QPack: Quantum Approximate Optimization Algorithms as universal benchmark for quantum computers

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Abstract

In this paper, we present QPack, a benchmark for NISQ era quantum computers using QAOA algorithms. Unlike other evaluation metrics in the field, this benchmark evaluates not only one, but multiple important aspects of quantum computing hardware: the maximum problem size a quantum computer can solve, the required run-time, as well as the achieved accuracy. This benchmark will also be available for quantum simulators, where it is able to assess the run-time and required memory that a simulator needs to run the application. The applications MaxCut, dominating set and traveling salesman are included to provide variation in resource requirements. We also discuss the design aspects that are taken in consideration for an optimal benchmark, with critical quantum benchmark requirements in mind. An implementation strategy is presented, providing practical metrics. The measurement results show how QAOA can be optimized using classical optimization algorithms, suggesting the use of a global/local optimizer hybrid implementation. The implementation of the MaxCut, dominating set and traveling salesman problem show that different QAOA applications use a wide variety of quantum resources. This will allow for a diverse benchmark that promotes optimal design considerations, avoiding hardware implementations for specific applications.

1. Towards a standard quantum benchmark

Currently, quantum computing is making large steps to becoming a mature technology. More companies are developing their own quantum hardware for both research and preparing for practical deployment. The main challenges in the past years have been an abundance of practical applications for the few-qubit Noisy Intermediate-Scale Quantum (NISQ) quantum hardware and scaling the qubits and depth of the quantum hardware. For these reasons, quantum computing was not yet at the maturity for a useful quantum benchmark.

Many quantum benchmarks have been developed, but these either aim at qubit level assessment or are lacking in practical usability. For a benchmark to be useful, the practical application of the quantum hardware needs to be reflected. For this a practical application is required and this was not yet achievable with current quantum hardware scales. Benchmarks at the component level (individual qubits, quantum logic gates) have been developed widely and are useful for the development of the hardware. This is however more aimed at basic quantum research rather than application [1]. This also serves a fundamentally different goal than a performance measure of quantum computers. Many different forms of quantum hardware are being used, without a clear dominating implementation. Each of these have different dynamics and metrics, and can therefore not be generalized [2]. For this reason, making a benchmark for low-level hardware aspects will not properly reflect its performance compared to other implementations of the quantum hardware.

Furthermore, while benchmarks for single qubit operations have been developed [3-6], these performances do not accurately reflect quantum operations on larger scales. Noise levels, for example, are an important metric in single gate performance. The noise however, varies per gate and due to qubit entanglement will propagate unpredictably throughout the system [2] [7] [8]. This makes it impossible to use single gate noise performance to extrapolate for the entire system, while for classical computers this would have been possible. These difficulties in determining the performance will require abstraction from the low level performance and an application level benchmark is needed to properly verify the performance.

Other benchmarks such as Random Benchmarking (RB) or quantum volume [9] are well known quantum benchmarks, but provide limited insight to practical use of quantum computers. RB is an example of a volumetric benchmark, which determines to which circuit depth, the quantum hardware can hold the required fidelity for a set number of qubits. RB can determine the fidelity for a random sequence of quantum gates, which should give a general idea of how the hardware performs. By using RB, or any other volumetric benchmark, the quantum volume can be determined. However, this gives little insight on the performance of a practical algorithm on the quantum hardware. Another challenge in developing a benchmark for quantum computing, is that there is no consensus on which metrics should be benchmarked to reflect
In this paper, we propose QPack: a benchmark targeted to measure the performance of applications executed on quantum computers and quantum computer simulators. The benchmark has three main components, as presented in Figure 1.

**Problem library**: A set of problems are provided to ensure practical relevance of the benchmark and a diverse means of evaluation. Alternative problems targeted by our benchmark are discussed in Section 5, 6 and Appendix B.

**Quantum algorithm**: A quantum algorithm must be chosen which can be applied to various problems and is applicable on current quantum hardware and quantum simulators. With current quantum hardware in mind, a hybrid classical-quantum optimizer is chosen as our first quantum algorithm. The selected quantum optimizer is QAOA (Quantum Approximate Optimization Algorithm). The selection of this optimizer is further elaborated in Section 3 and 4. The options and selection of the classical optimizer are discussed in Appendix C. Measurements of these classical optimizers are done as well, which is further elaborated in Section 7. The QPack benchmark is envisioned to grow as more quantum algorithms become applicable on quantum hardware.

**Performance evaluation**: The performance of quantum computers and simulators need to be evaluated according to a selection of metrics. Further discussion on these metrics is presented in Section 2 and 6.

In this paper, a set of metrics is proposed to suit the emerging quantum QAOA approach. QAOA is a promising quantum approach for optimization using relatively few qubits. With the current rate of development of scaling quantum hardware, this approach is expected to be one of the first to have practical applications. The contributions of this work are as follows.

- The general outline of the benchmark QPack, targeting essential metrics
- Analysis of classical optimizers to improve QAOA implementations
- Introducing the concept of quantum algorithm technology readiness level (QTRL), which gives a ranking of cutting edge QAOA implementations

In Section 2, a literature review on quantum benchmarks is presented, addressing concerns on current quantum benchmarks and providing the necessary metrics. Near term quantum algorithms will be discussed in Section 3 and the details on the QAOA algorithms will be examined in Section 4. Supplementary QAOA examples are provided in Appendix A. QAOA algorithms are implemented in a hybrid classical-quantum computing set-up, where a problem is defined in the classical computer, after which an approximate optimization is performed using QAOA, of which the parameters are optimized using the classical computer. Generally, the classical and quantum computer work in an alternating fashion until an optimal configuration is found. QAOA has a limited probability of finding the optimal solution, but aims to achieve a equal or higher probability than its classical counterpart with improved performance. When the QAOA algorithm is executed, it can be assessed, used and reinitialized from the classical computer. To further assess QAOA, the practical concerns will be
covered as well. This will cover issues such as parameter tuning, but also concerns with current quantum hardware and how to deal with its limitations. In current trends, not only are there newer implementations, but also various ways to improve on the original algorithm. The shortcomings will be discussed and emerging trends such as QUBO \(^{[10]}\), Quantum Alternating Operator Ansatz \(^{[11]}\) and machine learning \(^{[12]}-{[14]}\) to improve upon the shortcomings are discussed.

To understand whether this algorithm is applicable to NISQ era quantum computers, the implementation of the algorithm to various problems are presented in Appendix \(^{[B]}\). In Section \(^{[5]}\) the readiness of the implementations of the QAOA algorithm is evaluated as well, presenting a Quantum Technology Readiness Level (QTRL). This will give insight to how far the development of QAOA algorithms is, and whether these will be implemented in the near future. The benchmark implementation proposal is presented in Section \(^{[C]}\). The critical metrics are addressed, and method are presented to reliably test these. In Appendix \(^{[C]}\), a theoretical evaluation of various classical optimizers is supplied to find the expected best fit for the QAOA algorithm. From these optimizers, a selection will be made for numeric measurements. In Section \(^{[7]}\), classical optimizers and QAOA applications are respectively measured. From these measurements, insights are given for efficient implementations and possible further improvements. In Section \(^{[8]}\) the conclusions and future work regarding the benchmark are discussed.

2. Literature review on quantum benchmarking

As mentioned before, a popular metric to measure the performance of quantum computers is its quantum volume: the number of qubits and the quantum circuit depth it can run. The authors of the quantum volume benchmark mention in total four metrics to which the performance of a quantum computer can be evaluated \(^{[15]}\):

- The number of physical qubits
- The number of gates that can be applied before errors (quantum circuit depth)
- The connectivity of the quantum computer
- The number of operations that can be run in parallel

The number of physical qubits is only interesting if it can reach a required circuit depth, as such these metrics can be combined in the quantum volume. As argued before, quantum volume on itself does not reflect practical performance properly. Furthermore, the connectivity and number of operation run in parallel, certainly have value as metrics, however it can be argued whether these metrics have practical value. For example, a fully connected quantum computer is good on paper, but if it cannot scale it cannot be put in practice. From the perspective of this paper, it is considered that execution with limited connectivity will be handled by the compiler (additional qubit SWAPs to enable execution on limited connectivity). As a result, the connectivity will affect the number of quantum operations and with that the run time. An important characteristic of the benchmark, is that it will use non-native problems, meaning that the problem does not correspond to the qubit layout. This means more resources are required to compile the problem to the quantum hardware layout, which significantly impacts performance \(^{[16]}\), but is essential for practical application. Similarly, the number of operations run in parallel will decrease the critical path of the circuit and reduce the run-time. With this, both metrics can be abstracted by evaluating the run-time. As the quantum computers have progressed to a size that can run practical algorithms such as QAOA and VQE (variational quantum eigensolver), a higher abstraction level using application performance would be the proper method to evaluate the performance of current quantum computers.

Recently, a quantum benchmark which uses QAOA has been announced by Atos \(^{[17]}\) called the Q-score. This benchmark evaluates to which problem size a quantum computer can run an optimization algorithm for the MaxCut problem, to which the details are provided in Appendix \(^{[A.1.1]}\). While the benchmark is aimed at an algorithm to be used in practice, it only measures the problem size that can be executed. This however does not evaluate the following metrics:

- **Success-rate, accuracy**: How well is the algorithm executed
- **Performance**: How fast is the algorithm executed
- **Scaling**: How well does the quantum computer perform on different problem sizes

This way, the benchmark gives limited insight into the quality of the quantum hardware except for the fact that it can run the optimization algorithm and the quantum volume it can achieve for this application.

Another concern on the Q-score benchmark is the lack of universality. While it claims to run on every current quantum computer, it still only uses a single problem: MaxCut. The danger of using a single application is that quantum computers will be tailored to one specific problem but perform poorly with others. An extreme case is the D-Wave quantum computer, which is specialized to quantum annealing. Note that this is an extreme case as this quantum computer is not gate-based and can therefore not be programmed to do any other application. QAOA is a versatile algorithm that can be applied on a large variation of computational problems, as explored in Section \(^{[5]}\) To avoid single problem tailoring, multiple different
problems can be used to benchmark the quantum hardware. Further details on the requirements of quantum benchmarks are discussed in Section 5.

3. Near term quantum algorithms

Quantum algorithms have the potential to outperform classical algorithms, also called quantum supremacy. Many quantum algorithms have been developed and algorithms such as Shor’s algorithms are proven to perform better than their classical counterpart. Currently the development of quantum hardware is not yet at the scale to support such algorithms. In order to achieve practical quantum algorithms, with quantum supremacy in mind, algorithms have emerged to fit the current NISQ technology. With this technology, algorithms for 50-100 qubits could be supported. In this section, a selection of similar near term algorithms are discussed which are candidates for near term implementation.

3.1. Quantum Approximate Optimization Algorithm (QAOA)

The first algorithm discussed in this section is QAOA [18], introduced by Farhi et al. in 2014. This algorithm can be used to approximate a set of NP-Hard optimization problems with relatively few qubits. NP-Hard optimization problems are a large bottleneck for current computing systems, as these cannot be efficiently calculated using classical computers. The type of optimization problems that QAOA can be applied to, consist of a set of parameters with a set of constraints where the parameters need a specific configuration for finding the optimal solution. This has many practical applications, ranging from multiprocessor scheduling to warehouse order picking and flight timetable planning. The specifics of these applications will be further discussed in Appendix A and Section 5.

3.2. Variational quantum eigensolver (VQE)

The quantum variational eigensolver (VQE) is a quantum algorithm that finds the eigenvalues of a Hamiltonian $H$, representing the system to be solved [19]. It is used to minimize the objective function $⟨ψ(θ) | H | ψ(θ)⟩$. The minimum eigenvalue sought is represented by the ground state of the system. The state $|ψ(θ)⟩$ can be varied by changing $θ$ to converge tot the minimum, my means of a classical optimizer. This is a minimum eigenvalue problem and is a constraint satisfaction problem (CSP), which is generally NP-hard [20]. It is also one of the algorithms, like QAOA, that is believed to be one of the first algorithms to run effectively on a near-term quantum computer.

3.3. Quantum adiabatic algorithm (QAA)

The quantum adiabatic algorithm (QAA) is able to find the optimal solution to a satifyability problem when given enough time, by finding the ground state of the slowly varying hamiltionian $H(t)$ [21]. QAA uses the time-dependent Hamiltonian $H(t) = (1 - t/T)B + (t/T)C$. The algorithm starts in the highest energy state of $B$, and seeks the highest energy state of $C$. This makes use of the Perron-Frobenius theorem that the difference in energies between the top state and the one below is greater than 0 for $t < T$ [18]. This means that if $T$ is sufficiently large, the optimal solution can be found by slowly varying $t$ for $0 < t ≤ T$ [21]. A downside of QAA is that success probability is not a monotonic function of $T$. This means that the success probability can drop, whereas for QAOA the success probability always increases with $p$ [18, 22]. It is also shown that QAA can be trapped in a false minimum, which is not the case for QAOA [18]. It is also worth mentioning that QAA is not a gate-based algorithm.

4. Introduction to QAOA

As QAOA can be implemented to a larger variety of applications compared to VQE and has an advantage over QAA, QAOA was selected for this benchmark. To understand this algorithm better for implementation, further details are discussed.

QAOA is designed to find approximate solutions for combinatorial optimization problems with the help of quantum computing. To go in further detail, the algorithm will be explained using the equations given by Farhi et al. In combinatorial optimization problems, the goal is to maximize or minimize the number of clauses $(m)$ satisfied. A clause $(ψ)$ is a Boolean requirement, for example for a $n$-bit Boolean string $z = z_1, ... z_n$:

$$ψ_{example} : z_1 ∧ z_2$$

(1)

To satisfy the clause of the example $z_1$ and $z_2$ must satisfy $z_1 = z_2 = 1$. 

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The QAOA algorithm depends on a parameter $p \geq 1$, which determines the quality of the approximation. Quality is given as an approximation ratio. This ratio is defined as either the number of clauses satisfied by the QAOA algorithm divided by the number of clauses satisfied in the optimal assignment ($r = \frac{M_p}{M_{opt}}$), or as the number of clauses satisfied by the QAOA algorithm divided by the number of clauses ($r = \frac{M_p}{m}$). The latter is considered to be stronger [23]. The depth of the quantum circuit required to implement this algorithm grows in the worst case linearly with $p$ times the number of constraints $m$ [18].

The equation that needs to be maximized (cost Hamiltonian) is as follows:

$$C(z) = \sum_{\psi \in \Psi} C_{\psi}(z)$$  \hspace{1cm} (2)

Here, $C_{\psi}(z) = 1$ if clause $\psi \in \Psi$ is satisfied, and 0 otherwise. In the quantum approach we define the Boolean string as a vector $|z\rangle$ in the computational basis $\{|0\rangle, |1\rangle\}$. The operator for equation (2) then becomes

$$U(C, \gamma) = e^{-i\gamma C} = \prod_{\psi \in \Psi} e^{-i \gamma C_{\psi}}$$  \hspace{1cm} (3)

The terms of the product commute as these are diagonal in the computational basis and each term’s locality is the locality of clause $\psi$. The unitary is dependent on angle vector $\gamma$ and can be restricted to $[0, 2\pi]$ since $C$ has integer values [18]. Choosing the number of elements $\gamma$ is divided in, will impact precision and performance. To improve the precision of the QAOA algorithm, multiple cycles of the gates will be applied. The number of cycles is denoted as $p$. For integer $p \geq 1$, $\gamma$ is defined as $\gamma \equiv \{\gamma_1, \ldots, \gamma_p\}$, where each $\gamma_i$ with $1 \leq i \leq p$ is a vector within the range $[0, 2\pi]$.

To sum the outcomes of equation (3), the so-called mixer Hamiltonian $H_B$ or $H_B$ is introduced:

$$B = \sum_{j=1}^{n} \sigma_j^x$$  \hspace{1cm} (4)

Here, the Pauli X-gates operate on a single qubit $|z_j\rangle$. For integer $p \geq 1$, $\beta$ is defined as $\beta \equiv \{\beta_1, \ldots, \beta_p\}$, where each $\beta_i$ with $1 \leq i \leq p$ represents a angle vector $\beta$ for a single cycle. The general definition of the unitary applied to a single qubit then becomes:

$$U(B, \beta) = e^{-i\beta B} = \prod_{j=1}^{n} e^{-i \beta \sigma_j^x}$$  \hspace{1cm} (5)

Here, $\sigma_j^x$ is the Pauli-X operator on qubit $j$. The unitary $U(B, \beta)$ depends on angle vector $\beta$, which runs from 0 to $\pi$. The vector $|z\rangle$ is placed in superposition:

$$|s\rangle = \frac{1}{\sqrt{2^n}} \sum_z |z\rangle$$  \hspace{1cm} (6)

The angle dependent quantum state can then be written as

$$|\gamma, \beta\rangle = U(B, \beta_p)U(C, \gamma_p)\ldots U(B, \beta_1)U(C, \gamma_1) |s\rangle$$  \hspace{1cm} (7)

The expectation of $C$ then becomes:

$$F_p(\gamma, \beta) = \langle \gamma, \beta | C | \gamma, \beta \rangle$$  \hspace{1cm} (8)

The maximum expectation for $p$ qaoa cycles ($M_p$) is then defined as:

$$M_p = \max_{\gamma, \beta} F_p(\gamma, \beta)$$  \hspace{1cm} (9)

Since increasing parameter $p$ will increase the quality of the solution, in other words a equal or higher expectation will be found, we can state the following:

$$M_p \geq M_{p-1}$$  \hspace{1cm} (10)

With the intent that $\lim_{p \to \infty} M_p = \max_z C(z)$, which is proven by Farhi et al.[18].

To give an intuition on how the algorithm operates, an example will be given. In this example, a system with 2 (qu)bits per clause is examined. The general clause will be worked out for bits $j$ and $k$:

$$C = \sum_{j<k} C_{<jk>}$$  \hspace{1cm} (11)
This is derived from equation (3). The expectation from equation (8) becomes:

$$F_p(\gamma,\beta) = \sum_{jk} |s\rangle U^\dagger(C,\gamma_1) \cdot \ldots \cdot U^\dagger(B,\beta_p)C_{<jk>}U(B,\beta_p) \cdot \ldots \cdot U(C,\gamma_1) |s\rangle$$  \hspace{1cm} (12)

Here $U^\dagger$ denotes the conjugate transpose of unitary operator $U$.

The operator for a single clause then becomes:

$$U^\dagger(C,\gamma_1) \ldots U^\dagger(B,\beta_p)C_{<jk>}U(B,\beta_p) \ldots U(C,\gamma_1)$$  \hspace{1cm} (13)

The contribution for $p = 1$ can then be written as:

$$U^\dagger(C,\gamma_1)U^\dagger(B,\beta_1)C_{<jk>}U(B,\beta_1)U(C,\gamma_1)$$  \hspace{1cm} (14)

Using an example for $C$, used in MaxCut applications (Appendix A.1.1), it can be shown which operators contribute to this equation. MaxCut and other applications will be discussed later in greater detail. For this example, the definition for the maximized equation becomes:

$$C_{<jk>} = \frac{1}{2}(-\sigma_j^x\sigma_k^x + 1)$$  \hspace{1cm} (15)

Now substituting equation (5), gives rise to the following:

$$U^\dagger(C,\gamma_1)e^{i\beta_1(\sigma_1^x+...+\sigma_n^x)}\frac{1}{2}(-\sigma_j^x\sigma_k^x + 1)e^{-i\beta_1(\sigma_1^x+...+\sigma_n^x)}U(C,\gamma_1)$$  \hspace{1cm} (16)

All $\sigma$ terms in the second exponent except for $\sigma_j$ and $\sigma_k$ can be moved in front of the $\frac{1}{2}(-\sigma_j^x\sigma_k^x + 1)$ term as they do not interact with qubits $j$ and $k$, i.e. the operators commute ($\hat{A}\hat{B} = \hat{B}\hat{A}$). Because these operators can be moved to the front, they cancel out with their Hermitian conjugate. For increasing $p$, $U(B,\beta)$ will contain the qubits connected one step further from the original clause. For example, if qubit $j$ shares a clause with qubit $l$, the operators acting on qubit $j$ will be included as well. By expanding this for increasing $p$, more qubits are considered for each clause, effectively increasing the quality of the approximation. To expand this, the unitary $U(C,\gamma)$ must be understood. This unitary’s operator $C_\alpha$ is 1 if the condition is met and 0 otherwise. In the case of a graph (e.g. MaxCut), this means that the conditions are a connectivity matrix. This makes the term 1 if a connection between the qubits exists. The unitary of $\gamma_1$ will contain the $\sigma$ for $j$ and $k$, but also all qubits which are connected. This has consequence that $U(B,\beta_2)$ will keep $\sigma_j$ and $\sigma_k$ but also for all qubits connected to these qubits. This way, increasing $p$ will increase the qubits in the graph.

**Practical concerns on QAOA**

In order to apply QAOA algorithms to practical applications, some hard challenges must be achieved first. One of the major challenges is that even while QAOA uses much less resources than e.g. Grover’s algorithm, it still requires hundreds of qubits in order to achieve better performance than classical algorithms. Specifically for QAOA, the depth of a circuit can be a huge bottleneck if it does not make use of an optimized implementation [24]. Furthermore, the limited precision of QAOA will require a large parameter $p$ to achieve optimal results. This parameter is expected to grow almost linearly with the problem size, but finding the optimal value for $p$ is one of the big challenges for QAOA to become practical [25]. Another challenge is the tuning of parameters $\beta$ and $\gamma$. The original paper of QAOA [18], proposes an optimal configuration for the $\beta$ and $\gamma$ parameters, but is considered computationally expensive [24][26]. Instead, optimal parameters can be found for specific problem instances [24]. For specific problems, a value for $p$ can be chosen in such a way that the approximation is better than the classical counter part. For example, Crooks shows that for $p \geq 8$, the QAOA for MaxCut could outperform the Goemans-Williamson algorithm [24]. This way, a lower bound can be set on the $p$ parameter.

An emerging trend is to optimize the parameters for QAOA using machine learning [12][14]. Results of Khairy et al. show that training for an 8-qubit system, the training time can take up to 4.98 hours. While this optimization improves performance, this can only be applied if the algorithm is used many times for the same $n$-bit system in order to achieve speedup. Wauters et al. [15] aims to solve this problem by suggesting that a strategy learned from a small system, can be applied to a larger system to achieve similar speedup. Their results using local optimizations on larger systems show this is achievable. Alam et al. [12] applies machine learning to a classical optimizer that iteratively runs the QAOA algorithm with new parameters. Their implementations show an average reduction of iterations of 44.9% and is also a good solution for run-time optimization.
In terms of integration, Qiskit and Rigetti actively include QAOA in their repositories. Qiskit currently only supports Ising-type problems such as MaxCut [26], while Rigetti also has support for e.g. the partitioning problem and makes this publicly available on Github. Rewriting the problem to a format that can be optimized using QAOA is a challenge in itself as well. In recent papers, Quadratic Unconstrained Binary Optimization (QUBO) [27] is used to map problems to QAOA.

Another downside of QAOA could be the limited range of problems that it can solve. While all problems discussed in Section 5 are considered important challenges, the quantum algorithm is still limited to very similar problems. An generalization of QAOA is presented as the Quantum Alternating Operator Ansatz, which covers a wider range of problems [11]. As discussed in Section 5, some algorithms are not well suited for QAOA and other quantum algorithms will likely perform better results. The constraint density is also shown to impact the performance of QAOA [28]. This means that performance will depend not only on the size of a graph, but also the number of constraints compared to the size of the graph.

Another challenge is that while QAOA might perform good in theory and on a simulator, on real hardware the performance might be considerably worse [29] or could make an implementation unfeasible [30]. The relatively large amount of noise in current quantum hardware results in better performance for algorithms with lower depth [10] and will likely be a strong factor in implementing QAOA in practice.

5. Quantum algorithm technology readiness level

The QAOA implementations of the above discussed problems will be summarized and compared according to their technology readiness level (TRL). This is done, as not every paper provides an in-depth analysis of the proposed implementation. Providing an in-depth analysis of every implementation would be beyond the scope of this report. TRL was first introduced by NASA [31] in order to evaluate the state of development of technologies. The NASA TRL has 9 levels, from proposing basic principals (1) to flight proven (9). Currently, more adaptions have been made for both European projects and commercial projects [32].

![QTRL Graph](image.png)

Figure 2. A quantum technology readiness level (QTRL) evaluation of the presented QAOA implementations

In order to evaluate the maturity of quantum algorithm implementations appropriately, we propose a separate quantum TRL (QTRL). This QTRL is inspired by the TRL presented by NASA, but adapted to quantum algorithms to cover quantum algorithm specific challenges. The QTRL are ordered as follows:

1) **Theoretical proof of concept is presented:** The QAOA algorithm to a specific problem is worked out in such a way that both the Cost and Mixer Hamiltonian are presented. A theoretical proof is given that this implementation approximates the optimal solution.
2) **Demonstrated on quantum simulator:** The QAOA algorithm is implemented on a quantum simulator and provides meaningful results.

3) **Cost and performance analysis:** An in-depth analysis of the implementation is done, showing the required resources and complexity.

4) **Full stack:** The problem is implemented to a practical application and a classical application that uses the QAOA algorithm is presented. The system should work with the combination of a classical computer and a quantum simulator or on quantum hardware. The full system should provide useful results.

5) **Ready for application:** The full stack is ready for implementation using quantum hardware and can be applied to problems in practice. The application will likely need optimization or clever implementation to out perform classical implementations.

6) **Quantum supremacy:** The problem can be solved faster on a classical-quantum hybrid full stack compared to a classical implementation, using the quantum algorithm. This is currently an aim for the future, as no such implementations have been presented yet. The first quantum algorithm to do so, must either make use of very few resources, or the resources of quantum hardware have risen to such a level that high resource demanding algorithms can be run (think of Grover’s and Shor’s algorithm).

The QTRL of the problems is presented in Figure 2. Some notes on the results are:

- Publications on the Ising model have analytic results on complexity, but since it is considered not feasible and no resource analysis is done.
- Analysis has been done on the complexity of the set packing implementation, but no in-depth results on resources have been published.
- The traveling salesman has been implemented in full stack and on a practical application, but is not ready to work on available quantum hardware.

6. Benchmark outline

Having determined the algorithm to base the benchmark on, the outline of QPack is presented for implementation. In order to properly evaluate the performance of a quantum hardware implementation in practice, the following aspects need to be considered:

1) Run-time
   a) Classic computation
   b) Classic to quantum connection
   c) Quantum computation

2) Outcome accuracy / best approximation error

3) $|0\rangle$ bias [36]

4) Success probability

5) Performance scaling

**Run-time:** The run-time of an application is an obvious parameter to measure. Classically, apart from the functionality, this is the main parameter measured as it separates implementations on their practical performance. Since the quantum hardware is only practical in hybrid configuration, both the classical and quantum hardware need to be evaluated. While the quantum speedup should be most significant to the performance, for QAOA optimization it was found that the classical optimizer is crucial to the performance of the QAOA optimization [30]. Determining the performance of the classical hardware is therefore essential. For this reason the following run-times need to be observed:

- Overall run-time
- Run-time classical hardware
- Connection between classical and quantum hardware
- Preprocessing/placing and routing
- Run-time quantum hardware

The connection between quantum and classical hardware might very well be significant to the overall performance. Multiple calls need to be made to the quantum hardware in QAOA. Since quantum computing is a Compute as a Service (CaaS) in current implementations, the way the connection is organized as well as the relative slow internet connection can be crucial. In cases that the implementation is organized with a local classical computer sending instructions to the remote
quantum computer, most time will be lost by this connection. A more mature implementation would be both a remote classical computer and a remote quantum computer, which share a faster local connection. By explicitly measuring these parameters, much more crucial information is learned about the bottleneck of an implementation. As the benchmark does not optimize quantum instructions to suit specific hardware, the performance of the compiler will be reflected as well and will translate to the number of instructions generated and how the quantum circuit is scheduled. Other bottlenecks on the implementation could include: number of calls to quantum hardware from classical hardware and time required per quantum instruction.

Best approximation error: QAOA can only approximate an optimal solution. While this is dependent on parameter $p$ and the classical optimization strategy, it will also be dependent on the hardware. The qubit quality will determine the noise in a system and will determine $p$ and can significantly decrease performance. Furthermore, gate error and finite coherence time can introduce significant bounds on $p$, limiting not only compensation for noise, but also place significant bounds on scaling. Another effect on the accuracy could be $|0\rangle$ bias. This means that the states are more likely to be measured as a logical 0 rather than a logical 1, skewing the outcome and effecting the accuracy. The approximation can be evaluated in multiple ways.

1. The benchmark will be run on the hardware with optimal parameter $p$, determined iteratively. This way the maximum achievable accuracy can be found by comparing it to the solution of an exact algorithm. This has as downside that multiple runs will be required to find the correct parameter, and increasing $p$ will increase the run-time, which might not be properly reflected this way. If the run-time of the implementation is however presented for only the optimal parameter, it will likely better reflect how the optimization would be implemented in practice. This way a decision will be made for the trade-off between speed and accuracy, favoring accuracy. The difficult part is that, in the case that there are no bounds on $p$, $p$ might grow to infinity, approaching exact calculation. Recent research show that increasing $p$ will not always improve accuracy and will have a practical limit.

2. The other method is to test for, e.g., $p \in \{1, 2, 3, 4\}$ and compare these results. This way the run-time will not be determined by the choice of $p$, but the accuracy will reflect the quality of the quantum hardware. This will require more interpretation, as the accuracy shown will not be the optimal accuracy, but shows how the accuracy will be for low iterations of $p$. The difficulty in this approach lies in determining how $p$ scales for larger problem sizes. The size of $p$ is expected to grow with the problem size, but at which rate is not yet determined. Some research suggest that QAOA will only be practical for low depth (e.g. $p=2$) and therefore eliminated this issue. From both approaches, the latter appears to be the most fair and with fewer issues, but demands an explanation on how to interpret the results.

Alternatively, an approach can be taken where the accuracy is evaluated for a predetermined run-time. This however requires that the run-time will not be constant for each problem size as the run-time is expected to grow. Determining a starting point for the run time as well as how this will progress for the problem size is nontrivial. For this reason, method 1 is preferred.

Success probability: The probability of success is another measure of the quality of the quantum hardware. Preferably, the best approximation error of the QAOA implementation reaches 0 for some amount of runs. The probability of success can be determined by the percentage of runs that achieve the optimal solution and will, much like the best approximation error, reflect the quality of the quantum hardware. This method however requires that the implementation can in fact find the optimal solution, rendering the previous method obsolete.

Performance scaling: With concerns as bounds on $p$ and scaling issues, it is important to give insight on how the benchmark performance scales for larger problem sizes. By determining the run-time for increasing problem size, the scaling performance can be reviewed. Similarly, it can be evaluated on how the accuracy or success probability decreases for larger problem sizes.

While this benchmark is focused on quantum hardware, it could be extended to quantum simulators, evaluating run-time and memory consumption. This could give valuable insight to developers to find the optimal simulator to work with.

6.1. Implementation

The implementation of the benchmark will require universality, in the sense that it should run on every quantum computer. The LibKet library is suited for this task and will be used to implement the benchmark. The benchmark will require multiple steps. Multiple problems need to be tested in order to show that the hardware is not optimized for a single problem. The problems that will be tested are:

- MaxCut problem (MCP)
optimization algorithms will be applied for increasing problem size to compare the run-time performance and accuracy. In Appendix C, a preliminary study of various classical optimizers was done. In this section, various promising classical optimizers and QAOA applications are presented. These problems have been chosen due to the effectiveness of QAOA on them, and their technological readiness level as explored in Section 5. These problems will then need to be tested for increasing problem size, until the quantum hardware is unable to find a solution. This could be either due to not having enough qubits, or having a too low chance of finding the optima (< 50%). The QAOA runs themselves will need multiple runs to determine the success rate and average run-time and accuracy. The solutions found by the QAOA optimization, need to be compared to a pre-computed answer using a classical exact algorithm. If the hardware supports larger circuit depth, the QAOA algorithm can be adjusted to a maximum \( p \). As theoretically the best found solution is always larger or equal to solutions found for smaller QAOA depth \( p \), a maximum value can be found when the found solution does not improve or diminishes. Diminishing of the solution indicates that no larger circuit depth is possible. This search to a maximum \( p \) can be included as an additional step for the benchmark to find the best accuracy of the QAOA implementation. The maximum circuit depth and width of quantum hardware will translate to maximum resources per available memory for a quantum simulator.

To give insight on \( |0\rangle \) bias, a trivial circuit can be run beforehand. The measurements will indicate if there is a bias. The implementation of QAOA will be done using a classical optimizer which is further explored in Section 7.1.

As the benchmark needs to be reproducible, the configuration of the problems must be predetermined. Akshay et al. [28] show that the performance of QAOA in terms of configurations is mainly due to the density (e.g. in a graph: the number of edges with respect to the number of vertices). As the benchmark needs to scale to an undefined problem size, the problems configurations cannot be hard-coded. In the proposed benchmark, the density will remain the same, to make the performance predetermined. This can for example be achieved by a bounded connectivity. Alternatively, a set of connections can be predetermined and a regular structure will be applied and scaled. This however is not necessarily representative of practical applications. The number of "shots" for a single QAOA iteration will range between 10 and 100, as these give the best results [43]. The number of iterations to achieve an estimation of the accuracy must be further analyzed. Expected is that the estimation will saturate towards a maximum reliability. A lower bound must be determined for this reliability. Determining the parameter \( p \) is also not trivial. There are arguments that the accuracy of QAOA will not grow for \( p > 2 \) [10], but others argue that e.g. a minimum of \( p \geq 8 \) is required for the MaxCut application to compete with classical approaches [24]. Determining \( p \), possibly dependent on the application will require further numerical analysis.

The outline for QPack is given schematically in Figure 3. Here an initial \( |0\rangle \) bias test is done, and the QAOA applications are run for increasing problem sizes. The benchmark will stop if for all applications the maximum problem size has been reached. The maximum is determined if a) not enough qubits are available, or b) the probability of finding the correct result falls below 50%. The cut-off limit of 50% has been chosen as below this threshold, re-iterating the algorithm will not produce better results. Some design choices can be made to make sure the benchmark is as complete as possible. First of all, the generation of problems can be done every iteration of the QAOA optimization. It would be fairest to create a new configuration of the problem, as certain configurations might be easier to optimize and might give an unfair advantage. This however will require longer computation times for the benchmark itself. The number of QAOA runs is also debatable. More runs will give a better average, but a limit must be set to limit the run-time. Another interesting addition would be adding both weighted and unweighted problems for the problems. This can show if the hardware is optimized with e.g. using parameter "sensitive" edges [44]. This solution would preferably be implemented by the benchmark, but requires too much information about the hardware, which should be abstracted. A quantum instruction compiler would be tasked to implement the qubit SWAPs required for this method. A further concern is that the benchmark should allow for parallelism. With the current size of quantum hardware, it is unlikely that this will be fully exploited in practice. However, as quantum hardware will scale up, there should be support to apply the parallelism. For the suggested Nelder-Mead classical optimization algorithm, a parallel variant has been developed [45,47]. This will allow the use of more quantum resources to compute smaller problems.

### 7. Measurements

In this section, measurements of the different classical optimizer options and the different QAOA implementations are presented. These measurements were done using Qiskit qasm simulator, to show relative performances of classical parameter optimizers and QAOA applications.

#### 7.1. Measurements of classical optimizers

In Appendix C a preliminary study of various classical optimizers was done. In this section, various promising classical optimization algorithms will be applied for increasing problem size to compare the run-time performance and accuracy.

- Traveling salesman problem (TSP)
- Dominating set problem (DSP)
Apart from Nelder-Mead and BFGS, which are both discussed in Appendix C, other optimization algorithms available in open-source libraries are presented as well. The list of tested optimizers is:

1) Local optimizers
   a) Nelder-Mead
   b) BFGS
   c) NEWUOA
   d) BOBYQA
   e) COBYLA

2) Global optimizers
   a) Dual annealing
   b) SHGO (simplicial homology global optimization)
   c) ISRES
   d) MLSL / MLSL LDS (Multi-Level Single-Linkage, low-discrepancy sequence)
   e) DIRECT (DIviding RECTangles)
   f) StoGO
These algorithms were implemented in Python using either SciPy or the NL-Opt library [48]. Some of these algorithms are not included in the following results, as either no convergence was found (due to various reasons) or if the optimization had such a long run-time that it cannot be considered a contender in comparison to other algorithms. The algorithms included in this list are:

- Dual annealing
- NEWUOA
- BOBYQA
- ISRES
- MLSL / MLSL_LDS
- DIRECT
- StoGO

Perhaps with different implementations, these algorithms could be used for QAOA optimization. In the case of dual annealing, it was clear that convergence could be found, but takes significantly longer than other tested optimization algorithms. The MLSL implementation suffers from searching for every local optima (which can be very significant with noisy QAOA results). A variant of MLSL might work for QAOA, but with the current implementation no convergence could be found in reasonable time.

![Figure 4. Data of run-time measurements fitted to exponential functions. Any number in the legend indicates the convergence tolerance, which is default if not indicated.](image)

The run-time measurements were done on MaxCut problems with 3 to 23 nodes, as above 20 nodes run times become very large and simulating many data points becomes too time-consuming. The QAOA algorithm is implemented using Qiskit for the Qasm simulator [49]. The MaxCut problems are randomly configured, but have the same number of edges as nodes to maintain the problem complexity. The results are shown in Figure 4. The data is fitted to an exponential function, as the obtained data shows a clear exponential growth. In this figure, it can be seen that the Nelder-Mead algorithms which was expected to perform best, is in fact the slowest from the selected algorithms in practice. SHGO, COBYLA and BOBYQA perform much better in terms of run-time, with SHGO being the fastest.

For the accuracy measurements, the different algorithms solve the same MaxCut problem for different sizes and the best expectation values are compared. Preferably, a fine grid search (brute force) is implemented to compare the results to, but this proved to be too time consuming to collect data, even for small problems. In Figure 5 the found expected values are compared to the value found by the Dual-Annealing algorithm. Dual-Annealing was chosen, since it was a slower global optimizer, but allowed for reasonable computing times and expecting that this would outperform the faster algorithms. The difference in accuracy is calculated as

\[
\text{relative accuracy} = \frac{\text{DA expectation value} - \text{tested algorithm expectation value}}{\text{DA expectation value}}
\]

The results however show that Dual-Annealing does always find better solutions and is often outperformed. The \(\beta\) and \(\gamma\) parameters are not compared, as different local minima might find values very close to the optimal value. The results show clearly that
COBYLA using randomized starting points outperforms other algorithms, indicating that a hybrid approach finds the best solutions. This, however, significantly increases the search time. For the single algorithm approaches, Nelder-Mead finds the best expectation values, presenting a trade-off between accuracy and time. It should be noted that for larger problem sizes, the expectation values are much closer and it is expected that for scaling purposes it is better to choose a faster algorithm such as COBYLA, BOBYQA or SHGO. Some parameters such as the number of the QAOA iterations or the convergence tolerance are not optimized as this is expected to give minimal change to the results with respect to the comparison.

Considering the found results in terms of accuracy and run-time, a hybrid approach could be applied. Heuristics such as random starting points combined with a local optimizer are often applied, to counter the local optimizer of getting trapped in local optima. Another implementation is the use of a (fast) global optimizer with a more accurate local optimizer. In the case of optimizer QAOA parameters, using a fast algorithm such as SHGO combined with e.g. Nelder-Mead or BFGS would be a good approach. This approach needs to be be investigated with respect to which global optimizer accuracy specification (which translates to run-time), will outperform random starting points for a similar run-time. Furthermore, many combinations are possible of both local and global optimizers. These combinations are worth examining to find better run-times for a set accuracy and vice versa.

7.2. Measurements of applications

A common downside of computer benchmarks is that hardware vendors are tempted to tailor their systems to excel in the particular benchmarks. We have therefore included multiple applications to the QPack benchmark. Next to the MaxCut problem (MCP), the dominating set problem (DSP) and the traveling salesman problem (TSP) have been included. In this section, the details on the QAOA implementation will be discussed, as well as the effect on the measured performance.

The MaxCut application has been examined in detail in Appendix A.1.1. The QAOA implementation requires the following gates for $n$ vertices and $m$ edges(or clauses) and $p$ QAOA iterations:

| Gate type | # gates |
|-----------|---------|
| Hadamard  | $n$     |
| CNOT      | $2m \cdot p$ |
| RZ        | $m \cdot p$ |
| RX        | $n \cdot p$ |

From the applications explored, MaxCut QAOA requires the least gates and is therefore expected to run best on NISQ era devices. MaxCut will result in the smallest circuit depth and does not require additional ancilla qubits.
The QAOA for DSP is implemented according to the algorithm provided by Nicholas Guerrero [36]. This implementation uses logical OR gates, which can be implemented using CNOT gates and ancilla qubits. The number of required ancillas and CNOT per logical OR depends on the number of input qubits $k$. The number of required ancillas is $k-1$. The implementation by Guerrero uses the logical OR to control a RY gate. This OR-controlled RY gate requires one additional ancilla as target qubit. As the ancillas can be re-used, the ancillas per circuit add up to $k$ ancillas, with $2 \leq k \leq n$. The logical 2-OR uses 3 CNOT gates, as depicted in Figure 6. These 2-OR gates can be combined to a $n$-input logical OR. For $n$ inputs, this $n$-OR is implemented as:

```python
qc = QuantumCircuit(2*n)
qc.append(ORGate, [0, 1, n])
for i in range(2, n):
    qc.append(ORGate, [i, n+i-2, n+i-1])
qc.crx(gamma, 2*n-2, 2*n-1)
for i in range(n, 2, -1):
    qc.append(ORGate, [n-i-1, 2*n-2-i, 2*n-1-i])
qc.append(ORGate, [0, 1, n])
```

![Figure 6. Implementation of a 2-input logical OR using CNOT gates.](image)

The circuit can be implemented using the following resources (at most):

| Gate Type | # Gates |
|-----------|---------|
| Hadamard  | $n$     |
| X         | $2m \cdot p$ |
| CNOT      | $(6n - 5) \cdot m \cdot p$ |
| RZ        | $m \cdot p$ |
| RX        | $n \cdot p$ |

$n$ qubits are initialised in superposition, using $n$ Hadamard gates. Inverted controlled RZ-gates and OR-controlled RZ-gates are used to implement the $m$ clauses [36]. The $n$ RX gates are then applied to the $n$ qubits. Excluding the initialization, this is repeated for $p$ iterations.

The DSP QAOA implementation uses similar, but significantly more resources than the MCP implementation. The DSP implementation uses $(6n - 7) \cdot m \cdot p$ more CNOT gates and $2n \cdot p$ additional Pauli-X gates. This requires quantum computers to support larger circuit depth, but also more ancilla qubits and better CNOT mapping. The additional CNOT requirement will reflect the qubit connectivity of the quantum hardware implementation, as well as the handling of qubit SWAPS (if required) by the hardware scheduler.

The TSP QAOA implementation is a much more demanding quantum algorithm and with the current implementation also uses different resources. The implementation is done according to this github blog: [https://lucaman99.github.io/new_blog/2020/mar16.html][50], which is one of the few examples of a clear implementation. The author however indicates that the state preparation is suboptimal and is therefore altered to suit the algorithm better. The TSP algorithm, as other QAOA algorithm, consists of a state preparation, a mixer Hamiltonian and a cost Hamiltonian. Whereas the MCP and DSP QAOA need $n$ to $2n$ qubits for $n$ vertices, this implementation uses $n^2$ qubits. Other variations exist, such as presented by Ruan et al. [51], using $m$ qubits, which is at most $n(n - 1)/2$ qubits for a fully connected graph. This implementation will be considered a future improvement. This however means that the current implementation requires significantly more qubits compared to MCP and DSP.
For the state preparation $n$ binary strings of length $n$ are required with a Hamming weight of 2. The superposition of all possible strings with a set Hamming weight is called a Dicke state \[52\]. In the TSP implementation a Dicke state preparation is applied on each row of $n$ qubits for Hamming weight 2, using the implementation by Bärtchi and Eidenbenz \[53\]. The cost and mixer Hamiltonian are left unchanged. Considering the significant cost of both the Dicke state preparation and the QAOA cycles, it worth mentioning the costs separately. The gate counts are provided in the following tables:

| Dicke State Preparation Cost | TSP QAOA cycles Cost |
|-----------------------------|----------------------|
| **Gate type** | **# gates** | **Gate type** | **# gates** |
| Hadamard | $8n(n - 2)$ | RZ | $n^2 \cdot p$ |
| $T/T^\dagger$ | $49n(n - 2)$ | RZZ | $\frac{n^2 + n}{2} \cdot p$ |
| CNOT | $(31n - 28)n$ | RXX | $2n \cdot p$ |
| RY | $(6n - 10)n$ | RYY | $2n \cdot p$ |
| X | $2n$ |           |         |

This shows that while not only the circuit cost is significantly higher, many different gates are used. This will avoid fine tuning of quantum computers on solely Hademard, CNOT, RX and RZ Gates. To compare the impact of the different
applications, a run-time comparison was done. The applications are implemented using the SHGO classical optimizer. The results in Figures 7 and 8 show that the run-time corresponds to the increase of circuit depth and required qubits as expected. Note that Figures 7 and 8 do not show large problem sizes for DSP and TSP as the larger problem sizes result in simulator memory issues. Despite the smaller data range, the difference in run-times can be clearly distinguished.

8. Conclusion and future developments

In this paper, the theoretical background on QAOA has been explored to set a basic understanding of how the algorithm operates and what the trade-offs are. Increasing accuracy by increasing $p$ requires longer run-time and is required for larger problems. The performance is also determined by the clause density and makes the performance problem dependent. State of the art development of the QAOA algorithm in practice is shown to be advancing, with a wide variety of algorithms shown for different, but similar problems. While these NP-hard problems are similar, it has been shown that QAOA is not well suited for every problem [54]. In some cases, such as the Ising problem, current classical approximations are expected to perform better and alternatives like the quantum adiabatic algorithm might be a better fit. For most of the problems discussed, the QAOA algorithm appears to be a good solution, with applications even reaching a full-stack application. The development of each implementation has been evaluated according to a TLR fitted for quantum algorithms. In this evaluation it is shown that most applications have at least been developed to the point that the algorithm has been simulated on a quantum simulator to show the capability of the implementations. In the case of the packing, MCP, DSP and TSP applications, a proper resource and performance analysis has been done. The implementation of TSP by Sarkar et al. [30] is currently the only implementation to have reached the level of a full stack development. This implementation also shows that current NISQ technology cannot properly support QAOA algorithms for practical implementation. Either advances on quantum hardware must be made, or more resilient implementations of QAOA must be developed.

Using this assessment, the MCP, DSP and TSP applications have been selected to be included in the presented benchmark. Furthermore, a theoretical and numerical analysis is done on classical optimizers to find the implementation to best suit the QAOA algorithm. The results show that a clear trade-off exists between run-time and accuracy. A possible hybrid implementation using both a fast global optimizer and an accurate local optimizer might provide an optimal implementation, but needs further analysis.

A proposal for QPack, a benchmark using the QAOA applications is presented, with critical quantum benchmark requirements in mind [1, 2]. This benchmark will explore run-time and accuracy for available NISQ era quantum computers, using various applications. The benchmark will reflect the resources available, the implemented optimizations and the bottlenecks in the architectural implementation. The latter can specify the run-time on the quantum hardware, the classical hardware and the communication between both.

In future work, the benchmark can be further tailored for a proper implementation. We are currently working on a reference implementation of the QPack benchmark in LibKet [42], to ensure that the benchmark will run on all major publicly available quantum computers. The initial version is expected to be presented as open-source in Q3 of 2021. The implementation in C++ will also allow for better performance measurements for both run-time and memory consumption. Fine-tuning of the applications is also required, as a trade-off can be made between accuracy in run-time and precision when choosing the classical (hybrid) optimizer and the QAOA depth $p$. Finding the minimal requirements for the QAOA application to compete with classical approaches will need further examination. Furthermore, the QAOA applications currently implemented are not optimal in terms of resources and can be further improved upon as mentioned in section 7.2 Finally, support for parallel processing is desired. As classical optimizers such as Nelder-Mead Simplex can be run in parallel [43-47], more objective functions need to run in parallel. If the quantum hardware can support a multiple of the qubits required by the objective function, such a parallel implementation can be supported. With current quantum hardware sizes, such implementations are not yet of importance, as practical problem sizes do not fit on the current hardware [55]. As the quantum hardware scales further, this parallelism can result in significant speedup.

The QPack benchmark aims to expand its repertoire of algorithms in the future, as applications based on Shor's and Grover's algorithm [56] will become implementable on quantum computers. Currently, the quantum hardware cannot support these algorithms as more qubits and larger circuit depths are required. As more applications become practical on quantum computers, the QPack benchmark is envisioned to grow correspondingly to set the standard as a practical quantum algorithm benchmark.

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Appendix A.

General optimization problems

The general optimization problems discussed in this section will be the combinatorial satisfaction problems (CSP) max-
kSAT and max-kXOR. Here, k denotes the exact number of variables contained in a clause. The special cases of CSP will be discussed: the one with typicality and the MaxCut problem. These problems represent general applications from which other practical applications can be derived. These practical applications are discussed in further detail in Appendix B to determine which optimization problem solutions are most developed and suited for the benchmark.

A.1. Max-kSAT and max-kXOR

In max-kSAT the objective function needs to be maximized, as discussed in section 3. Max-kSAT is the general set of problems where the number of Boolean constraints satisfied is maximized. Individual constraints can have their own weight. Giving a weight to constraints can be beneficial for certain problems. For now the unweighted problems are examined, i.e. weight = 1. There exist problems where not all constraints can be satisfied. In these cases the maximum number of constraints, but not all need to be satisfied. The problem can take form of any constraint that applies to k parameters.
Currently, the most common max-$k$SAT problem discussed, is the max-$k$XOR. For this variant of max-$k$SAT problems, the objective function is defined as [23]:

$$C = \frac{1}{2} \pm \frac{1}{2} \prod_{i=1}^{k} x_i$$

(17)

A.1.1. MaxCut. This is by far the most discussed problem with regard to QAOA [12, 18, 23, 24, 29, 43, 55]. The MaxCut problem is a max-2XOR problem, that can be visually represented as a graph. The individual parameters are presented as vertices, while the clauses can be represented as edges. The objective of MaxCut is to find as may edges $j_k$ as possible, where $j = (1 - k)$. A visualization is shown in Figure 9.

MaxCut is a known NP-complete problem and therefore serves as a good example of what can be accomplished with QAOA [58, 59]. The performance of MaxCut can be increased with pre-processing. If the input graph has a regular shape, e.g. with a bounded degree, the graph can be divided into sub-graphs that occur multiple times. This way, only the unique graphs need to be analyzed, and their expectation value multiplied with their corresponding occurrence [18]. An example is the 3-regular graph, which only has 2 possible sub-graphs, as shown in Figure 10. With pre-processing, only the occurrence of the different sub-graphs need to be found, and the QAOA needs to find the expectation value of the 2 possible graphs. This however implies that the classic algorithm needs to find the occurrences of the sub-graphs with high performance. How this carries over to practical applications is not yet explored, and will be very application dependent. A mayor concern is that finding the subgraphs, known as the clique problem, is in itself one of Karp's NP-complete problems [55].

MaxCut can be applied to challenges as circuit layout design [60], data clustering [61], network design and statistical physics [62]. This shows that MaxCut can be applied in a large variety of industry level optimization problems.

A.1.2. Typicality. A CSP is considered typical if [23]

$$\mathbb{E}_{\psi}[\psi(x) - \psi(\emptyset)] = \sum_i P(\psi_i)(\psi_i(x) - \hat{\psi}_i(\emptyset)) = 0, \quad \psi_i \in \Psi$$

(18)

where $P$ denotes the probability distribution for a constraint, with $\sum_i P(\psi_i, l) = 1$ where $l$ is the $l$th constraint. Applying the Fourier transformation on $\hat{\psi}(x)$ gives:

$$\mathbb{E}_{\psi}[\hat{\psi}(K)] = 0 \quad \forall K \neq \emptyset$$

(19)
This means that the Fourier coefficients associated with $P(\psi)$ have 0 mean. Note that the MaxCut problem does not have typicality. Typicality is interesting in CSP, as this leads to analytical derivation of the satisfaction ratio for this set of problems. Lin et al. have proven that for every CSP with a bounded degree and typicality, a satisfaction ratio of $\mu + \Omega(1/\sqrt{D})$ can be found with a probability of $1 - O(D^2/m)$ [23]. Here the maximum number of constrains in which a variable occurs is $D$. The number of variables per constraint is constant, as the CSP has a bounded degree. With this probability, a high success rate can be achieved for $m \gg D$.

Appendix B.
Overview of NP-Hard problems with QAOA implementations

B.1. MaxCut

The details of the MaxCut problem have been discussed in detail in Appendix A.1.1. The optimization can be applied for circuit layout design [63], Data clustering [61] or implementing the Ising model. The MaxCut problem for QAOA has been studied extensively [23, 24, 29, 43]. It has been shown that the approximation of QAOA achieves better results than the classical Goemans-Williamson [64] for $p \geq 8$ [24]. For the general MaxCut algorithm, the gates required are $O(N^2P)$ and can be run in $O(NP)$ assuming $O(N)$ gates can be run in parallel. The classical Goemans-Williamson algorithm, in contrasts, requires a run time of $O(Nm)$ for $m$ edges [24].

B.2. Ising model

The Ising model can be approximated by the MaxCut algorithm [65]. Implementations for the Ising model can be found in physics for simulation of e.g. phase separation, lattice-based liquid-gas model or spin glasses. Applications for this model can also be found in biology for the protein folding problem [34]. The model is also supported in Qiskit [66], alongside the popular MaxCut algorithm. The Ising model has in recent publishing been compared for both classical and QAOA algorithms [67]. It becomes apparent that for large clause density, QAOA shows reachability deficits [28] and is therefore no improvement on the classical algorithms. For a large enough search space, the QAOA algorithm can reach a Grover scaling of $O(\sqrt{N})$.

B.3. Set packing

In the set packing problem a set of subsets is given. A minimal selection of the subsets must be chosen to cover all elements of the set [35]. A visual representation of this problem is shown in Figure 11.

This problem is also covered by Ruan et al. by adjusting the Hamming distance to $d(x, x') = 1$. The complexity achieved with their method is $O(n)$ for $n$ subsets.

B.4. Vertex cover

In the vertex cover, all edges of a graph $(V, E)$ must be covered by selecting the minimum amount of nodes. This problem is implemented by Ruan et al. with an alteration on the previous method [33]. The vertex cover problem has implementations in, e.g., monitoring. Examples are security camera placement or network link monitoring.
B.5. Dominating set problem

The dominating set problem is very similar to the vertex covering problem, but instead of covering edges, there must be an edge to each vertex from a vertex from the selected set. The applications of both problems are very similar as well. An implementation of QAOA and an analysis of the algorithm is presented by Nicholas Guerrero [36]. In the circuit presented, for \( n \) vertices the following is required [36]:

- \( 18n^2 - 6n \) single qubit gates
- \( 16n^2 - 12n \) controlled Pauli-X gates
- \( 2n \) qubits (of which \( n \) are ancillary)

B.6. Traveling salesman problem

The traveling salesman problem is a well known problem where a salesman needs to visit all cities (vertices) which are connected by roads (weighted edges). A special case of the problem, the undirected Hamiltonian circuit, is also one of Karps’s 21 problems. A (naive) classical approach would check all routes and would have a complexity of \( O(n!) \) [68]. An implementation based on Grover’s algorithm has shown a quadratic speedup to \( O(\sqrt{(n!)})) \) [68], but such an implementation would require a lot of quantum resources and would currently not be applicable to quantum hardware. A QAOA solution has been presented by Radzihovsky et al. [69] and by Henry and Dudas [70]. The respective source codes for implementation on a Rigetti (pyquil and the Rigetti QVM) quantum computer are available at [https://github.com/murphyjm/cs269q_radzihovsky_murphy_swofford][69] and [https://github.com/danielhenry1/QAOA_TSP][70]. Radzihovsky et al. show that the number of gates in the cost Hamiltonian scales with \( n^2 \) for \( n \) cities, and a circuit depth of \( 2n \) for even \( n \) and \( 2(n - 1) \) for uneven \( n \). Ruen et al. also published an implementation using \( n^2 \) qubits. The traveling salesman problem has a large range of applications, such as computer wiring, drilling PCB and order-picking in warehouses [71]. A recent implementation of QAOA on the traveling salesman problem is presented by Sarkar et al. [30]. In this implementation, the QAOA is applied for quantum accelerated de Novo DNA sequence reconstruction. An application and QAOA simulation are presented, but does not feature a hardware implementation as the currently available quantum hardware are not sufficient to support meaningful results [30].

B.7. Tail assignment problem

The tail assignment problem deals with the scheduling of a set of flights to a set of aircraft to create a feasible flight schedule, while keeping the lowest cost. This problem is an optimization of a packing problem with additional constraints. Vikstal et al. propose an implementation of QAOA for this problem [37]. In their publication, they show that for \( p = 2 \), 99.9% can be achieved, but requires 74 measurements for 25 route instances. This case performs better than quantum annealing. Using more measurements instead of increasing \( p \) is computationally less expensive.

B.8. Facility placement problem

The facility placement problem aims to place a node (facility) with the least transportation cost (this in itself is a Weber problem [72]), while considering other constraints. A QAOA implementation is presented by Quiñones and Junqueira [38]. This paper, however, shows that the QAOA implementation has a much higher cost and lower optimal solution probability than a VQE for the investigated case. This might indicate that this type of problem is not suited for QAOA.

B.9. QAOA for Grover’s algorithm

An interesting approach has been presented in [39], where the principals of QAOA have been applied to Grover’s algorithm. Much like the implementations discussed before, it uses \( p \) iterations to improve fidelity/accuracy. This implementation could potentially make the algorithm that is proven to perform better than classical algorithms (quadratic speed-up), executable on relatively few qubits. This would allow it to run on near-future devices. Some critical issues however exist with this implementation. QAOA has limited accuracy, while Grover’s algorithm can only be applied practically (e.g. database searching) if an exact solution can be found. The authors mitigate this problem by checking with multiple rounds whether the found solution is correct. This might require the algorithm to run for many iterations before the solution is found. Furthermore, the chance of success of the algorithm is only 50%, making it impractical for implementation. Error-correction schemes might make this implementation worthwhile, but it is unclear whether such a solution can be found. Quantum error correction in adiabatic models is still a challenge [73], but could make this application implementable.
Appendix C.
Parameter optimization

This section explores the strategies to optimally determine the $\beta$ and $\gamma$ parameters. The optimization of these parameters is considered to be the main bottleneck of QAOA [30], and the selection of the optimizer could make or break the application. This single objective real-parameter optimization is done classically and many algorithms have been developed for this problem. Critical parameters for choosing the classical optimization are:

- Number of parameters
- Problem size
- Smoothness of the objective function
- Local optima

C.1. Gradient-based optimization

Gradient-based optimization uses the gradient of the problem function to find a (local) optimal. Gradient-based optimizers converge generally faster than gradient-free ones and would therefore be favorable [74]. However, gradient-based optimization only works well on smooth functions and is prone to getting stuck in local optima. Due to the dependency on smooth functions, any function that is either discontinuous or noisy will cause problems for the optimization. In the case that a smooth function is available, the problem of local minima could be averted by choosing multiple starting points and running the optimization multiple times or in parallel if possible. This, however, increases the computational complexity and choosing an efficient algorithm for the starting value is not trivial. Often random points are chosen, but a more efficient algorithm based on the Discrete Fourier Transform (DFT) is presented by [43] but is not open-source.

C.2. Gradient-free algorithms

Gradient-free algorithms do not depend on a gradient of the function, as the name suggests. This means that these algorithms can be applied to objective functions that are noisy, discrete or discontinuous [75]. Gradient-free can be more resilient with respect to local minima, depending on the algorithm. The downside of these algorithms is that these generally take more computation time or more iterations.

C.3. Problem instances

The objective function is evaluated with the above mentioned critical aspects, in order to find the optimization algorithm that fits best. The objective functions are considered in general and not per individual problem. The reason for this will become apparent in the evaluation.

**Number of parameters**: For all problems, the number of parameters are 2: $\beta$ and $\gamma$. Optionally, $p$ can be taken as a parameter as well, but since publications show that QAOA is most effective in low depth, i.e. low $p$, this parameter will not contribute significantly. Generally a value for $p$ is chosen beforehand (e.g. Crooks [24] shows that $p \geq 8$ is required to outperform the Goemans-Williamson algorithm) after which $\beta$ and $\gamma$ are optimized. Theoretically, an optimizer would increase $p$ to infinite as this would give the best results. In practice, $p$ can be included as well, as performance is likely to decrease with higher circuit depth on quantum hardware.

**Problem size**: The problem size is expected to grow very large, as scalability needs to be considered. This does not differ per problem type.

**Smoothness of objective function**: The smoothness of the objective function is expected to differ per problem type. However, due to the probabilistic nature of the results, as well as noise in quantum hardware, the objective function is never smooth in practice.

**Local optima**: The presence of local optima is dependent on each individual problem, but due to noise in quantum hardware, local optima might still occur. Local optima might not be as strong as local minima inherent to the objective function. This could give room to optimizers that have some trouble escaping from strong local optima.

C.4. Selection of optimizer

Considering how all QAOA problem instances will suffer from noise, discontinuities and local optima, no gradient-based optimizer can be applied. From the gradient-free algorithms the following are considered:

**Nelder-Mead Simplex**: Nelder-mead is efficient for non-smooth objective functions. It is however not very efficient for 10 or more design variables. Considering that only 2 variables are optimized, the Nelder-Mead optimizer fits well.
Nelder-Mead is also more resilient with regard to local optima compared to other local optimizers.

**Genetic Algorithms:** Genetic algorithms generally require large number of function evaluations, but is applicable to multi-objective optimizations. Genetic algorithms are not well suited, since QAOA problems only have one objective function. The large number of iterations are therefore inefficient.

**Simulated Annealing (SA):** Simulated annealing has more freedom than other gradient-free optimization algorithms, but comparison to other algorithms shows that the computation per iteration of SA is less efficient. Alternatively, SA could be accelerated with VQE, but the performance is not yet adequately explored and will be more demanding of the quantum hardware. Potentially, this could be used in the future when quantum hardware is more mature and scalable.

**Particle swarm optimization (PSO):** Particle swarm optimization can converge fast, has a short computational time and has very few parameters to adjust. The downsize is that it is prone to get trapped in local optima, especially with complex problems [76]. Since large problem instances need to be considered with regards to scalability, PSO might not be suited for QAOA. PSO could be considered for problem instances with no inherent local optima (i.e. local optima due to noise). Unfortunately, it could be difficult to tune initial parameters for PSO. Considering that QAOA should be applied to multiple different problems, tuning the parameters could create a bottleneck. PSO could be considered an option for similar problems and a custom PSO parameterization. A custom PSO could be considered for the Ising model, with seemingly no inherent local optima [77], but not for the more popular and more developed MaxCut [13].

**Symmetric Rank-1 Update Method (SR1):** The SR1 method is not a gradient-free algorithm, but is included for special cases. SR1 uses a first-order derivative, as opposed to a second-order derivative like the Newton method. This means that the smoothness requirement on the objective function is less strict. In the case that the hardware has sufficiently low noise and multiple measurements per iteration are performed, the SR1 method might be applicable. The main difficulty, is that it is subjective to how smooth an objective function needs to be for SR1 to perform well, as no clear comparison is done between noise levels in objective functions and performance of the algorithm. It would also require the objective function to be evaluated, meaning it would be unclear per implementation if the algorithm works well. Quasi-Newton methods such as SR1 and BFGS only work for finding local minima. This means that if multiple local minima exist in the solution landscape, the global minima might not be found. With this in mind, SR1 can only be applied to objective functions with only one minimum and would require extensive evaluation of the objective function. Another Quasi-Newton method that is commonly used is the BFGS algorithm, but as long as the problem field has a limit constraint (in this case $\gamma, \beta \in [0, 2\pi]$), SR1 converges faster.

More state-of-the-art algorithms exist, as competitions in the field of single objective real-parameters optimization are organized by IEEE yearly (CEC Real-Parameter Optimization Competitions) but since the winning algorithms have not been found as either open-source or a library, the winning algorithms are not considered for application. Regardless, the best algorithm for low dimensions was found to be UMOEA [78].

From the evaluated optimizers, Nelder-Mead is considered the best fit for QAOA. Numerical comparison of classical optimizers [79] show that in terms of performance, BFGS and Nelder-Mead differ very little in run-time and find identical results in sufficiently smooth functions. This raises the argument that if the objective function is sufficiently smooth, Nelder-Mead could be used as well and no custom optimizer needs to be applied. This saves development time for the application. PSO or SR1 could be considered only for very special cases. For the general case, UMOEA could be implemented to possibly further improve performance.