Instance Space Analysis of Quantum Algorithms

Supervisors: Prof. Kate Smith-Miles, Prof. Lloyd Hollenberg

PhD Completion Seminar

Vivek Katial

The University of Melbourne

2024-11-26

Agenda

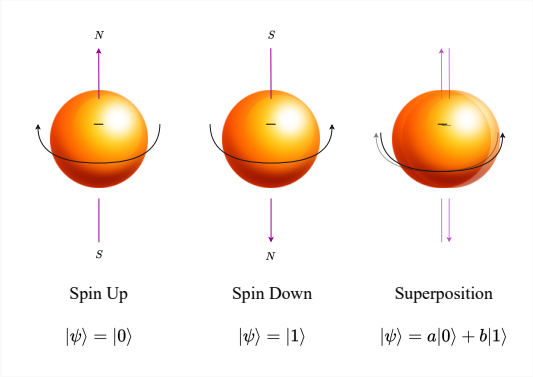
1. Introduction
2. Quantum Approximate Optimisation Algorithm (QAOA)
3. Instance Space Analysis
4. Evolving Instances for QAOA
5. Software for QAOA Parameter Initialisation
6. Conclusion and Future Work

Introduction

Why Quantum?

1. Quantum Computers can *theoretically solve* can solve some problems much faster than classical computers
2. What problems?
   - **Shor's algorithm** for factoring large numbers - could break RSA encryption [15]
   - **Grovers Search** - Quadratic speedup over classical search [7]
   - **Simulation of physical systems** - Quantum Chemistry, Material Science
3. What's the catch?
   - Hardware is **hard** - assuming no errors we need several 1000s of qubits
   - With current error rates - need millions of qubits + 100s of millions of gates
   - **NISQ** - Noisy Intermediate-Scale Quantum (NISQ) devices - 50-100 qubits, noisy, error-prone

How does Quantum Computing work?



Superposition

- Quantum bits (qubits) can exist in a superposition of states
- For $N = 2$ qubits: $|\psi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2 = \mathbb{C}^4$
- Represented by a vector in a complex vector space $|\psi\rangle \in [\mathbb{C}^2]^{\otimes n}$
- For $N = 300$, there are 2^{300} possible states - more than the number of atoms in the universe!

- Currently we're in the NISQ-era of Quantum Computing
- Need to design algorithms that can run on NISQ-devices

Need to find algorithms that can:

1. Can run on small (100-1000 qubit devices)
2. Solve useful problems
3. Shouldn't require extensive error correction

This has led to the development of **Variational Quantum Algorithms (VQAs)** [9], which are hybrid algorithms specifically designed for NISQ devices

Aims of the Thesis

- VQAs are a promising class of quantum algorithms tailored for NISQ devices
- Two prominent examples:
  1. **Quantum Approximate Optimisation Algorithm (QAOA)** [4]
  2. **Variational Quantum Eigensolver (VQE)**
- QAOA in particular is a low-depth algorithm designed to solve optimisation problems
  - Many problems can be mapped to a Hamiltonian and solved using QAOA (e.g. MaxCut, TSP, Vehicle Routing, 3SAT)

Partition a graph $G = (V, E)$ into two sets S and $V \setminus S$ such that the number of edges between the two sets is maximised.

$$\max_{\mathbf{s}} \sum_{(i,j)\in E} w_{ij}(1 - z_i z_j)$$

where $z_i \in \{0, 1\}$ and $w_{ij} \in \mathbb{R}$ is the weight of edge (i, j).

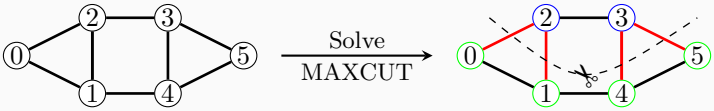


Figure 1: An example of a six-node MaxCut problem

Solution is a binary string $\mathbf{s} = (s_1, s_2, \ldots, s_n)$ where $s_i \in \{0, 1\}$ and the optimal objective value is $C_{\max}$ where $C_{\max} = \sum_{(i,j)\in E} w_{ij}$ for the edges in our **maximum cut**.

We map the MaxCut problem to a *Hamiltonian* for quantum optimisation.

Classical Formulation

Objective:

$$\max_{\mathbf{s}} \sum_{(i,j)\in E} w_{ij}(1 - z_i z_j)$$

State Space:

$$\mathbf{s} \in \{0,1\}^n$$

Solution:

$$\mathbf{s}^* = \operatorname*{argmax}_{\mathbf{s}} \sum_{(i,j)\in E} w_{ij}(1 - z_i z_j)$$

map

Quantum Formulation

Objective:

$$H = \sum_{(i,j)\in E} w_{ij}(I - Z_i Z_j)$$

State Space:

$$|\psi\rangle \in \mathcal{H}_2^{\otimes n}$$

Solution:

$$|\psi_{\text{ground}}\rangle = \operatorname*{argmin}_{|\psi\rangle} \langle\psi|H|\psi\rangle$$

Quantum Approximate Optimisation Algorithm (QAOA)

- QAOA prepares a parameterised "trial" (ansatz) state of the form:

$$
\begin{aligned}
|\psi(\theta)\rangle &= |\psi(\vec{\gamma}, \vec{\beta})\rangle \\
&= \prod_{j=1}^{p} e^{-i\beta_j \hat{H}_B} e^{-i\gamma_j \hat{H}_P} |+\rangle^{\otimes n}
\end{aligned}
$$

- Where $\hat{H}_P = \sum_{(i,j)\in E} w_{ij}(1 - \hat{Z}_i\hat{Z}_j)$ is the problem Hamiltonian and $\hat{H}_B = \sum_{i=1}^{n} \hat{X}_i$ is the mixing Hamiltonian.
- The parameters $\vec{\gamma} = (\gamma_1, \ldots, \gamma_p)$ and $\vec{\beta} = (\beta_1, \ldots, \beta_p)$ are optimised to minimise the expectation value of the problem Hamiltonian.

- The QAOA Ansatz Energy is given by taking the expectation value of the problem Hamiltonian with respect to the trial state:

$$
\begin{aligned}
F_p(\vec{\gamma},\vec{\beta}) &= \langle +|^{\otimes n} \left(\prod_{j=1}^{p} e^{-i\beta_j \hat{H}_B} e^{-i\gamma_j \hat{H}_P}\right)^{\dagger} \hat{H}_P \left(\prod_{j=1}^{p} e^{-i\beta_j \hat{H}_B} e^{-i\gamma_j \hat{H}_P}\right) |+\rangle^{\otimes n} \\
&= \langle \psi(\vec{\gamma},\vec{\beta})|\hat{H}_P|\psi(\vec{\gamma},\vec{\beta})\rangle
\end{aligned}
$$

- The goal is to find the optimal parameters $\vec{\gamma}^*, \vec{\beta}^*$ that minimise the energy $F_p(\vec{\gamma},\vec{\beta})$.

$$
(\vec{\gamma}^*,\vec{\beta}^*) = \arg\min_{\vec{\gamma},\vec{\beta}} F_p(\vec{\gamma},\vec{\beta}), \qquad \alpha = \frac{F_p(\vec{\gamma}^*,\vec{\beta}^*)}{C_{\max}}
$$

Key Design Decisions

1. **Circuit Depth** (p)
   - Controls the expressivity of the ansatz
   - As $p \to \infty$ QAOA can find the exact solution
2. **Classical Optimiser**
   - Gradient-free: Nelder-Mead, COBYLA
   - Gradient-based: ADAM, SPSA
3. **Initial Parameters** $(\vec{\gamma}_0, \vec{\beta}_0)$
   - Various strategies for initialisation (e.g. TQA [11], INTERP [18])

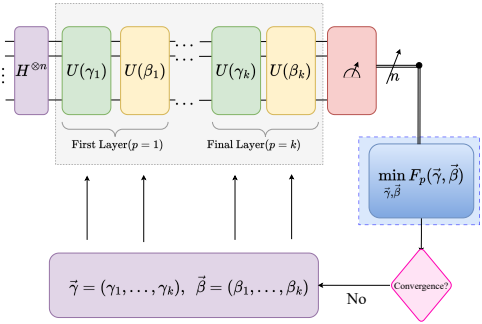


Figure 2: QAOA Circuit Architecture

Key Findings

- Recent studies show optimal QAOA parameters for depth p are transferable across a small class of instances [2]
- Optimal QAOA depth is instance-dependent [12]
- Algorithm performance heavily influenced by:
  - Choice of classical optimiser [5]
  - Initial parameter selection [18],[8],[14],[16]

Current Limitations

- Narrow focus on specific instance classes ($d-$regular graphs, random graphs, no weights)
- Predominantly shallow depth circuits ($p \leq 3$) [12],[16]
- Limited understanding of instance feature impacts on QAOA performance and design decisions
- Lack of standardised parameter initialisation frameworks [1]

RQ1

How can we generate diverse MaxCut instances beyond current QAOA research?

RQ2

How do instance characteristics influence key QAOA design decisions?

RQ3

Can we develop methods to automatically optimise QAOA parameters based on instance features?

- **Landscape Evolution with Depth:**
  - Higher p – more complex optimisation landscape [3]
- **Weight Distribution Impact:**
  - Cauchy distributions $\rightarrow$ more rugged landscapes [13]
  - Weight scaling heuristics show promise
  - Convergence to unweighted case under rescaling [16]
- **Practical Implications:**
  - More complex landscapes require more calls to the QPU, classical optimisers can falter $\rightarrow$more resource use!

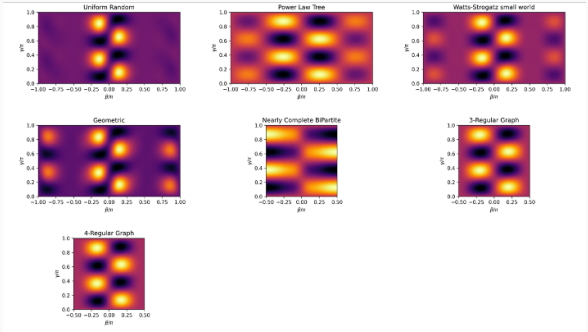


Figure 3: QAOA Landscape Variation Across MaxCut Instances (p=1, unweighted)

Instance Space Analysis

- Based on the *No Free Lunch Theorem* [17]: Algorithms have strengths and weaknesses
- Identify features that differentiate instances from each other and influence algorithm performance
- Identifies which algorithms are best suited for which instances - instead of reporting "on-average" performance
- ISA projects instances onto a 2D space to visualise the strengths and weaknesses of algorithms

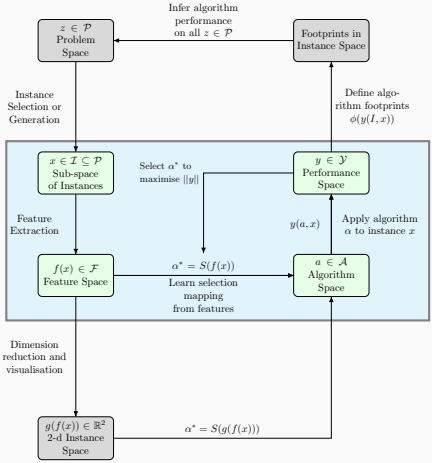
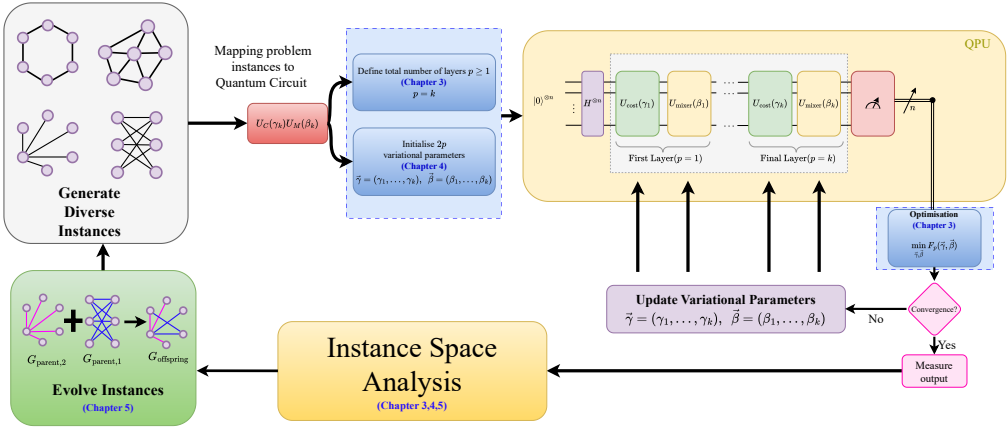


Figure 4: Instance space analysis workflow

Our Approach



IS I & II: Network Structures

- Random
- 3-regular
- 4-regular
- Geometric
- Watts-Strogatz
- Nearly complete bipartite

IS III & IV: Weight Distributions

- $\mathcal{U}[0, 1]$ (Uniform)
- $\mathcal{U}[-1, 1]$ (Uniform)
- Exp(λ) (Exponential)
- $\Gamma(k, \theta)$ (Gamma)
- $\mathcal{N}(\mu, \sigma^2)$ (Normal)
- LogNorm(μ, σ^2) (Lognormal)

Total Instance Classes: $7 \times 6 = 42$

Structural Features

- Number of Edges, Nodes
- Bipartite Graph
- Clique Number
- Connected Graph
- Density
- Edge Connectivity
- Max, Min Degree
- Min. Dominating Set size
- Regular Graph
- Smallest Eigenvalue
- Vertex Connectivity

Spectral Features

- Algebraic Connectivity
- Laplacian Largest Eigenvalue
- Ratio of Two Largest Laplacian Eigenvalues
- Ratio of Two Smallest Laplacian Eigenvalues

Cycle & Path Features

- Acyclic Graph
- Average Distance
- Diameter
- Eulerian Graph
- Number of Components
- Planar Graph
- Radius

Literature

- Distance-Regular Graph
- Group Size
- Number of Cut Vertices
- Number of Minimal Odd Cycles
- Number of Orbits
- Graph Entropy:
  $I(G) = \frac{1}{n} \sum_i |A_i| \log |A_i|$

Weight Features

- Mean, Median, Standard Deviation, Variance
- Min/Max, IQE, Skewness, Kurtosis
- Coef. of Variation
- Weighted Avg Clustering
- Weighted Avg Path Length
- Weighted Diameter
- Weighted Radius
- Max Weighted Degree
- Min Weighted Degree

Instance Space III and IV only

---

48 Features

- **Why?** Most algorithms achieve good approximation ratios
- **Components:**
  - Function evaluations
  - Approximation ratio (α)
- **Method to compute performance (κ):**
  1. Find $\alpha_{\max}$ (best ratio)
  2. Set $\alpha_{\text{acceptable}} = 0.95\alpha_{\max}$
  3. Count iterations (κ) to reach $\alpha_{\text{acceptable}}$
  4. If never reached, set penalty $\kappa = 10^5$

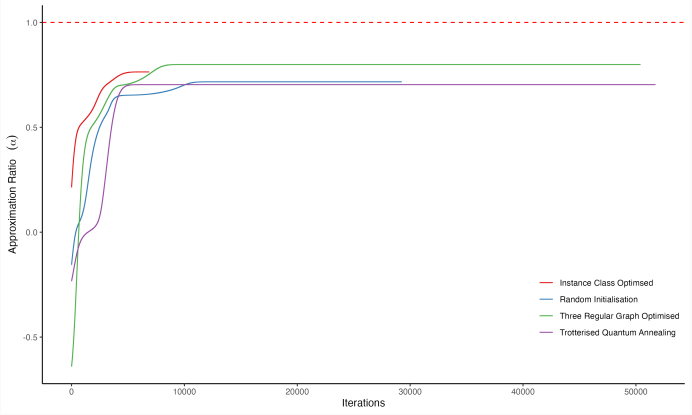


Figure 5: Approximation ratio α for various instances

Design Choices Across Independent Studies

- **IS I:** Layer Depth (p)
  - How many layers are needed for different instances?
  - $p \in 2, 5, 10, 15, 20$
- **IS II:** Classical Optimiser Selection
  - Which optimiser requires fewer calls to the quantum device?
  - Nelder-Mead, Conjugate Gradient, Powell, SLSQP, L-BFGS-B
- **IS III/IV:** Initialisation Technique
  - Can we have faster convergence to optimal parameters?
  - Random, TQA, INTERP, Constant, QIBPI, Three-Regular

Fixed meta-data

- Features
- Instances
- Performance Measure

All choices represent design decisions

Each study isolates one key design choice while maintaining other parameters constant

Instance Space III: Parameter Initialisation

Input: Number of nodes $N = 8$, Allowed Number of layers $L = 15$
Output: Median optimal parameters $\vec{\gamma}$ and $\vec{\beta}$ for each class
Procedure `GenerateGraphInstances()`:
    for $p \leftarrow 1$ **to** L **do**
        foreach *graph type* T *in* $T_1, \ldots, T_{42}$ **do**
            for $i \leftarrow 1$ **to** 100 **do**
                Generate graph instance $G_{i,T}$ with N nodes; `optimiseQAOAParameters`$(G_{i,T}, p)$;
            end
            `CalculateMedianParameters`(T_p);
        end
    end
Function `optimiseQAOAParameters`(G, p):
    Input: Graph instance G
    Output: Optimal parameters $(\vec{\gamma}_G, \vec{\beta}_G) = (\gamma_1, \ldots, \gamma_p), (\beta_1, \ldots, \beta_p)$
    Run QAOA on graph instance G with random initialisation to find optimal parameters for depth p; **return** $(\vec{\gamma}_G, \vec{\beta}_G) = (\gamma_1, \ldots, \gamma_p), (\beta_1, \ldots, \beta_p)$;
Function `CalculateMedianParameters`(T):
    Input: Graph type T, Set of parameters $\vec{\gamma}i, p, T$, $\vec{\beta}i, p, T$
    Output: Median parameters $\vec{\gamma}$median, T, $\vec{\beta}$median, T
    Calculate the median of the parameters $\gamma_{i,p,T}$ and $\beta_{i,p,T}$ for all instances of type T; Store median parameters in a parameter class corresponding to T; **return** $\vec{\gamma}$*median*, T, $\vec{\beta}$*median*, T;

Algorithm 1: Generate Initial QAOA Parameters using QIBPI

Random:

- $\gamma_i \sim \mathcal{U}(-\pi, \pi)$
- $\beta_i \sim \mathcal{U}(-\pi/2, \pi/2)$

TQA [11]:

- $\gamma_i = i \cdot \Delta t/p$
- $\beta_i = (1 - i/p) \cdot \Delta t$

CONSTANT [6]:

- $\gamma_i = 0.2$
- $\beta_i = -0.2$

FOURIER: [18]

- Frequency domain approach
- $\gamma_i = \sum_k u_k \sin((k - \frac{1}{2})(i - \frac{1}{2})\frac{\pi}{p})$

INTERP: [18]

- Parameter interpolation
- $[\gamma_0^{(p+1)}]_i = \frac{i-1}{p}[\gamma_L^{(p)}]_{i-1}$

QIBPI:

- Uses QIBPI pre-optimised parameters

3-Regular:

- Uses 3-regular pre-optimised parameters

The projection transformation is given by the matrix $\mathbf{Z}$:

$$\mathbf{Z} = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} -0.5225 & 0.2301 \\ -0.5939 & 0.7398 \\ 0.3977 & -0.2637 \\ -0.1423 & -0.2023 \\ -0.0091 & 0.5056 \\ 0.4226 & -0.019 \\ 0.0843 & 0.6528 \\ -0.0033 & -0.0937 \\ -0.2002 & -0.3513 \\ 0.3448 & -0.3839 \end{pmatrix}^{\top} \begin{pmatrix} \text{algebraic connectivity} \\ \text{average distance} \\ \text{clique number} \\ \text{diameter} \\ \text{maximum degree} \\ \text{maximum weighted degree} \\ \text{number of edges} \\ \text{radius} \\ \text{skewness weight} \\ \text{weighted average clustering} \end{pmatrix}$$

Plotting 4,200 instances across $\mathbb{R}^2$.

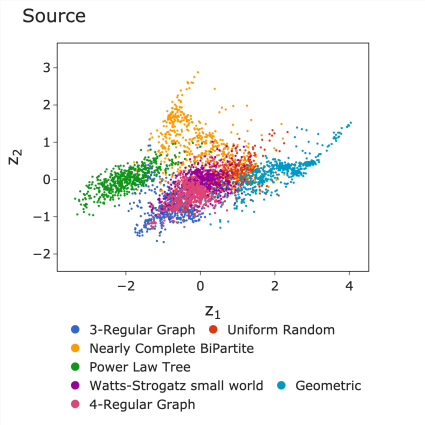
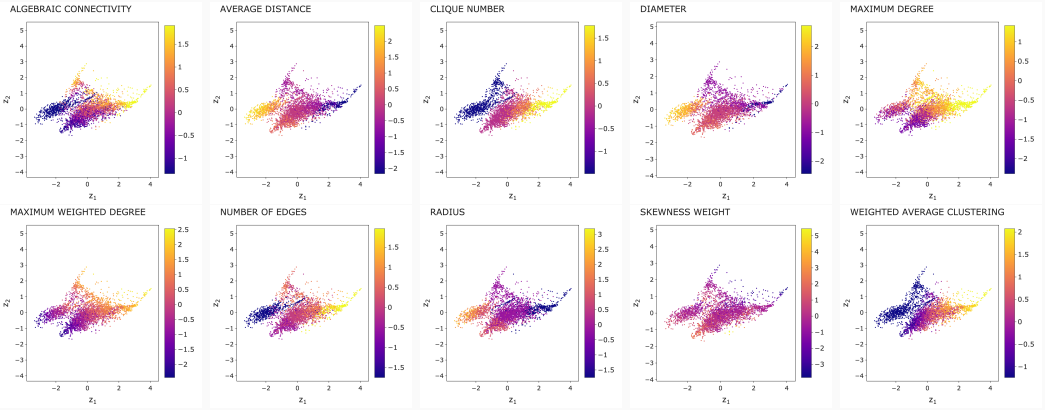


Figure 6: Source Distribution


ALGEBRAIC CONNECTIVITY
AVERAGE DISTANCE
CLIQUE NUMBER
DIAMETER
MAXIMUM DEGREE
MAXIMUM WEIGHTED DEGREE
NUMBER OF EDGES
RADIUS
SKEWNESS WEIGHT
WEIGHTED AVERAGE CLUSTERING
z_1
z_2

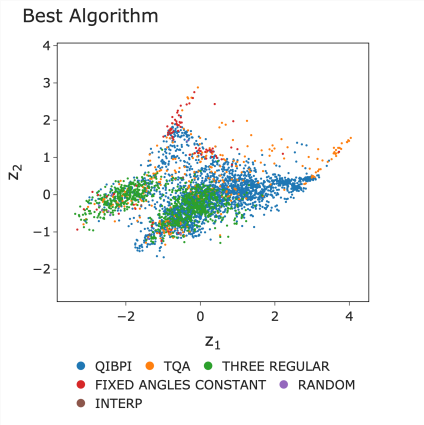


Figure 7: Best Algorithm

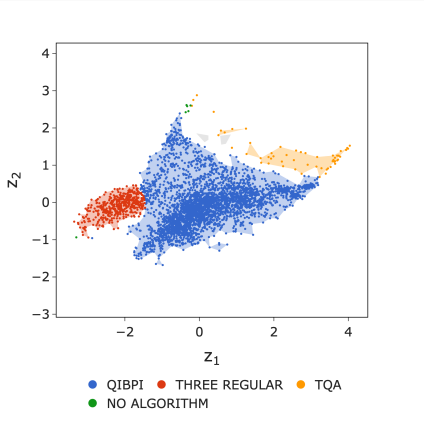
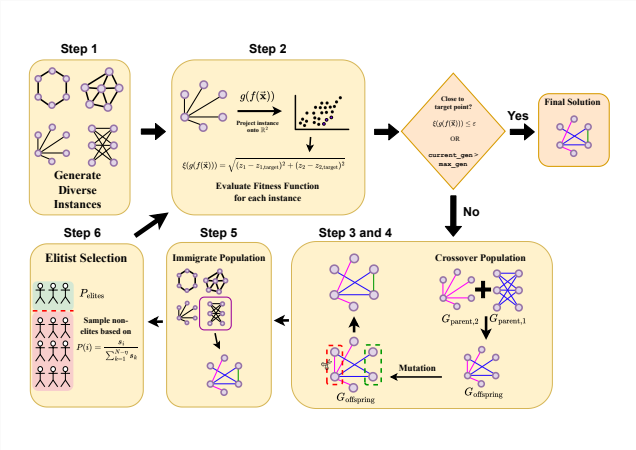


Figure 8: Algorithm Distribution

Initialisation Strategy	P_{good} (%)	CV Accuracy (%)	CV Precision (%)
CONSTANT	3.20	96.70	33.3
INTERP	0.10	99.90	–
QIBPI	70.90	75.80	78.00
Three-Regular	44.80	78.50	73.80
TQA	11.10	90.10	87.50
Selector	**77.90**	–	**78.10**

Table 1: Performance metrics for various initialisation strategies

Evolving Instances for QAOA



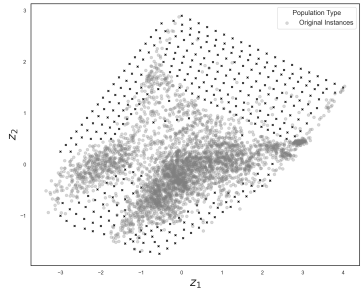


Figure 9: Gaps in Instance Space

We identify 360 target points in the instance space and evolve instances to reach these targets.

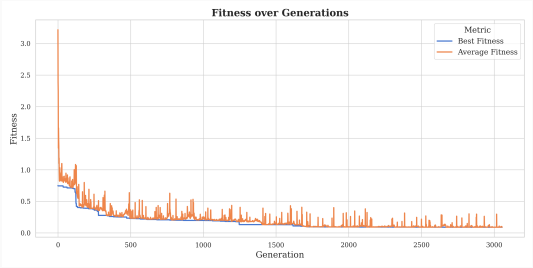


Figure 10: Fitness over Generations

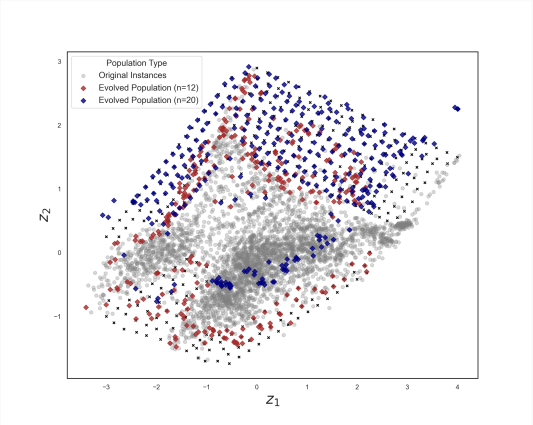
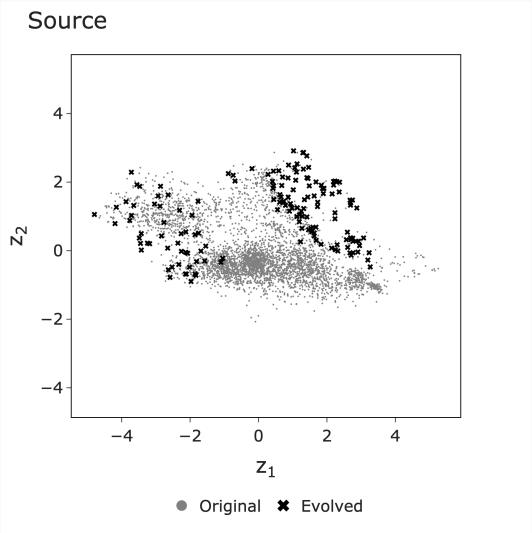
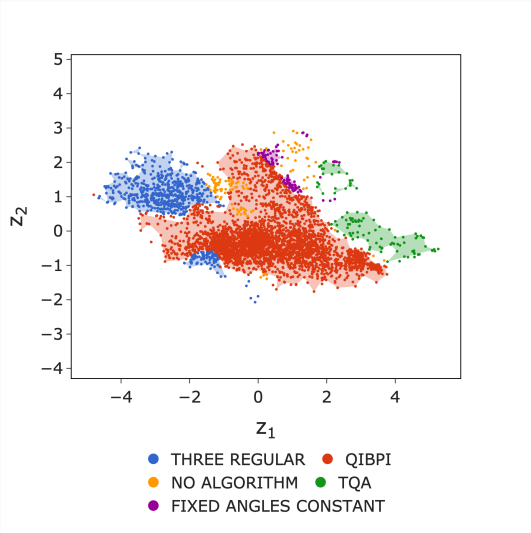


Figure 11: Gaps in Instance Space


Source
4
2
0
−2
−4
z_2
−4
−2
0
2
4
z_1
Original
Evolved


5
4
3
2
1
0
−1
−2
−3
−4
z_2
−4
−2
0
2
4
z_1
THREE REGULAR
QIBPI
NO ALGORITHM
TQA
FIXED ANGLES CONSTANT

Software for QAOA Parameter Initialisation

- Parameter initialisation significantly impacts QAOA's performance and convergence
- Current challenges:
  - Overwhelming number of initialisation techniques
  - Implementations are coupled with the various quantum libraries (e.g. Cirq, Qiskit, PyQuil)
  - Lack of standardization and comparison across different techniques

Key Features:

- Consolidates multiple strategies (Random, QIBPI, QAOAKit, TQA, Constant)
- RESTful API for easy integration
- Modular and extensible
- Built-in validation and error handling
- Automatic documentation generation

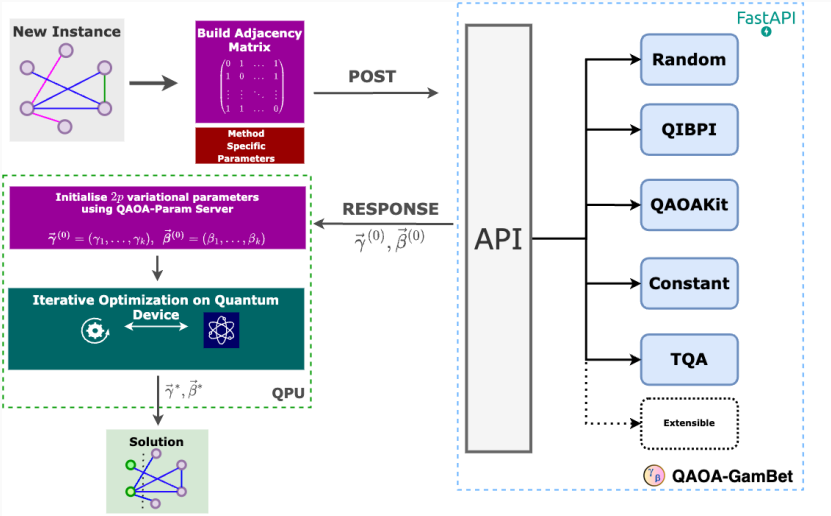


Figure 12: FastAPI Workflow

Request

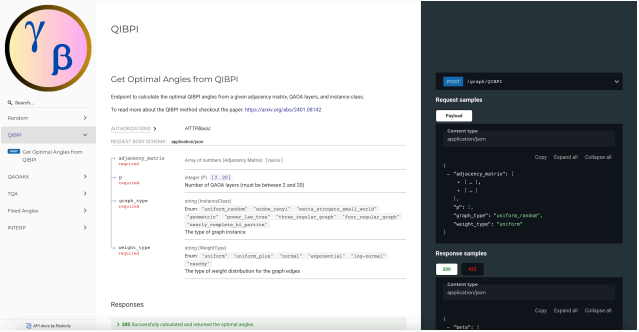
```
# Prepare the request data
data = {
    "adjacency_matrix": adjacency_matrix,
    "p": 2,
    "graph_type": "three_regular_graph",
    "weight_type": "uniform"
}

# Send a request to get optimal angles
response = requests.post(
    "http://localhost:5000/graph/QIBPI",
    json=data,
    auth=('username', 'password')
)
```

Response

```
{
  "beta": [0.1, 0.15, 0.2],
  "gamma": [0.3, 0.35, 0.4],
  "source": "QIBPI"
}
```

Example



- Auto-generated documentation from docstrings
- Rendered using Swagger UI and redoc

Conclusion

- Key Contributions:
  - Expanded QAOA research scope with diverse test suite of MaxCut instances
  - Conducted Instance Space Analysis (ISA) to understand instance-feature impacts on QAOA design choices
  - Quantum Instance-based Parameter Initialisation (QIBPI)
  - FastAPI for QAOA Parameter Initialisation
- Instance Space Analysis:
  - Parameter transfer effective within instance classes, but not across
  - Gaps in instance space identified and applied instance evolution

- Expand analysis scope
  - Extend to larger problem sizes
  - Include more weight distributions and network structures
  - Apply ISA to other quantum algorithms (VQE, F-VQE)
- Bridge theory-practice gap
  - Test on real quantum hardware (e.g., IBM's 128-qubit machine [10])
  - Create ML-based approaches leveraging experimental data

Thank You - Questions?

- Link to QAOA-GamBet
- Link to ISA's

[1] Amira Abbas et al. **"Quantum Optimization: Potential, Challenges, and the Path Forward".** In: *arXiv preprint arXiv:2312.02279* (2023).

[2] Fernando G. S. L. Brandão et al. **"For Fixed Control Parameters the Quantum Approximate Optimization Algorithm's Objective Function Value Concentrates for Typical Instances".** Version Submitted. In: *arXiv* (Aug. 2023). DOI: 10.48550/arXiv.1812.04170.

[3] Sergey Bravyi, David Gosset, and Robert König. **"Quantum advantage with shallow circuits".** In: *Science* 362.6412 (2018), pp. 308–311. DOI: 10.1126/science.aar3106. eprint: https://www.science.org/doi/pdf/10.1126/science.aar3106. URL: https://www.science.org/doi/abs/10.1126/science.aar3106.

[4] Edward Farhi, Jeffrey Goldstone, and Sam Gutmann. ***A Quantum Approximate Optimization Algorithm.*** 2014. arXiv: 1411.4028 [quant-ph].

[5] Mario Fernández-Pendás et al. **"A study of the performance of classical minimizers in the Quantum Approximate Optimization Algorithm".** In: *Journal of Computational and Applied Mathematics* 404 (2022), p. 113388. ISSN: 0377-0427. DOI: https://doi.org/10.1016/j.cam.2021.113388. URL: https://www.sciencedirect.com/science/article/pii/S0377042721000078.

[6] Igor Gaidai and Rebekah Herrman. ***Performance Analysis of Multi-Angle QAOA for $p > 1$.*** 2023. arXiv: 2312.00200 [cs.ET].

[7] Lov K. Grover. **"A fast quantum mechanical algorithm for database search".** In: *Proceedings of the twenty-eighth annual ACM symposium on Theory of computing - STOC '96* (1996). DOI: 10.1145/237814.237866. URL: http://dx.doi.org/10.1145/237814.237866.

[8] X. Lee et al. **"Parameters Fixing Strategy for Quantum Approximate Optimization Algorithm".** In: *2021 IEEE International Conference on Quantum Computing and Engineering (QCE)*. Los Alamitos, CA, USA: IEEE Computer Society, Oct. 2021, pp. 10–16. DOI: 10.1109/QCE52317.2021.00016. URL: https://doi.ieeecomputersociety.org/10.1109/QCE52317.2021.00016.

[9] Alberto Peruzzo et al. **"A variational eigenvalue solver on a photonic quantum processor".** In: *Nature Communications* 5.1 (2014), p. 4213. DOI: 10.1038/ncomms5213. URL: https://doi.org/10.1038/ncomms5213.

[10] Natasha Sachdeva et al. **"Quantum optimization using a 127-qubit gate-model IBM quantum computer can outperform quantum annealers for nontrivial binary optimization problems".** In: *arXiv preprint arXiv:2406.01743* (2024).

[11] Stefan H. Sack and Maksym Serbyn. **"Quantum annealing initialization of the quantum approximate optimization algorithm".** In: *Quantum* 5 (July 2021), p. 491. ISSN: 2521-327X. DOI: 10.22331/q-2021-07-01-491. URL: https://doi.org/10.22331/q-2021-07-01-491.

[12] Ruslan Shaydulin et al. **"Classical symmetries and the quantum approximate optimization algorithm".** In: *Quantum Information Processing* 20 (2021), pp. 1–28.

[13] Ruslan Shaydulin et al. **"Parameter Transfer for Quantum Approximate Optimization of Weighted MaxCut".** In: *ACM Transactions on Quantum Computing* 4.3 (Apr. 2023), pp. 1–15. ISSN: 2643-6817. DOI: 10.1145/3584706. URL: http://dx.doi.org/10.1145/3584706.

[14] Ruslan Shaydulin et al. **"QAOAKit: A Toolkit for Reproducible Study, Application, and Verification of the QAOA".** In: *2021 IEEE/ACM Second International Workshop on Quantum Computing Software (QCS)*. IEEE, Nov. 2021. DOI: 10.1109/qcs54837.2021.00011. URL: https://doi.org/10.1109/qcs54837.2021.00011.

[15] P. W. Shor. **"Algorithms for quantum computation: discrete logarithms and factoring".** In: *Proceedings 35th Annual Symposium on Foundations of Computer Science*. 1994, pp. 124–134.

[16] Shree Hari Sureshbabu et al. **"Parameter Setting in Quantum Approximate Optimization of Weighted Problems".** In: *Quantum* 8 (Jan. 2024), p. 1231. ISSN: 2521-327X. DOI: 10.22331/q-2024-01-18-1231. URL: https://doi.org/10.22331/q-2024-01-18-1231.

[17] David H Wolpert and William G Macready. **"No free lunch theorems for optimization".** In: *IEEE transactions on evolutionary computation* 1.1 (1997), pp. 67–82.

[18] Leo Zhou et al. **"Quantum Approximate Optimization Algorithm: Performance, Mechanism, and Implementation on Near-Term Devices".** In: *Phys. Rev. X* 10 (2 June 2020), p. 021067. DOI: 10.1103/PhysRevX.10.021067. URL: https://link.aps.org/doi/10.1103/PhysRevX.10.021067.