs are to being isomorphic. This cannot be posed as a ‘yes-no’ problem, as many magnitudes of similarity must meaningfully captured. There are multiple measures of graph similarity. Some examples include:

- *Graph Edit Distance (GED)*: Counts how many ‘edits’ are required to transform one graph into another, where ‘edits’ include inserting/deleting a vertex or edge, or substituting one vertex or edge with another. The lower the distance, the more similar the two graphs are. TODO: CITATIONS
- *Maximum Common Subgraph (MCS)*: Finds the largest induced subgraph that is common to the two given graphs. The larger the subgraph, the more similar the two graphs are.
- *Frobenius Distance*: Calculates the distance between two graphs using the difference between their adjacency matrices. The lower the distance, the more similar the two graphs are.
- *Edge Overlap*: Finds the proportion of matching entries in the adjacency matrices of the graphs. The greater the proportion, the more similar the two graphs are.[3]

The choice of measure often depends on the specific application and the properties

of the graphs being compared. Considerations such as cost, time, and interpretability inform which measure is best for a practical problem.

Koutra et al. [4] formalised a set of axioms that graph similarity measures should conform to: TODO: MAPPING OUTPUTS TO  $(0,1]$ .

1. Identity:  $\text{sim}(G_1, G_2) = 1 \iff G_1 \cong G_2$
2. Symmetric:  $\text{sim}(G_1, G_2) = \text{sim}(G_2, G_1)$
3. Zero: For a clique graph  $G_1$  and a empty graph  $G_2$ ,  $\lim_{n \rightarrow \infty} \text{sim}(G_1, G_2) = 0$

The measures listed above can all be minimally adapted to satisfy these axioms.

Most graph similarity measures assume a given mapping between the vertices of the graphs. Unlike in graph isomorphism, this vertex mapping doesn't need to be a bijection, since there exists a notion of similarity between graphs with a different number of vertices. For graph similarity methods such as those listed previously, the choice of vertex mapping can change the final result. However, Koutra's axiom 1 requires that graph similarity measures can identify isomorphic graphs by giving them a similarity of 1.

So to satisfy Koutra's axioms, we must find a mapping between the graphs that maximises their similarity.

To find the best mapping between labelled graphs, one can simply ‘pair up’ the vertices in the graphs so that each pair consists of one vertex from each graph that share the same label. This significantly reduces the number of possible mappings (often to just 1), so finding the mapping with the maximum similarity is simple.

To find the best mapping between unlabelled graphs is very challenging. In the general case, the similarity associated with every possible permutation of mappings must be checked until either a mapping that shows isomorphism (or another verifiable global maximum) is found, or the entire space of mappings has been searched.

As such, the unlabelled graph similarity problem can be defined in terms of a

combinatorial optimisation problem.

### 2.2.1 Problem Definition

A formal definition for the unlabelled graph similarity problem is as follows:

Let  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  be two finite, simple graphs and considered *unlabelled* in the sense that vertex identifiers carry no intrinsic meaning.

Let  $\Pi(V_1, V_2)$  denote the set of all maps  $\pi : V_1 \rightarrow V_2$ .

Given a base similarity function  $f : \mathcal{G} \times \mathcal{G} \rightarrow \mathbb{R}$  that compares labelled graphs from the class  $\mathcal{G}$  of all finite simple graphs, the *unlabelled similarity* between  $G_1$  and  $G_2$  is then defined as

$$\text{Sim}(G_1, G_2) = \max_{\pi \in \Pi(V_1, V_2)} f(G_1, \pi(G_2)),$$

where  $\pi(G_2)$  denotes the relabelling of  $G_2$  induced by  $\pi$ .

The unlabelled graph similarity problem is the problem of computing  $\text{Sim}(G_1, G_2)$ . Since  $\Pi$  is set of maps between two finite sets, the size of the set  $|\Pi|$  scales super-exponentially. In the case that  $|V_1| = |V_2|$  and the maps  $\pi$  denote permutations of  $n$  vertices (),  $|\Pi| = n!$ .

This problem is known to be NP-hard, meaning that there is no known polynomial-time algorithm to solve it for all instances. As a result, various heuristic and approximation techniques have been developed to tackle the graph similarity problem. This thesis will explore an approximate quantum algorithm, described in the remainder of this chapter.

## 2.3 Quantum Computing

Quantum computing is based on the principles of quantum mechanics, which describe the behaviour of particles at the atomic and subatomic levels.

This section provides a brief overview of the fundamental concepts of quantum

computing that are relevant to understanding the non-variational QWOA and its application to the graph similarity problem.

### 2.3.1 Qubits and Quantum Superposition

The fundamental unit of information in classical computing is the bit, which can exist in one of two states, typically written as 0 or 1.

In quantum computing, the basic unit of information is the quantum bit or qubit. Unlike classical bits, which can only be in one state at a time, qubits can exist in a superposition of states.

Qubits are physically realised with two-state quantum systems, such as the spin of an electron in which the two states can be taken as spin up or spin down. Qubits are mathematically described by their two-dimensional complex state vectors. Systems of qubits are described in a  $2^n$  dimensional complex vector space, where  $n$  is the number of qubits. A qubit's state (or the state of a collection of qubits) can be represented as the complex weighted sum of its basis states. A common choice of basis states is called the standard or computational basis, consisting of the positive and negative eigenvalues of the Pauli Z operator, commonly notated as  $|0\rangle$  and  $|1\rangle$ , respectively. A general state of a single qubit can be expressed in the standard basis as:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

where  $\alpha$  and  $\beta$  are complex numbers that satisfy the normalisation condition  $|\alpha|^2 + |\beta|^2 = 1$ . The Born rule states that the coefficients  $|\alpha|^2$  and  $|\beta|^2$  represent the probabilities of measuring the qubit in the states  $|0\rangle$  and  $|1\rangle$ , respectively.

When multiple qubits are combined, their joint state is represented by the tensor product of their individual states. For example, the state of a two-qubit system

can be expressed as:

$$\begin{aligned}
 |\psi_{12}\rangle &= |\psi_1\rangle \otimes |\psi_2\rangle = (\alpha_1 |0\rangle + \beta_1 |1\rangle) \otimes (\alpha_2 |0\rangle + \beta_2 |1\rangle) \\
 &= \alpha_1\alpha_2 |00\rangle + \alpha_1\beta_2 |01\rangle + \beta_1\alpha_2 |10\rangle + \beta_1\beta_2 |11\rangle \\
 &= \alpha_1\alpha_2 |00\rangle + \alpha_1\beta_2 |01\rangle + \beta_1\alpha_2 |10\rangle + \beta_1\beta_2 |11\rangle
 \end{aligned}$$

where  $|00\rangle, |01\rangle, |10\rangle$ , and  $|11\rangle$  are the basis states of the two-qubit system.

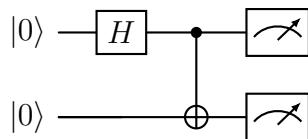
This allows a quantum computer with  $n$  qubits to represent  $2^n$  states simultaneously, which is a key feature that enables quantum parallelism, allowing quantum computers to perform certain computations more efficiently than classical computers.

Despite this parallelism, the computational power is limited by the fact that measuring a quantum state collapses it to one of its basis states, yielding only a single outcome. Therefore, quantum algorithms must be carefully designed to manipulate the amplitudes of the quantum states such that the desired outcomes have higher probabilities of being measured.

### 2.3.2 Quantum Gates, Entanglement

Quantum gates are the building blocks of quantum circuits, analogous to classical logic gates. They manipulate the states of qubits through unitary transformations, which are reversible operations that preserve the total probability of the quantum system. Common quantum gates include the Hadamard gate, which creates superposition, and the CNOT gate, which entangles two qubits.

We can visually represent a series of quantum gates acting on qubits using a quantum circuit diagram. For example, the following diagram shows a simple quantum circuit with two qubits and two gates:



This diagram represents a circuit where the first qubit is put into superposition by the Hadamard gate (H), and then a CNOT gate acts on the second qubit depending on whether the first qubit is in a  $|1\rangle$  state or the  $|0\rangle$  state. Finally, both qubits are measured.

The quantum state begins as:

$$|\psi\rangle = |00\rangle$$

Then after the Hadamard gate is applied, the quantum state is:

$$|\psi_H\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle)$$

Finally the CNOT gate is applied and the quantum state is:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

The measurements can be performed relative to any basis in the qubit's vector space. Commonly, measurements are performed in the same basis as that is used to describe the qubits.

This state is an example of entanglement, a unique quantum phenomenon where the states of two or more qubits become correlated such that the state of one qubit cannot be described independently of the state of the other qubit(s). For example, in the entangled state above, if one were to measure the first qubit to be in the state  $|0\rangle$ , that necessarily requires the second qubit to also be in the state  $|0\rangle$ .

The measurement of one of the entangled qubits has collapsed the superposition for both qubits. This surprising result was initially deemed unphysical on the grounds that it violates local realism by Einstein, Poldowsky, and Rosen, the first to describe this behaviour[5]. Nevertheless, quantum entanglement and its implications have been repeatedly verified through experimentally violating Bell's inequality[6], establishing that the correlations produced from quantum entanglement cannot be explained by local hidden variables[7, 8, 9]. These correlations are fundamental to quantum algorithms. Without entanglement, quantum computers could be efficiently simulated by classical computers, negating any advantage[10].

### 2.3.3 Quantum Algorithms and Challenges

Quantum algorithms seek to leverage properties of qubits and quantum gates to solve specific problems more efficiently than classical algorithms. Notable examples include Shor’s algorithm for integer factorisation[11], which runs exponentially faster than the best-known classical algorithms, and Grover’s algorithm for unstructured search[12], which provides a quadratic speedup over classical search algorithms.

Large, universal, fault-tolerant quantum computers that can run these algorithms at useful scales will require large numbers of qubits. While researchers have made significant progress in error correction, coherence times, qubit connectivity, and gate fidelities, fault tolerant quantum computing may take decades to achieve. In the meantime, Noisy Intermediate-Scale Quantum (NISQ) computers already exist, and can run small-scale quantum algorithms that can provide insights into quantum behaviour and inform the development of larger systems.

These NISQ devices are limited by the number of qubits, gate fidelities, and coherence times. As a result, quantum algorithms designed for NISQ devices must be efficient in terms of qubit usage and circuit depth to minimise the impact of noise and errors.

Even if NISQ devices cannot solve problems faster than the best classical computers using the best classical algorithms (particularly with the emergence of exascale supercomputing), they could still provide an economic advantage by using less energy or by being lower cost to build and operate.

NISQ algorithms are designed to work within these low-resource constraints. These algorithms typically involve a hybrid approach, where a quantum computer is used to prepare and measure quantum states, while a classical computer optimises parameters based on the measurement results. Some examples of NISQ-era algorithms are described in the following sections.

## 2.4 Variational Quantum Algorithms

### 2.4.1 VQAs in General

Variational Quantum Algorithms (VQAs) are a class of hybrid quantum-classical algorithms that leverage the strengths of both quantum and classical computing to solve optimisation problems. They are particularly well-suited for NISQ devices due to their relatively low resource requirements and robustness to noise.

VQAs implement a parametrised quantum circuit (PQC) whose unitary evolution is governed by a set of  $d$  classically tunable parameters  $\theta \in \mathbb{R}^d$ . The quantum device prepares the state

$$|\psi(\theta)\rangle = U(\theta) |0\rangle^{\otimes n}$$

where  $U(\theta)$  is a depth-restricted circuit composed of parameterised single- and multi-qubit gates, and  $n$  is the number of qubits in the input to the quantum computer. Commonly,  $d = \mathcal{O}(\text{poly}(n))$ , since we seek efficient circuits that are polynomial in resources. TODO: CITATION

The objective function of the algorithm is typically expressed as the expectation value of a Hermitian operator  $H$  with respect to the variational state:

$$C(\theta) = \langle \psi(\theta) | H | \psi(\theta) \rangle$$

This cost function is estimated on the quantum device via repeated projective measurements in appropriate bases. A classical optimiser updates  $\theta$  with the aim of minimising (or maximising)  $C(\theta)$ , thus driving the quantum circuit towards a state that approximates the optimal configuration with respect to the target problem. The algorithm repeatedly prepares this variational quantum state, measures its expectation value, and optimises the parameters until a certain number of iterations is complete or until measurements of the quantum state have an approximation ratio sufficiently close to 1.

To summarise, VQAs consist of a two-step loop: a quantum computer evolves the initial state to a final state via a PQC, then a classical computer measures the

expectation value of the final state and uses this data to update the PQC. At the end of this loop, the quantum computer's output is now a good approximation of the optimal configuration.

### 2.4.2 QAOA

The Quantum Approximate Optimisation Algorithm (QAOA) is a subclass of VQAs designed to solve combinatorial optimisation problems, introduced by Farhi et al. [13] In this formulation, the PQC is defined by alternating applications of unitaries. One is a quality mixer associated with the problem instance and the other is a mixing operation that induces interference.

The quantum state begins in the equal superposition state over the computational basis states:

$$|s\rangle = \frac{1}{\sqrt{2^n}} \sum_z |z\rangle$$

where  $n$  is the number of qubits.

Define a unitary operator  $U(\gamma)$  which depends on: an angle  $\gamma$ , which lies between 0 and  $2\pi$ ; and a quality operator  $Q$ , which is a diagonal operator that contains the objective function value for each solution.

$$U(\gamma) = e^{i\gamma Q}$$

Define operator  $U(\beta)$  which depends on the parameter  $\beta$ , which lies between 0 and  $\pi$ .

$$U(\beta) = \prod_{j=1}^n e^{-i\beta \sigma_j^x}$$

Here,  $\sigma_j^x$  denotes the Pauli X operator applied to the  $j$  register. This is the mixing unitary, which induces interference between related solutions. Other mixers are introduced for use in the NVQWOA in section 2.5.

Now, for any integer  $p \geq 1$ , and  $2p$  angles  $\gamma = (\gamma_1, \dots, \gamma_p)$  and  $\beta = (\beta_1, \dots, \beta_p)$  we define the final quantum state:

$$|\gamma, \beta\rangle = U(\beta_p)U(\gamma_p)\dots U(\beta_1)U(\gamma_1)|s\rangle$$

This quantum state is acquired by repeatedly applying  $U(\gamma)$  then  $U(\beta)$ . The action that  $U(\gamma)$  has on each individual state is to apply a local phase shift to its complex amplitude proportional to the quality of the solution represented by that state. Because this results in the phases of the solutions being separated from one another, this unitary is called the phase separation unitary. The action that  $U(\beta)$  has on each individual state is equivalent to performing a quantum walk on a graph representing the connections between different states.

We can now do the usual VQA method of measuring the expectation value, optimising the parameters  $\gamma$  and  $\beta$ , and repeating to obtain good approximations of the optimal solution.

### 2.4.3 Challenges

Although VQAs are a promising platform for NISQ computing, their effective performance relies on the computationally expensive tuning of an often prohibitively large number of variational parameters. Additionally, the performance of these variational algorithms is highly dependent on the initialisation of the variational parameters.

Therefore, it can be argued that VQAs replace one difficult optimisation problem with another difficult optimisation problem.

## 2.5 Non-Variational Quantum Walk-based Optimisation Algorithm

### 2.5.1 Overview

The NVQWOA is a novel algorithm introduced by Bennett et al. that builds upon and addresses the variational challenges of the QAOA[1, 2]. Like the QAOA, it alternates between applying two unitaries: a phase-separation unitary that encodes the objective function into the complex phase of the states and a mixing unitary that induces quantum interference between the solutions. Unlike QAOA or other VQAs, the parameters defining the unitaries are not variationally tuned

by a classical optimiser. Instead, they are predetermined by the choice of only three hyperparameters  $\gamma, t, \beta$ . Additionally, the structure of the mixer is chosen to match the structure of the problem, to connect nearest-neighbour solutions to one another.

Simulations have demonstrated that this non-variational approach yields rapid convergence to global optima across diverse problem types, including MaxCut, maximum independent set, k-means clustering, capacitated facility location, and the quadratic assignment problem, using only modest circuit depths and a handful of iterations [2].

### 2.5.2 Algorithm Description

Using the terms and definitions of combinatorial optimisation problems from Section 2.1:

The algorithm begins with an initial superposition over all possible solution states:

$$|s\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{x} \in S} |\mathbf{x}\rangle$$

Each iteration of the NVQWOA applies two unitaries:

$$U_Q(\gamma) = e^{-i\gamma Q}, \quad U_M(t) = e^{-itA}$$

where  $Q$  is a diagonal operator such that  $Q|\mathbf{x}\rangle = f(\mathbf{x})|\mathbf{x}\rangle$  encodes the objective function values, and  $A$  is the adjacency matrix of a mixing graph whose vertices correspond with feasible solutions and whose edges connect nearest-neighbour solutions to one another.

The phase-separation unitary applies a phase to each solution states, proportional to the objective value of that solution  $f(\mathbf{x})$ , while the mixing unitary  $U_M(t)$  implements a continuous time quantum walk (CTQW) on the mixing graph, redistributing complex amplitudes through neighbouring solutions. Repeated alternating application of these unitaries produces a designed interference process in which

amplitudes associated with optimal or near-optimal solutions interfere constructively, amplifying their measurement probabilities.

The final quantum state after  $p$  iterations of each unitary is

$$|\gamma, t, \beta\rangle = \left[ \prod_{i=0}^{p-1} U_M(t_i) U_Q\left(\frac{\pm\gamma_i}{\sigma}\right) \right] |s\rangle$$

where the  $\pm$  accounts for whether the goal is minimisation ( $-$ ) or maximisation ( $+$ ),  $\sigma$  is the standard deviation of the initial objective function landscape (which can be efficiently approximated through random sampling of  $p = 0$ ),  $t_i$  and  $\gamma_i$  are obtained from specific formulae in terms of  $\gamma, t$ , and  $\beta$  and where  $\gamma > 0, t > 0$ , and  $0 < \beta < 1$ :

$$\gamma_i = \left( \beta + (1 - \beta) \frac{i}{p-1} \right) \gamma, \quad t_i = \left( 1 - (1 - \beta) \frac{i}{p-1} \right) t$$

So the angles  $\gamma_i$  increase linearly with  $i$  and the mixing times  $t_i$  decrease linearly with  $i$ .

### 2.5.3 Mixing Unitary

A key conceptual advance of the NVQWOA lies in the explicit construction of a problem-structured mixing graph (also referred to as mixing unitary or mixer). The vertices of the graph represent feasible solutions, and edges connect nearest neighbour configurations, typically those separated by a minimal Hamming distance or by a single elementary move. The resulting adjacency matrix  $A$  defines a vertex-transitive graph whose degree  $d$  is polynomial in problem size.

#### 2.5.3.1 Mixer Examples

In his work, Bennett provides some examples of mixing graphs with known efficient implementations on a quantum computer [1, 2]:

*Binary Mixer:* For problems with  $n$  binary decision variables  $x_j \in \{0, 1\}$ , the mixing graph is a  $n$ -dimensional hypercube, which is identical to the transverse-

field Hamiltonian from the QAOA. Solutions are connected to the  $n$  other solutions which differ by one bit-flip.

*Integer Mixer:* For problems with  $n$  integer decision variables  $x_j \in \{0, 1, \dots, k-1\}$ . Solutions are connected to the  $n(k-1)$  other solutions which differ in the choice of one decision variable.

*Permutation Mixer:* For problems with  $n$  integer decision variables  $x_j \in \{0, 1, \dots, k-1\}$  where the solutions are constrained to not have repeated decision variables. Solutions are connected to the  $\frac{1}{2}n(n-1)$  other solutions which are transpositions of each other.

The choice of mixing graph directly determines how probability amplitudes are propagated, making it possible to exploit problem structure, unlike the transverse-Hamiltonian mixer in the QAOA, which applies the same mixer to all combinatorial optimisation problems[13].

### 2.5.3.2 Mixer Subshells

The distance  $dist(u, v)$  between two vertices  $u, v$  on a graph is the minimum length of the paths connecting them. A subshell is a subset of the vertices of the mixing graph, defined in relation to a reference vertex  $u$ . The subshell  $h_u$  contains all vertices that are a distance  $h$  away from  $u$ . The set of all subshells for a graph form equivalence classes on the set of the vertices of the graph.

For the NVQWOA to perform well on a combinatorial optimisation problem, it is expected to satisfy two conditions. First, the action of the mixer on an arbitrary solution state  $|\mathbf{u}\rangle$  must be as follows:

$$U_M(t) |\mathbf{u}\rangle = \sum_{h=0}^D \left( e^{-ih\phi(t)} \sum_{\mathbf{x} \in h_u} r_{\mathbf{x}}(t) |\mathbf{x}\rangle \right),$$

where  $D$  is the diameter of the mixing graph and (for sufficiently small  $t$ )  $r_{\mathbf{x}}$  and  $\phi$  are positive real-valued functions, and  $0 < \phi(t) < \pi$ . In essence, probability amplitude from an initial vertex is distributed to other vertices such that the complex phase of the distributed probability amplitudes are proportional to their

distance from the initial vertex.

The second condition is that the following relationship should be at least approximately satisfied,

$$(\mu_{h\mathbf{x}} - f(\mathbf{x})) \approx -m_h(f(\mathbf{x}) - \mu),$$

where  $\mu_{h\mathbf{x}}$  is defined as the mean objective function value of solutions contained in  $h_{\mathbf{x}}$ ,  $\mu$  is the mean objective function value of all solutions in  $S$ , and  $m_h$  is a positive constant. Also, the proportionality  $m_h$  should increase monotonically with increasing  $h$  (up to a distance which is a considerable fraction of the graph's diameter  $D$ )

# Chapter 3

## Methods

We simulated the application of the NVQWOA to the graph similarity problem. The measure of graph similarity chosen was Edge Overlap, as it is a low-cost measure that still serves as a interpretable measure of similarity. The aim was to maximise this objective function through matrix exponentiation and multiplication,analytically computing the manipulation of state vector such that the states which corresponded with the optimal solutions (those with the greatest similarity) had an amplified probability of being measured.

There were two phases to the analysis. First, we applied the algorithm to one problem at a time and small problem sizes up to  $n = 9$ , using standard matrix exponentiation. Then we applied the algorithm to several problem instances simultaneously and had problem sizes up to  $n = 10$ .

### 3.1 Simulation

To investigate the performance of the NVQWOA on graph similarity problems, we chose to perform classical simulations of a quantum computer, rather than directly performing the algorithm on a quantum computer. Simulation allows for computation with negligible stochastic or decoherence errors and complete analysis of the evolving quantum state, something which is inaccessible on real quantum hardware but useful for characterising performance and benchmarking.

Simulation of quantum algorithms and computers can be approached in many different ways. Tensor networks simplify circuits into lower-entanglement systems but has exponentially degrading performance as circuit depth and entanglement entropy. Stabiliser-based approaches can efficiently simulate Clifford-only circuits and certain restricted non-Clifford extensions but cannot capture the parameterised unitaries used in the NVQWOA. State vector simulation computes the full evolution of the state vector, but can be costly in computational resources.

TODO: CITATIONS

State vector simulation was chosen as the strategy for its accuracy. The Qiskit Aer simulator and related packages were not suitable as the permutation mixer required is a sparse operator, which is inefficient to simulate under the requirements of using tensor products of standard gates. Instead, we directly computed the relevant matrix operations. For the first phase of analysis, the matrix exponentiation and multiplication was able to be performed on local hardware using the well-known SciPy package. For the second phase of analysis, the large problem sizes required parallel computation. To implement this, we used QuOp, a Python framework for parallel simulation of quantum variational algorithms[14, 15]. QuOp provides efficient handling of large, sparse unitaries and supports MPI-based parallelisation, allowing simulation of high-dimensional state vectors across multiple compute nodes without loss of precision.

Parallel simulations of the non-variational QWOA would not be possible without high-performance computing (HPC) resources, which were provided by the Pawsey Supercomputing Centre.

To simulate NVQWOA using QuOp, a parameter mapping was used to translate the hyperparameters of the NVQWOA to the individual parameters of a QVA. The quantum circuit was defined to be the two unitaries of the NVQWOA; the phase separator  $U_Q$ , and the mixer  $U_M$ . With these modifications, QuOp could simulate the NVQWOA.

## 3.2 Graph Similarity Measure

As described in section 2.2, there are many options for the choice of which graph similarity measure to use.

Graph edit distance is the most common choice, but is costly to compute, as it requires the equivalent of a pathfinding search, such as an  $A^*$  search algorithm. Maximum common Since computational resources were a significant pressure, we chose one of the least computationally expensive similarity measures to compute, the edge overlap.

To calculate the edge overlap, the number of matching entries in the adjacency matrices of the graphs are counted and the sum is divided by  $n^2$ , which corresponds to the size of the adjacency matrices and the maximum possible overlap. This easy calculation also makes the edge overlap highly interpretable. One can imagine the vertex mapping as translating the vertices of one graph to the corresponding vertices in the other graph, and the edge overlap represents how much the edges line up correctly. The edge overlap also works on directed graphs, but directed graphs were not investigated in this thesis.

When the best vertex mapping is known between the two graphs, the edge overlap satisfies Koutra’s similarity measure axioms, making it a ‘good’ measure of graph similarity.

A drawback of using edge overlap is that it is not well-defined for graphs with differing numbers of nodes,  $|V_1| \neq |V_2|$ . This restricts our investigation to graphs with an equal number of nodes.

The choice of graph similarity measure is not expected to have a strong effect on the observed results. The vertex mappings that give strong similarity with any particular measure usually give strong similarity with most measures. For the choice of a specific graph similarity measure to affect the results, it would have to give a different problem structure which significantly alters the structure of qualities.

### 3.3 Problem Instance Construction

There does not exist a universally used set of graph similarity problem instances. To test the algorithm on a wide group of fairly-chosen problems, we randomly generated the graphs using the Erdős-Rényi-Gilbert random graph model[16, 17]. The number of nodes  $n$ , was varied to investigate how changing problem sizes changed the performance of the algorithm  $n = 8, 9, 10$  were used for problem instance generation. The probability of edge inclusion was fixed at 0.5 for simplicity and repeatability. For each value of  $n$ , 30 graphs were generated using the NetworkX Python library [18]. The seeds were selected starting from 0 and increasing by 1 for each successive problem instance. Any seeds that generated a graph isomorphic with any previously generated graphs would have been removed from the list of valid seeds. Ultimately, none of the seeds we used generated graphs isomorphic to one another for  $n = 8, 9, 10$ , so the list of seeds was equivalent to the integers in  $[0, 29]$ .

Instead of calculating the similarity between the generated problem instances, the similarity was calculated between each graph and a copy of itself. This was to ensure similar distributions of similarity would arise between the different problem instances.

### 3.4 Phase Separator and Mixer Construction

The phase separating unitary was constructed in QuOp. For each vertex mapping, the quality (given as edge overlap) was calculated and stored as an array. This array was converted into a diagonal unitary operator in QuOp.

The mixer was constructed as a column oriented array in Numpy [19] and converted to a compressed sparse row format for storage. This sparse matrix could was loaded into QuOp using HDF5 parallel I/O operations[20].

Since we are considering graphs with an equal number of nodes  $n$ , vertex mappings match the arbitrary vertex indices of each graph to one another with some ordering,  $\pi : \{1, \dots, n\} \rightarrow \{1, \dots, n\}$ . (In the unlabelled graph problem, the vertices in each graph can still have indices, just not information that can inform how to

match those indices together.) Each  $\pi \in \Pi$  corresponds to a distinct reordering of the vertex indices. Therefore, vertex mappings can be equivalently written as permutations of  $n$  distinct decision variables.

From this, we can conclude that the correct choice of mixer is the permutation mixer, which connects solutions that are one swap of decision variables away from one another. In terms of vertex mappings, the permutation mixer connects solutions corresponding to mappings which differ only by two vertices that have had their targets swapped. Since these are the nearest neighbours to one another, we can also conclude that the minimum hamming distance from one solution to another is 2.

### 3.5 Hyperparameter Optimisation

The NVQWOA has three hyperparameters:  $\gamma, t, \beta$ . Although sub-optimal parameters can produce quantum circuits that significantly amplify optimal and near-optimal solutions, it is expected that finding optimal values for these hyperparameters through three-dimensional numerical optimisation will give the best possible results.[2]

We used three different objective functions as inputs to the optimiser:

1. *Expected Value (EV)*: The expected value of the state vector after amplification. This would require the fewest shots to compute on real quantum hardware, and is a natural choice for optimisation [21].
2. *Optimal Solution Probability (OSP)*: The probability of measuring an optimal solution. This is impractical to measure on quantum hardware, as it requires foreknowledge of the optimal solution and an unfeasible number of shots. It is included in our investigation here to provide an upper bound by finding the best possible parameters.
3. *Conditional Value at Risk (CVaR)*: The expected value of the  $\alpha$ -tail of the state vector. This takes more shots to measure on quantum hardware than the expected value, but has been shown to give faster convergence to better

solutions[22].

Optimisation of the NVQWOA hyperparameters was done in QuOp during the NVQWOA simulation, using the Nelder-Mead method of numerical optimisation [23]. This method was chosen for its efficiency. Since it does not require the computation of derivatives, the method is faster to compute than other alternatives. One downside of using Nelder-Mead is that it can converge to a locally optimal set of hyperparameters, rather than a globally optimal set. Additionally, it does not have an in-built method to set boundaries on the possible parameters, so it is possible that it could converge to non-physical parameters such as  $t < 0$ .

## 3.6 Procedure

### 3.6.1 Amplification Analysis

For each of  $n = 8, 9, 10$ , the probability distribution for the different solutions was compared before and after the algorithm was applied. We expected that solutions with high similarity would be more likely to be measured after the algorithm was applied. Additionally, the probability to measure the optimal solution was calculated.

### 3.6.2 Solution Distance Analysis

To supplement the verification of amplification, it is useful to obtain statistics on the distance between solutions. This is because we expect that near-optimal solutions, which will have a low distance to the optimal solutions, should be amplified more than other solutions, which have a greater distance to the optimal solutions.

There are two useful notions of distance between solutions: subshell distance and Hamming distance, which are defined and explained below.

#### 3.6.2.1 Subshell Distance

In this thesis, we use the term subshell distance to refer to the minimum distance on the mixing graph between a solution and an optimal solution. The term subshell

in this notion of distance comes from the description in section 2.5.3.2, and is used to distinguish this distance measure from other approaches. The mixer we are using is the permutation mixer, so the subshell distance is defined as:

$$\text{SD}(\mathbf{x}^1, \mathbf{x}^2) = \min\{m \in \mathbb{N}_0 : \exists \tau_1, \dots, \tau_m \in \mathcal{T} \text{ with } \tau_m \dots \tau_1 \mathbf{x}^2 = \mathbf{x}^1\}$$

where  $\mathcal{T} = \{(ij) : 1 \leq i \leq j \leq n\}$  is the set of all transpositions in the symmetric group  $S_n$  and transpositions act by reindexing coordinates. For this analysis  $\mathbf{x}^1$  is always an optimal solution. If there were multiple optimal solutions, the subshell distance from each optimal solution was found and the minimum value was used.

Subshell distance is a useful metric in the analysis because it directly represents how close the solutions are to each other on the mixing graph. By analysing how amplification is applied to solutions depending on their subshell distance, we can observe how probability is being moved by the mixing process. Additionally, if one were to perform a local search after finding a near-optimal solution, it would likely be a search of solutions with low subshell distance to the found solution, so analysing how the subshell distance of different solutions is relevant to the application of the NVQWOA.

### 3.6.2.2 Hamming Distance

Hamming distance is a simple yet powerful and highly interpretable measure for comparing objects. It measures the number of different decision variables for a solution. The Hamming distance for two solutions is defined as

$$\text{HD}(\mathbf{x}^1, \mathbf{x}^2) = \sum_{i=0}^n \delta(x_i^1, x_i^2)$$

where  $\delta$  is 1 if  $x_i^1 \neq x_i^2$  and 0 otherwise. For this analysis  $\mathbf{x}^1$  is always an optimal solution. If there were multiple optimal solutions, the Hamming distance from each optimal solution was found and the minimum value was used.

Hamming distance is a useful metric in the analysis because it gives a measure of distance that is not related to the structure of the algorithm and can be easily

compared to other combinatorial optimisation problems and algorithms.

### 3.6.3 Subshell Analysis

Using the notion of subshell distance and the conditions described in section 2.5.3.2, we can characterise the suitability of this mixer to the problem of graph similarity.

To do so, we analysed the qualities of solutions within each subshell. The average difference in quality between the optimal solutions and the solutions in each subshell were found. This was called the mean quality gap. It is expected that solutions that have a high subshell distance are of lower quality, so the mean quality gap should ideally increase monotonically with subshell distance. If the mean quality gap was not monotonically increasing, then

The variance in quality within each subshell was found. This was called the subshell variance. The variance of the average variances was found. This was called the second-order variance.

### 3.6.4 Hyperparameter Analysis

The hyperparameters were selected by the optimisation procedure outlined in section 3.5, beginning with the initial parameters  $\gamma = 1.0, t = 0.1, \beta = 0.4$ . This set of initial parameters were recommended by Tavis et al. [1].

We stored the hyperparameters obtained for each problem instance with each optimisation objective, producing a set of nine hyperparameters for each problem instance.

# Chapter 4

## Results and Discussion

This chapter presents and interprets the results of classical simulations of the non-variational quantum walk-based optimisation algorithm (NVQWOA) applied to the unlabelled graph similarity problem. The primary objective is to evaluate the performance of NVQWOA in amplifying the probability of optimal and near-optimal solutions, to examine how its dynamics reflect the structure of the solution space, and to understand how its limited hyperparameter set interacts with different objective functions.

When referring to the hyperparameter optimisation objective functions explained in section 3.5, we use the acronyms EV for expectation value, OSP for optimal solution probability, and CVaR for conditional value at risk.

### 4.1 Single Graph Analysis

The first part of the analysis was performed on a randomly chosen graph. The seed 2025 was arbitrarily chosen to create a random graph by the method described in section 3.3. The NVQWOA was applied to this graph with fixed initial hyperparameters,  $\gamma = 1.0, t = 0.1, \beta = 0.4$ , in order to see if suboptimal hyperparameters can still produce amplification. The number of iterations was increased to  $p = 30$ .

Figures 4.1 and 4.2 analyse the effect of the NVQWOA when applied to the graph

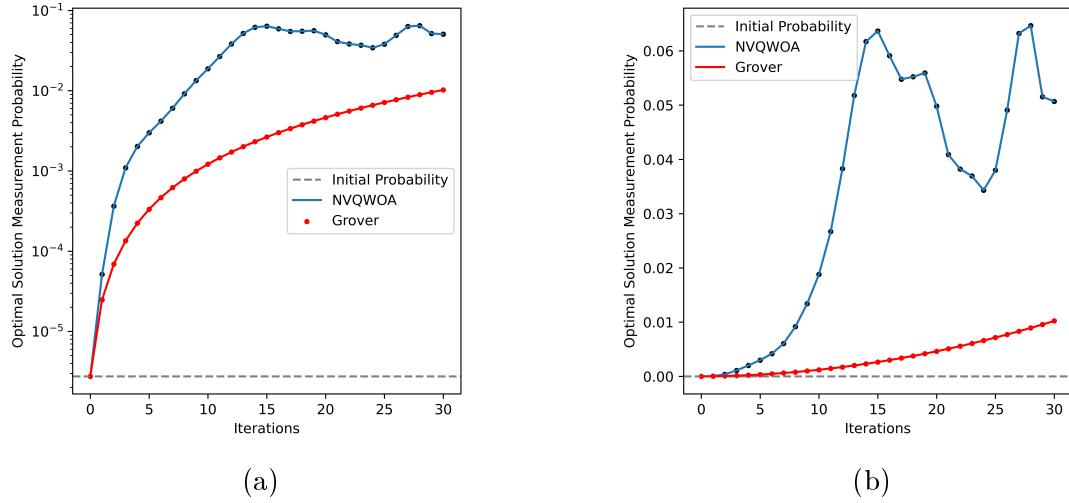


Figure 4.1: Simulation results for  $p = 30$  NVQWOA applied to seed 2025 and Grover’s algorithm for an unstructured database of equivalent size. Probability of measuring the optimal solution at each iteration. (a) log scaled y-axis, (b) linear y-axis.

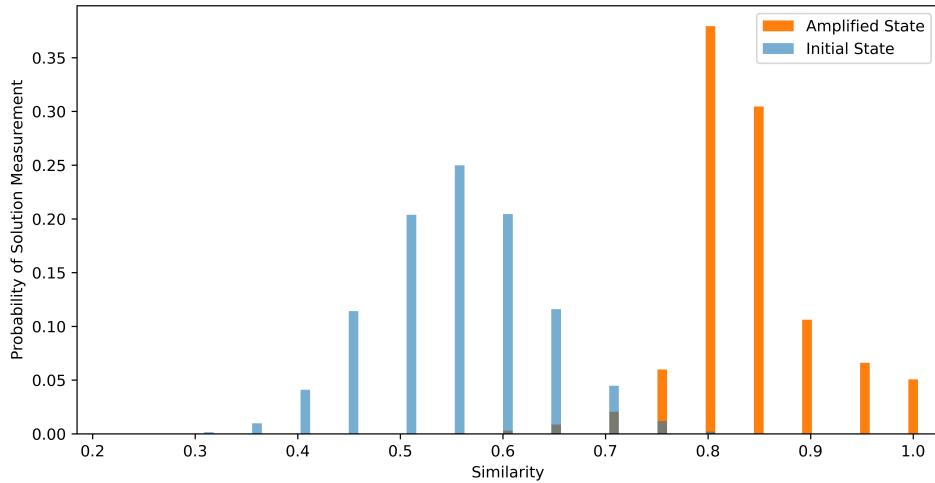


Figure 4.2: Simulation results for NVQWOA applied to seed 2025. Probability distributions for similarity as measured from the initial equal superposition state (blue) and the final amplified state (orange).

$n = 9$ , seed= 2025. From these results it is clear that probability amplitude has been channelled primarily into optimal and near-optimal solutions.

In Figure 4.1, the NVQWOA outperforms Grover’s algorithm for an equivalent number of iterations. Since Grover’s algorithm is optimal for searching an unstructured database [24], this suggests the the NVQWOA is successfully using the structure of the problem (as embedded in the phase separation and mixing unitaries) to amplify the optimal solutions. Another feature of note is that after  $p = 15$  iterations, the  $\text{OSP} = 0.0636607501$  is at a maximum, and after this point, the OSP decreases with further iterations until it reaches 0.0342996063. The OSP appears to oscillate between those values, and ends on a value of 0.0506801642.

In Figure 4.2, the expected value for the similarity has increased from 0.556927 to 0.840676. The mode of the distribution has moved from a similarity score that had 90690 states to a similarity score with only 748 states. Even though the probability of measuring the optimal solution has increased, it is not the new mode of the probability distribution. This is because there is only 1 optimal solution, so even though the other solutions have less amplification applied to them, they greatly outnumber the optimal solution usually by two or three orders of magnitude. Therefore, any small amount of probability that they receive can sum up to be greater than the solution receiving the most amplification.

This is further verified in Figure 4.3. Solutions with similarity below 0.75 are attenuated by the NVQWOA, and solutions with similarity greater than 0.75 are amplified, with the amplification increasing exponentially with similarity. The amount of amplification that the optimal solution receives is greater than any other solution, with an amplification factor of 18391. The similarity score of the solutions with the most attenuation is 0.25925926, with an amplification factor of  $3.73 \times 10^{-5}$ . Interestingly, the solutions with the most attenuation are not those with the minimum similarity scores. The minimum quality solutions, which have a similarity of 0.20987654, received an average amplification of  $3.33 \times 10^{-3}$ , which is more amplification than was applied to any other solutions with similarity score less than 0.6. This reduction in attenuation is due to the mapping of qualities onto the unit circle as part of the algorithm. EXPAND ON THIS.

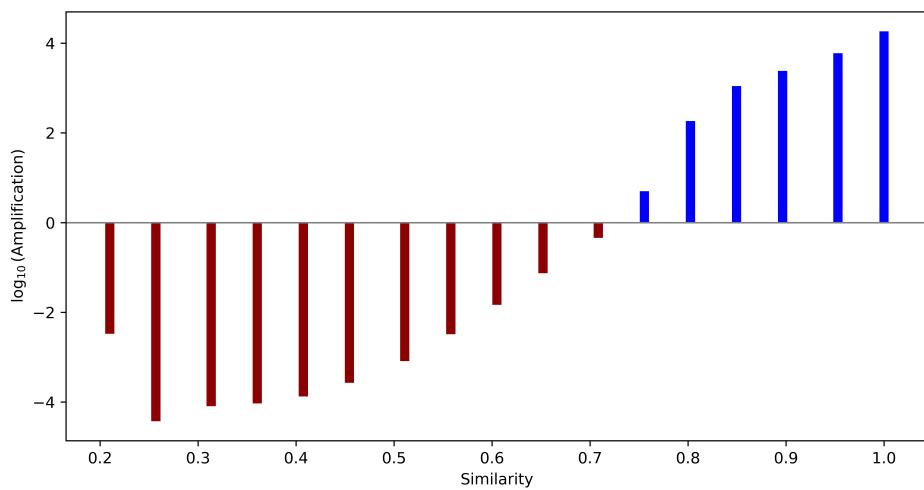


Figure 4.3: Simulation results for NVQWOA applied to seed 2025. Logarithmic scale solution amplification as a function of solution similarity.

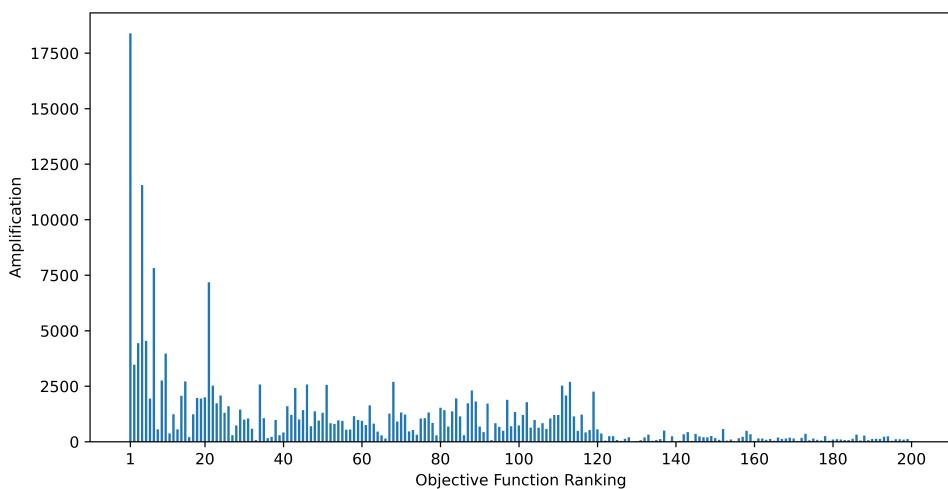


Figure 4.4: Simulation results for NVQWOA applied to seed 2025. Amplification applied to the best 200 solutions.

## 4.2 Multiple Graph Analysis

The next phase in the analysis was to perform simulations on many different graphs and observe how the algorithm performs in the average case. For these simulations, the number of iterations was decreased to  $p = 10$ , and hyperparameter optimisation was used to find suitable hyperparameters for each problem. As discussed in section 3.5, the hyperparameter optimisation objective functions used were expected value (EV), optimal solution probability (OSP), and conditional value at risk (CVaR).

### 4.2.1 Algorithm Behaviour and Amplification

To expand on the results from the previous section, probability distributions for the similarities were analysed. Figures 4.5 and 4.6 show the average probability distributions over the possible similarity scores, using a linear probability scale for Figure 4.5 and a log probability scale for 4.6. After amplification, the distributions are skewed towards higher-similarity solutions compared to the initial distribution. In the distributions representing the average final state for OSP, the modes are not shifted as much as the modes for EV or CVaR. This is because CVaR and EV can be improved by shifting up the mode of the probability distribution, even if the optimal solution probability decreases.

Unexpectedly, it appears that for some seeds at  $n = 8$ , optimising the hyperparameters for EV did not amplify the distribution at all. Rather disquieting. find an explanation for this.

It is evident in Figure 4.7 that the NVQWOA performs well in the average case to increase the probability of measuring the optimal solution. Additionally, comparing the fixed hyperparameter from the previous section to the optimised hyperparameters in the equivalent  $n = 9$  problem set here, we see that the final optimal solution probability has increased on average from 0.06366 to 0.23 for OSP, and 0.07 for EV and CVaR. However, given that the final optimal solution probability can vary over several orders of magnitude, whether hyperparameter optimisation assists in directly measuring the optimal solution appears to be in doubt.

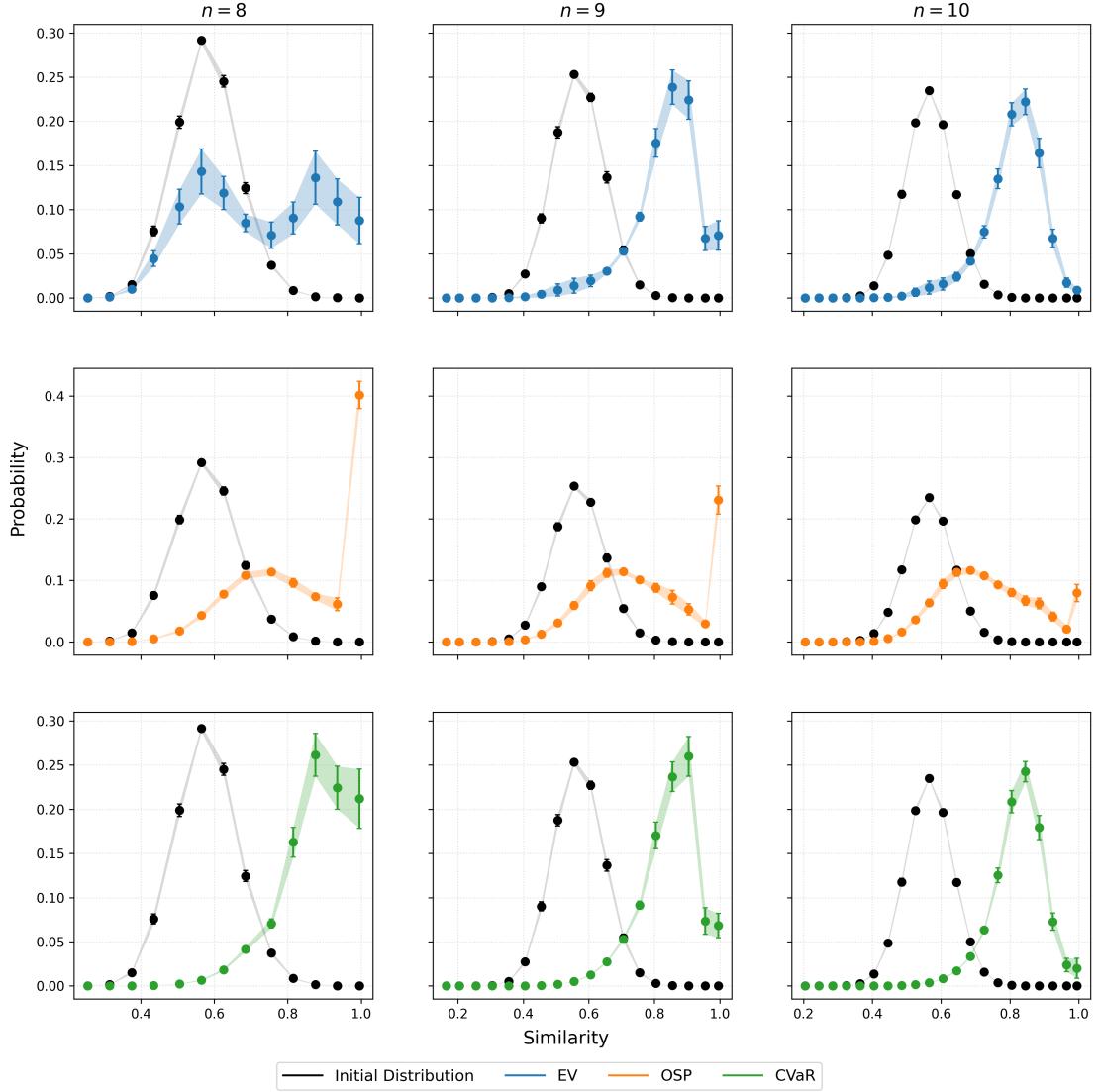


Figure 4.5: Probability distributions for similarity as measured from the initial equal superposition state (black) and the final amplified state. Average simulation results for NVQWOA applied to 30 graphs at (left)  $n = 8$ , (center)  $n = 9$ , (right)  $n = 10$ . (Top) hyperparameters optimised for EV. (Middle) hyperparameters optimised for OSP. (Bottom) hyperparameters optimised for CVaR.

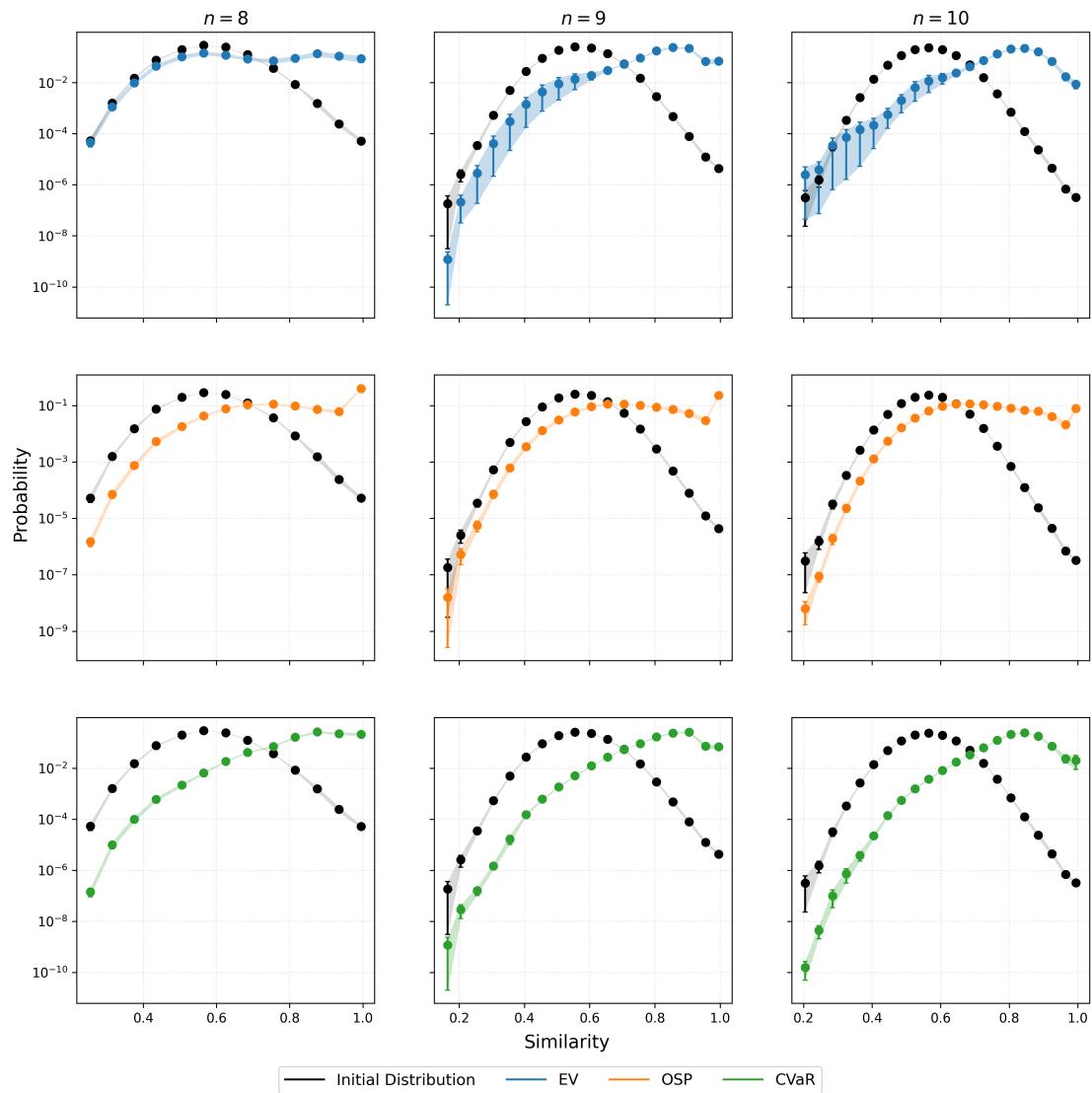


Figure 4.6: Depicts the same distributions as Fig 4.5 with a logarithmic y-axis.

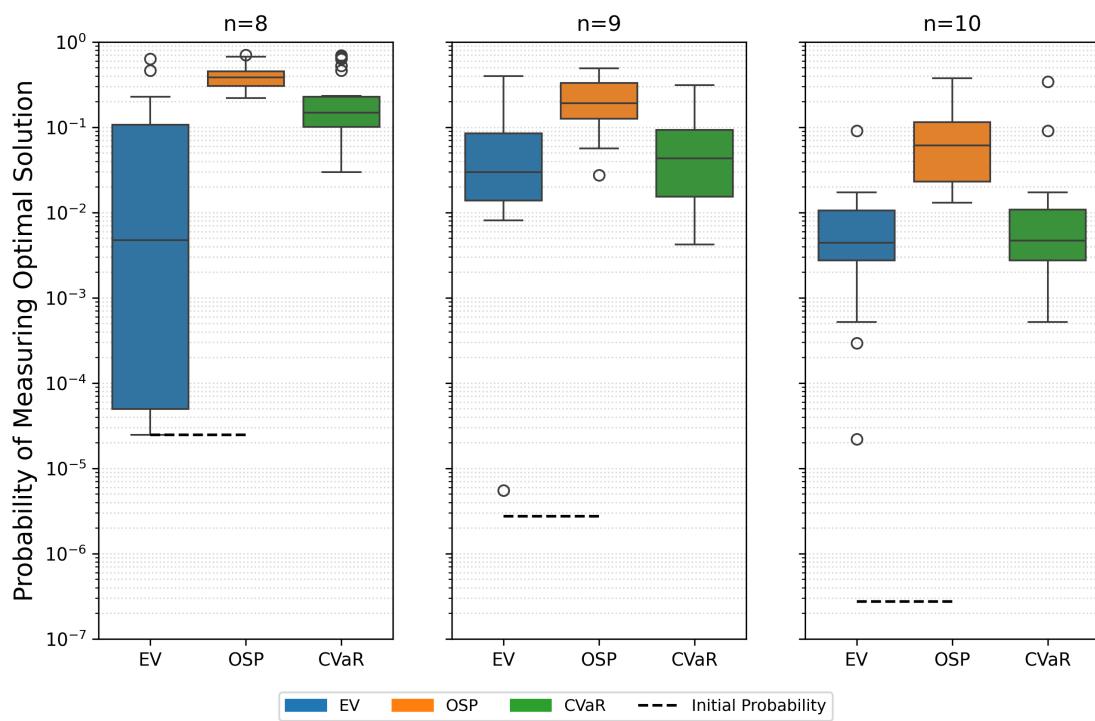


Figure 4.7: Simulation results of the NVQWOA applied to 30 graphs at (left)  $n = 8$ , (center)  $n = 9$ , (right)  $n = 10$ . Boxplots represent the distribution in probability to measure the optimal solution.

### 4.2.2 Distance Analysis

We next analysed the distance between each solution and the optimal solution(s) to determine the degree to which amplification favours solutions close to the optimum in the solution space. The measures of distance used were Hamming distance and subshell distance, described in section 3.6.2.

As shown in Figure 4.8, the mean Hamming distance decreased significantly after amplification, with X and Y and Z as the average reductions.

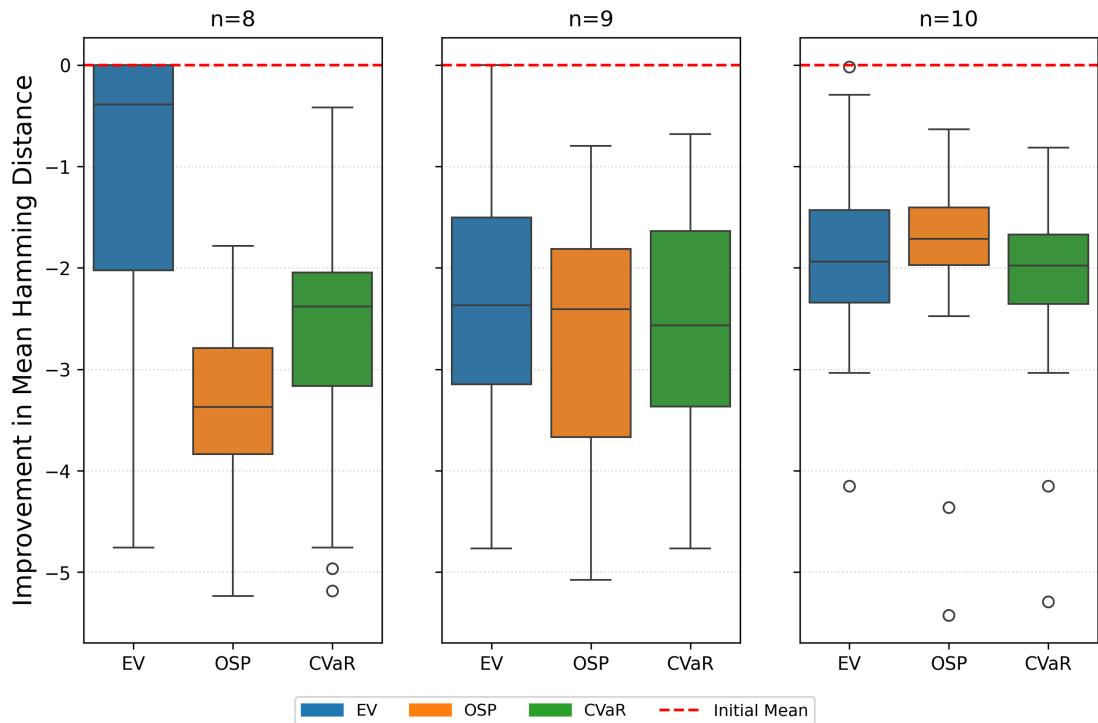


Figure 4.8: Simulation results of the NVQWOA applied to 30 graphs at (left)  $n = 8$ , (center)  $n = 9$ , (right)  $n = 10$ . Boxplots representing the distribution of improvements in mean Hamming distance. The Initial Mean (red)

Figure 4.9 shows how much amplification was applied to each solution based on their Hamming distance. The optimal solutions received average amplifications of X, Y and Z.

We also analysed the subshell distance between each solution and the optimal

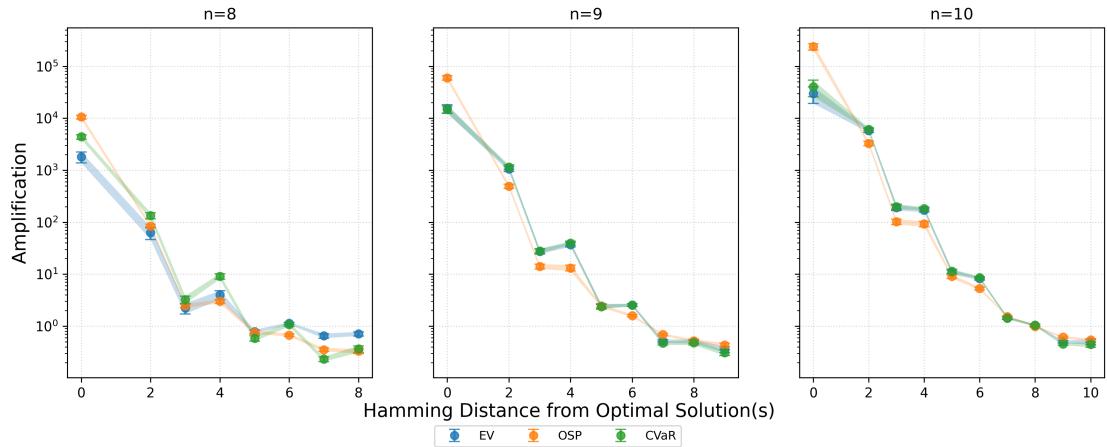


Figure 4.9: Mean amplification applied to each solution grouped by their Hamming distance from the optimal solution.

solution(s), which directly reflects the structure of the permutation mixer and the connectivity of the mixing graph.

Figure 4.10 shows the difference in mean subshell distance after amplification.

Figure 4.11 shows how much amplification was applied to each solution based on their subshell distance. These plots are monotonically decreasing.

### 4.2.3 Hyperparameter Analysis

We optimised the three NVQWOA hyperparameters  $\beta, \gamma, t$  under three different objective functions applied to the final state: the expected value (EV), the probability of measuring an optimal solution (OSP), and the conditional value at risk (CVaR).<sup>4.1</sup>

Table of mean hyperparameters:

$n = 8$	$\beta$	$\gamma$	$t$
EV	0.47(5)	0.2(2)	0.09(2)
OSP	0.78(2)	1.01(2)	0.180(2)
CVaR	0.55(2)	1.15(3)	0.169(3)

Table 4.1: Optimisation results for  $n = 8$ . Mean hyperparameters for each optimisation objective function.

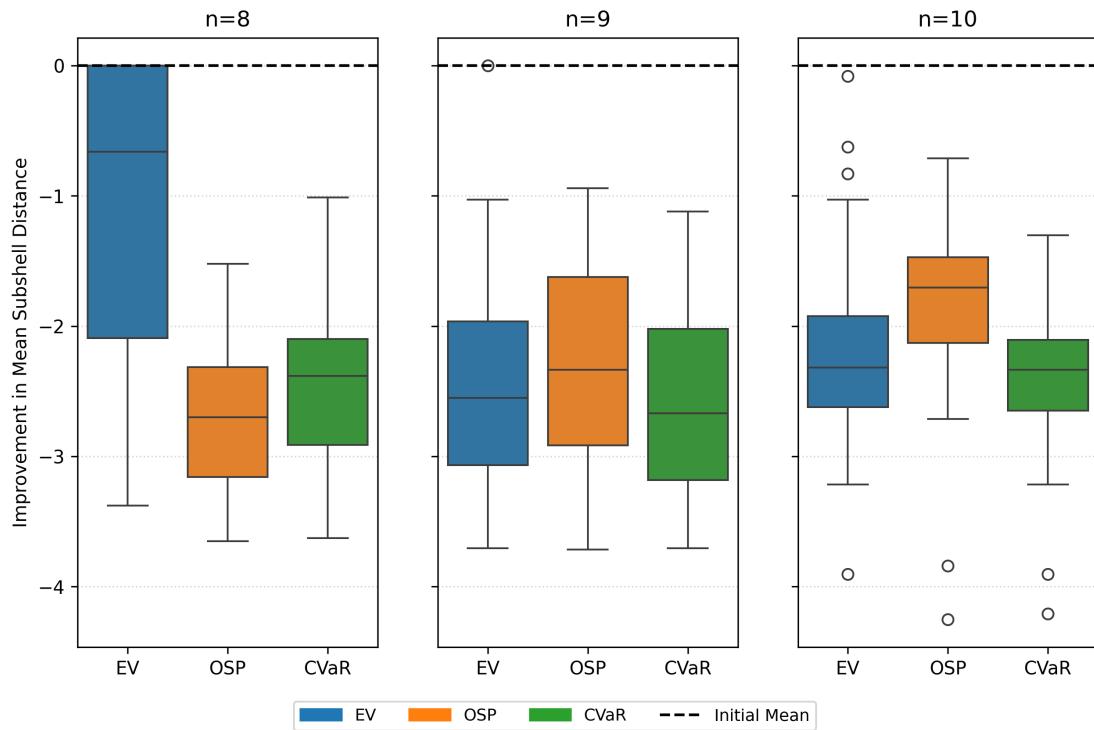


Figure 4.10: Improvement in subshell distance boxplot.

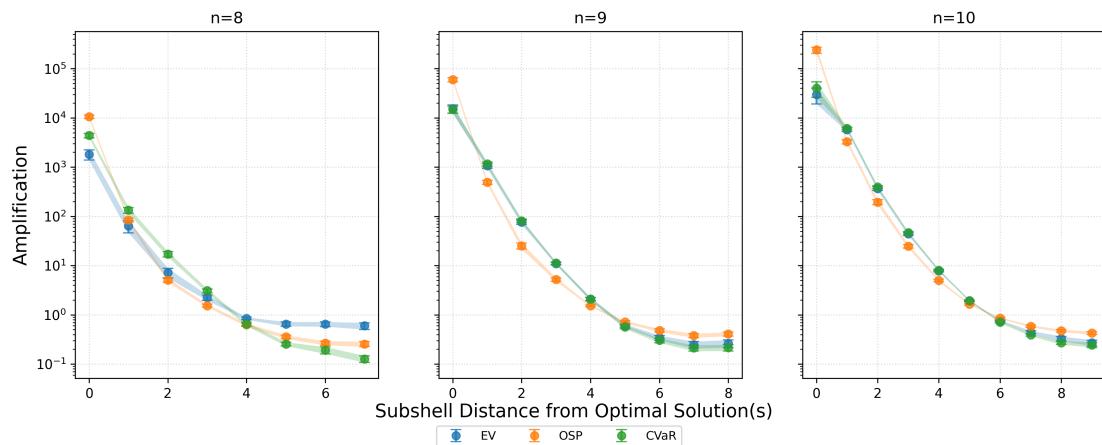


Figure 4.11: Mean amplification applied to each solution grouped by their subshell distance from the optimal solution.

$n = 9$	$\beta$	$\gamma$	$t$
EV	0.56(2)	-1.12(9)	0.144(7)
OSP	0.81(2)	1.05(2)	0.164(2)
CVaR	0.586(8)	1.19(2)	0.142(2)

$n = 10$	$\beta$	$\gamma$	$t$
EV	0.47(6)	-1.28(4)	0.15(1)
OSP	0.78(2)	1.12(2)	0.151(1)
CVaR	0.580(6)	1.28(1)	0.124(2)

### 4.3 Subshell Analysis

Figure 4.12 shows the mean quality gap between the optimal solutions and the subshells. For all problem instances, the mean quality gap was a monotonically increasing function with subshell distance.

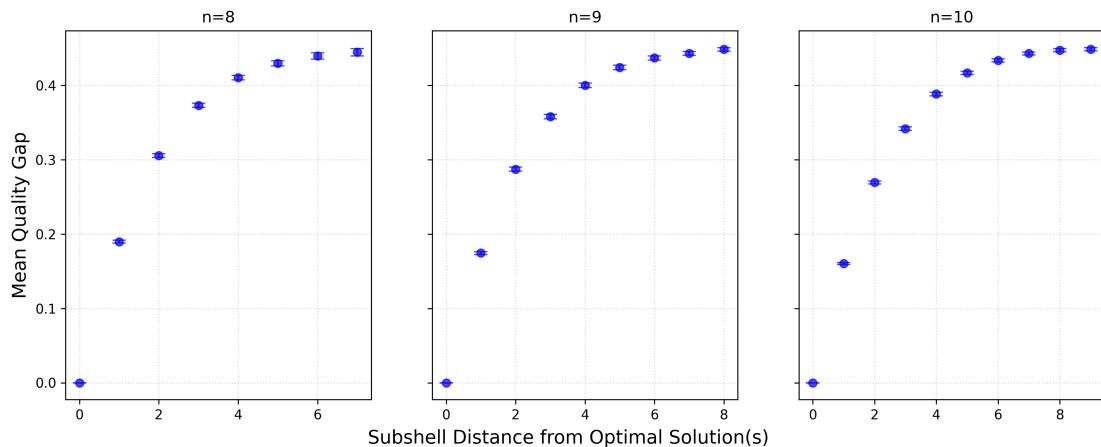


Figure 4.12: Mean quality gap vs subshell distance

Figure 4.13 shows the amount of variance in the objective values for each subshell. Lower variance indicates more phase-coherence within the shell, and therefore more potential for constructive interference with the target solution under optimisation of  $t$  and  $\gamma$ . The maximum subshell variance was  $X$ , for subshell  $h$  in problem  $k$ . FIND THIS

The second-order variance for  $n = 8$  was 4.7e-06,  $n = 9$  was 3.2e-06,  $n = 10$  was 2.0e-06.

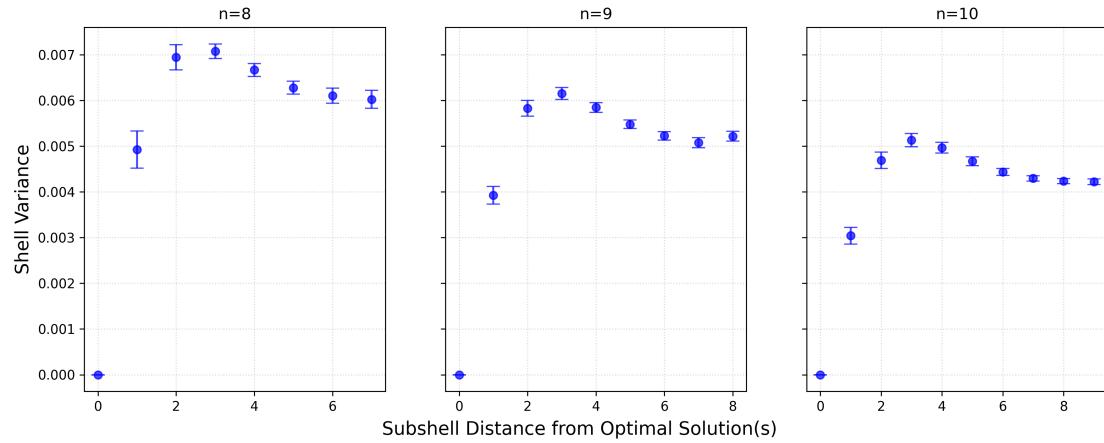


Figure 4.13: Shell variance vs subshell distance

# Chapter 5

## Future Work

### Exploration of Graph Similarity Measures

In this thesis, we explored the use of edge overlap as a measure of graph similarity. This corresponded well with the structure of the mixing graph. Investigation into other measures of graph similarity, such as maximum common subgraph or graph edit distance, may find that those measures yield better results.

### Random Graph Generation

The graphs generated for analysis were simple, undirected, unweighted graphs created using the Erdős-Rényi-Gilbert random graph model[16, 17]. Firstly, extending the problem to directed or weighted graphs would expand the possible applications to many practical fields where these graphs are common. Secondly, changing the random graph model to the Watts-Strogatz, Barabasi-Albert, or any other random graph model will change the characteristics of the problem instances, which could change the optimal hyperparameters. If the optimal hyperparameters do not significantly change depending on the structure and characteristics of the graph, this would greatly reduce the required number of shots to run the NVQWOA.

### Performance on Quantum Hardware

These classical simulations were performed assuming no noise in the gates and no decoherence in the qubits. Hyperparameter optimisation was determined by

objective functions that did not measure the quantum state using random shots but instead had access to the complete state vector. These assumptions, although useful for mathematical analysis as a proof of concept, are fundamentally unphysical. To improve the analysis of the NVQWOA, its real performance on quantum hardware should be calculated by simulating noise and decoherence.

# Chapter 6

## Conclusions

This thesis analysed using the NVQWOA on the unlabelled graph similarity problem. Using classical simulation techniques, we characterised the performance of the algorithm and assessed its potential for use in graph similarity tasks.

Our results demonstrate that the NVQWOA consistently amplifies optimal and near-optimal solutions across a range of problem sizes. The amount of amplification applied to each solution closely tracks the solution's proximity to the optimum, quantified by either Hamming distance or subshell distance, and align with expected behaviour for the continuous-time quantum walk on the mixing graph. The stability of the hyperparameters suggest that these hyperparameters could be used in a parameter transfer to instances with a larger problem size  $n$ .

TBD.

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# **Appendix A**

## **First**

Other results I guess.

# **Appendix B**

## **Research Proposal**

Application of a Non-variational Quantum Walk-based  
Optimisation Algorithm for Graph similarity

Dylan O'Donoghue

Supervisors: Tavis Bennett, Jingbo Wang

May 26, 2024

### **B.1 Introduction**

#### **B.1.1 Background**

Complex systems characterised by extensive interconnectivity, such as social networks, electrical power grids, circulatory systems, and database architectures are frequently modelled using network graphs [25]. Measuring the similarity between these graphs is crucial for enabling quantitative comparisons and gaining valuable insights. However, challenges arise when dealing with very large graphs, which significantly impact the scalability and efficiency of existing similarity algorithms. Moreover, the graph similarity problem becomes computationally intractable (re-

quiring exponential time) for graphs without known labelling using conventional methods [26]. This project aims to address these challenges by exploring the application of the non-variational quantum walk-based optimisation algorithm (non-variational QWOA) [1], potentially offering a breakthrough in solving the graph similarity problem more efficiently and effectively.

### B.1.2 Literature Review

Network graph models have become crucial components in systems that are used in everyday life, such as search engines and social networks [27]. Graph similarity (or graph distinguishability, as it is sometimes referred [28]) is often important in these contexts. For example, social networks are compared to identify certain interaction patterns [29], traffic networks are compared to help detect abnormal changes in traffic patterns [30], and web networks are compared for anomaly detection [31]. In all these cases, the similarity between two graphs with overlapping sets of nodes is assessed and the detection of changes in the patterns of connectivity is important. For graphs which match approximately, it is useful to obtain a quantitative measure of similarity. For example, classification techniques in machine learning match objects that are within a certain tolerance.

Graph similarity measures are quantitative calculations based on comparisons made between the structure of network graphs. Different measures of graph similarity will produce a variety of results due to differences in how the structures of the graphs are analysed. There are many measures of graph similarity, including Maximum Common Subgraph [32], Graph Edit Distance [33], Frobenius Distance [34], and Graph Eigendecomposition [35]. These measures are all successful at indicating the degree to which two graphs are similar and can also detect small differences between them.

#### Graph similarity in detail:

Let  $G_1(V, E_1), G_2(V, E_2)$  be two graphs defined by a set of vertices  $V$  and edge sets  $E_1, E_2$ . Define  $\text{sim}(G_1, G_2) \in [0, 1]$  as the similarity of these graphs and define  $A_1, A_2$  as the adjacency matrices of  $G_1$  and  $G_2$ , respectively.

Koutra et al. formalised a set of axioms that graph similarity measures should conform to [4]:

1. Identity:  $\text{sim}(G_1, G_2) = 1 \iff G_1 \cong G_2$
2. Symmetric:  $\text{sim}(G_1, G_2) = \text{sim}(G_2, G_1)$
3. Zero: For a clique graph  $G_1$  and a empty graph  $G_2$ ,  $\text{sim}(G_1, G_2) \rightarrow 0$  as  $n \rightarrow \infty$

They also raise that similarity algorithms should factor in the structural importance of each edge, the weight of removed edges, and the total number of edges in a graph. They also say a good graph similarity measure should be able to distinguish targeted and random changes, and should be scalable to large, generated graphs. However, this scalable criterion has only been fulfilled by algorithms applied to graphs with known node correspondence.

The failure of the scalability criterion for algorithms applied to graphs with unknown node correspondence (hereafter referred to as unlabelled graphs) is due to problem of finding the correct corresponding vertex labels between the graphs. Observe that due to Axiom 1, similarity algorithms should be able to identify isomorphic graphs (and assign them a similarity of 1), but confirming isomorphism requires checking each permutation of vertex labelling. Using this fact, the similarity of an unlabelled  $G_1$  and  $G_2$  can be expressed as:

$$\text{sim}(G_1, G_2) = \max_{\pi} \text{simscore}(A_1^{\pi}, A_2)$$

Here,  $\pi$  ranges over all permutations of the vertex set  $V$ ,  $A_1^{\pi}$  denotes the adjacency matrix obtained from  $G_1$  by permuting rows and columns according to  $\pi$ , and *simscore* is a function that assigns a scalar in the range  $[0, 1]$ , called the similarity score, to a particular pair of adjacency matrices. The structure of *simscore* depends on the measure of graph similarity that is being used. Note that in this scope, the graph similarity problem is the problem of finding the optimal alignment of two graphs such that their similarity score is maximised.

Since the unlabelled graph matching problem is NP-complete [26], existing al-

gorithms to measure graph similarity take exponential time to compute. Therefore, it is desirable to use quantum algorithms.

### **Quantum Optimisation Algorithms:**

Using the previously established framework, we can reduce the problem of graph similarity to a combinatorial optimisation problem (COP) suitable for quantum algorithms. The COP consists of  $n$  integer decision variables  $x_i \in \{0, 1, 2, \dots, n - 1\}$  where the solutions are characterised by vectors  $\mathbf{x} = (x_1, x_2, \dots, x_n)$ , which represent a particular labelling of vertices of  $G_1$  onto  $G_2$  (similar to  $A_1^\pi$ ), and the space of feasible solutions  $S$  contains all such vectors without repeating elements, such that there are  $N$  feasible solutions where  $N = n!$ . The system is initially in an equal superposition of all solutions,

$$|s\rangle = \frac{1}{\sqrt{N}} \sum |\mathbf{x}\rangle,$$

and we seek to amplify the probability of measuring the solution  $\mathbf{x}$  that maximises  $f(\mathbf{x})$ , where  $f$  is the objective function that represents the equivalent *simscore* for a particular  $\mathbf{x}$ .

One potential quantum algorithm that could be used is the quantum approximate optimisation algorithm (QAOA) [13], which uses a variational approach to solving COPs. The algorithm repeatedly applies two Hamiltonians to  $|s\rangle$ , where the application times of each Hamiltonian are classically controlled parameters. These parameters are initially random and must be tuned via a classical optimisation process. The parameters that globally maximise the expected value of the objective function must be selected for optimal performance of the algorithm [36].

Another variational algorithm is the quantum walk-based optimisation algorithm (QWOA), which is closely related to the main algorithm of this project. The QWOA is a more general form of the QAOA, where the time-based application of the transverse-field Hamiltonian is replaced by a continuous-time quantum walk (CTQW) on a graph that contains basis states encoding the feasible solutions to the COP [37]. The other Hamiltonian is unchanged and phase-shifts basis states depending on their associated objective function values.

The first concern in the use of variational algorithms is that the process of tuning the parameters is costly. The requirement to globally maximise these parameters means that gradient-based methods are more sensitive to the initial parameters, but the space of possible initial parameters grows exponentially in parameter count [38]. In essence, variational algorithms solve the maximisation of the objective function, but also present the challenge of solving the maximisation problem of their own parameters. As such, a non-variational approach is preferred for our problem.

Another problem with the above algorithms is that they are built on a quadratic unconstrained binary optimisation (QUBO) framework, and as such, the decision variables  $x_i$  must be binary. This conflicts with the structure of the graph similarity problem, which requires the use of non-binary decision variables. Although studies have shown that non-binary problems can be implemented into the QUBO framework [39], it requires introducing a penalty component to the objective function, further increasing the number of parameters. As such, an approach not restricted to only binary decision variables is preferred.

To address these issues, this project will implement a non-variational, non-binary-restricted quantum algorithm.

### **The Non-variational Quantum Walk-based Optimisation Algorithm:**

The main algorithm of this project is the non-variational quantum walk-based optimisation algorithm (non-variational QWOA) [1], which replaces the QWOA CTQW graph with a mixing graph that connects nearest-neighbour solutions.

For the graph similarity problem, the mixing graph connects each solution state to the set of  $\frac{1}{2}n(n - 1)$  possible transpositions (obtained by swapping two elements in  $\mathbf{x}$ ). As such, the adjacency matrix of the mixing graph can be expressed as

$$A = \sum_{i=0}^{n-2} \sum_{i+1}^{n-1} \text{SWAP}_{i,j},$$

where  $\text{SWAP}_{i,j}$  is defined as the permutation matrix associated with swapping the  $i^{\text{th}}$  and  $j^{\text{th}}$  entry in  $\mathbf{x}$  and applying identity to the remaining entries.

There are two important unitaries driving the interference process in the non-variational QWOA. The first is the phase-separation unitary,

$$U_Q = e^{-i\gamma Q}.$$

$Q$  is the quality, a diagonal operator such that  $Q |\mathbf{x}\rangle = f(x) |\mathbf{x}\rangle$ . Hence, the phase-separation unitary applies a phase-shift to each solution state proportional to its objective function value.

The second unitary is called the mixing unitary or mixer, and it performs the CTQW for time  $t$  on the mixing graph,

$$U_M = e^{itA}.$$

After establishing these unitaries and given a pre-selected number of iterations  $p$ , the amplified state is defined as:

$$|\gamma, t, \beta\rangle = \left[ \prod_{j=0}^{p-1} U_M(t_j) U_Q \left( \frac{\gamma_j}{\sigma} \right) \right] |s\rangle$$

Where  $\gamma$ ,  $t$ , and  $\beta$  are classically controlled positive-valued parameters that determine the applied phase separations and mixing times for each iteration. The values of  $\gamma_j$  increase linearly over the domain  $[\beta\gamma, \gamma]$ , and the values of  $t_j$  decrease linearly over the domain  $[\beta t, t]$ .  $\sigma$  is standard deviation of  $f(x)$ , controlling the different possible measures of graph similarity such that  $\gamma \approx 1$ . An approximate value of  $\sigma$  is sufficient and so can be found through random sampling of  $f(\mathbf{x})$ . An appropriate value of  $\beta$ , which is in the interval  $(0, 1)$ , is unique to a particular problem type. As such, it is expected that once found, a single value of  $\beta$  will be suitable for all graph similarity problems. Notably, Bennett et al. observes that optimal values of  $\beta$  range from approximately 0.4 down to  $\frac{1}{p}$  for the problems of Weighted Maxcut, Maximum Independent Set, K-Means Clustering, Capacitated Facility Location, and the Quadratic Assignment Problem [1].

## B.2 Project

### B.2.1 Aims

The primary goal of this project is to explore the uses of the non-variational QWOA for computing graph similarity, particularly investigating how modifications to the objective function and parameter tuning method influence the performance.

Secondary goals include benchmarking the performance of the algorithm using high performance computing (HPC) resources as well as generalising the implementation of the algorithm to work on weighted graphs, directed graphs and graphs with differing numbers of nodes. Additionally, I may show a proof-of-concept application of the algorithm on a practical case, such as small social network similarity.

### B.2.2 Significance

This numerical simulation project is part of a larger project to benchmark the non-variational QWOA across various combinatorial optimisation problems. The non-variational QWOA has shown promising preliminary results, which may indicate that it is a practical quantum algorithm that could outperform equivalent classical or quantum methods. By contributing to the development and benchmarking of the non-variational QWOA, this project aims to advance the field of quantum computing and algorithms, potentially impacting areas such as network security, design, and logistics.

## B.3 Research Plan

### B.3.1 Methodology and Problems

The code developed to run the numerical simulations on local hardware is in Python, due to the need for high clarity and readability to perform investigations of the performance of the non-variational QWOA. An important aspect of this part of the project is the ability to rapidly prototype the simulation in response to the obtained results. The performance of the code on local hardware is not high prior-

ity, as the number of qubits a serial program is able to simulate is highly restricted anyway. The HPC benchmarking simulations will be run on the supercomputer Setonix, at the Pawsey Supercomputing Centre, and the best programming language for these benchmarking simulations will be identified as part of the project.

To analyse the effect of changing the measure of graph similarity, the objective function of the non-variational QWOA will be modified to reflect the required calculation associated with the *simscore* for various measures of graph similarity. Comparisons between the performance of the algorithm using different measures of graph similarity will be used to explore how the algorithm is affected by changes in the measure of graph similarity.

The method by which the  $\gamma$ ,  $t$ , and  $\beta$  parameters are tuned will also be an area of inquiry. This will involve investigating which tuning method produces the greatest amplification in the optimal solution state, as well as attenuation on the non-optimal solution states.

A potential problem that may arise in benchmarking is that due to the overhead that quantum algorithms require, the benefit of a speed up is normally only achieved for problems with a large size  $n$ . Thus, the size of the benchmarking simulations would likely need to have a large  $n$ . This may involve excessive time or resources which could cause problems with the size of the scope of the project.

### B.3.2 Preliminary Work

This semester I have focused on building an in-depth understanding of the non-variational QWOA and similar quantum algorithms. Additionally, I have worked on obtaining preliminary results, building on the code originally developed by Tavis Bennett.

A graph  $G_1$  was randomly generated using an Erdős-Rényi random graph model [16] with  $N = 9$  nodes and probability for edge inclusion  $p = 0.5$ . The second graph  $G_2$  was a copy of the first graph, but with a single edge removed. The implemented objective function was the number of matching entries in the adjacency matrices of the graphs, divided by the total number of entries in the adjacency matrix. Since

only one edge was different between  $G_1$  and  $G_2$ , that meant two entries in the adjacency matrices  $A_1$  and  $A_2$  differed, giving an expected similarity of  $\frac{79}{81} \approx 0.97$

I tuned the  $\gamma$ ,  $t$ , and  $\beta$  parameters using two different methods. The first tuning method selected the parameters that would maximise the expected value of the objective function,  $\langle f(x) \rangle$ . The second tuning method selected the parameters that would maximise the probability to measure the optimal solution state,  $P(\text{opt})$ . These methods produced the values shown in Table B.1.

Tuning Method	$\gamma$	$t$	$\beta$
$\langle f(x) \rangle$	1.4745	0.2194	0.3545
$P(\text{opt})$	1.2378	0.2269	0.6568

Table B.1: Optimal parameter values from different tuning methods

Using these values for the parameters, numerical simulations of the non-variational QWOA was applied to  $G_1$  and  $G_2$  with a number of iterations  $p = 10$ , and the plots B.1, B.2, and B.3 were created.

Using these values for the parameters, numerical simulations of the non-variational QWOA was applied to  $G_1$  and  $G_2$  with a number of iterations  $p = 10$ , and the plots B.1, B.2, and B.3 were created.

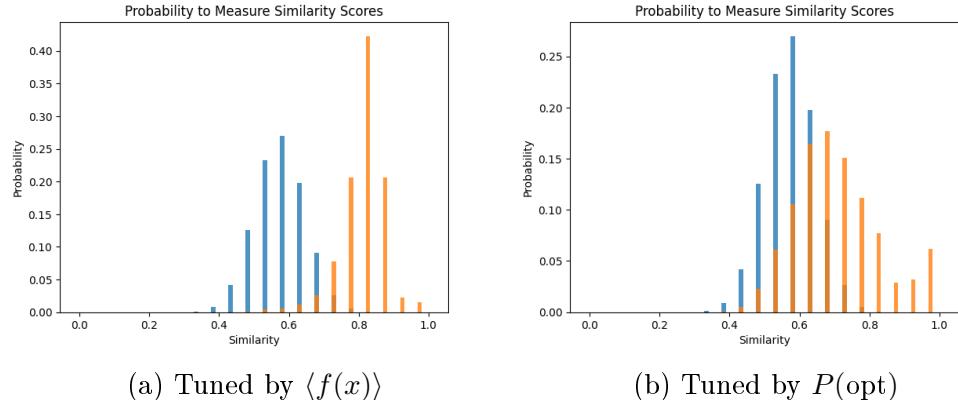


Figure B.1: Similarity score probability distributions for different tuning methods.

These plots show that for both tuning methods, the optimal solution was successfully amplified more than any other solution. However, the results also reveal

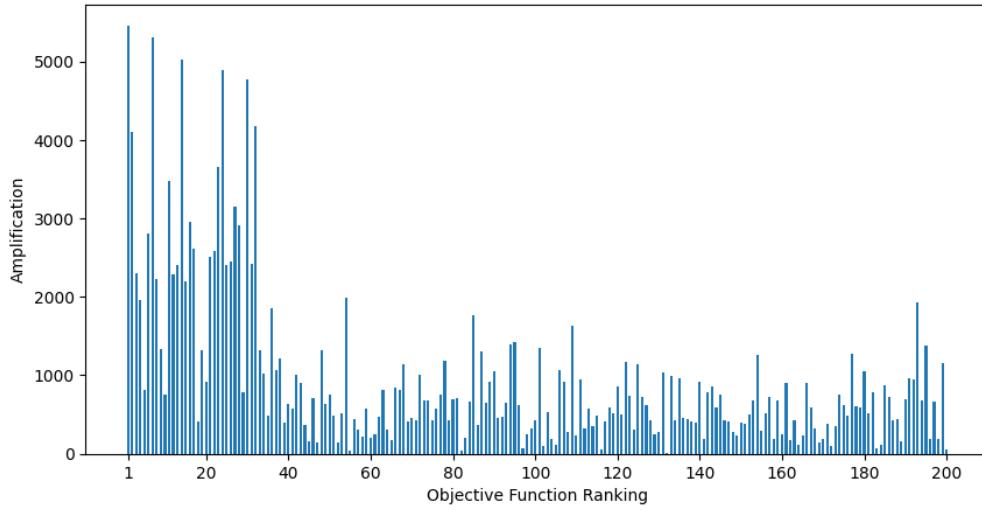


Figure B.2: Amount of amplification applied to the top 200 solutions when tuned by  $\langle f(x) \rangle$

several concerns. Firstly, we expect that tuning for  $\langle f(x) \rangle$  and tuning for  $P(\text{opt})$  should yield similar parameters, yet they produce very different  $\beta$  values in Table B.1. Bennett et al. suggest that  $\beta$  should be  $\approx 0.4$  or less, but the value of  $\beta$  obtained from tuning for  $P(\text{opt})$  significantly exceeds this guideline.

Secondly, when tuning for  $\langle f(x) \rangle$ , the amplification of non-optimal solutions is extremely high. The distribution of amplification in B.2 is spread out, and the amount of amplification applied to the optimal solution is much lower than in B.3.

Finally, as a result of these previous behaviours, the most likely similarity score to measure from both simulations is not the similarity score corresponding to the optimal solution.

All of these behaviours warrant further investigation into the configuration of the non-variational QWOA and adaptation of the tuning process is recommended to better align the results with theoretical predictions and practical requirements.

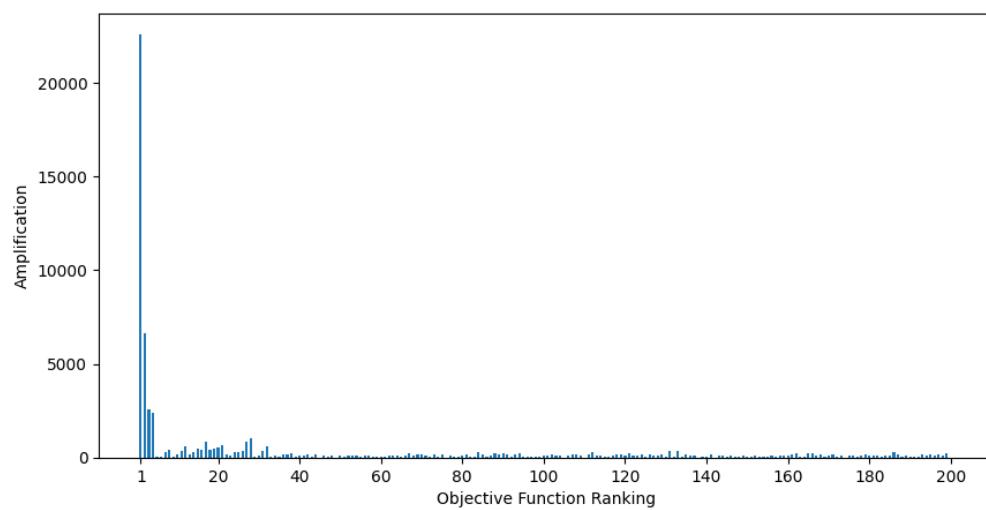


Figure B.3: Amount of amplification applied to the top 200 solutions when tuned by  $P(\text{opt})$