To quantum or not to quantum: towards algorithm selection in near-term quantum optimization

Charles Moussa,¹Henri Calandra,² and Vedran Dunjko¹

¹LIACS, Leiden University, Niels Bohrweg 1, 2333 CA Leiden, Netherlands
²TOTAL SA, Courbevoie, France

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The Quantum Approximate Optimization Algorithm (QAOA) constitutes one of the often mentioned candidates expected to yield a quantum boost in the era of near-term quantum computing. In practice, quantum optimization will have to compete with cheaper classical heuristic methods, which have the advantage of decades of empirical domain-specific enhancements. Consequently, to achieve optimal performance we will face the issue of algorithm selection, well-studied in practical computing. Here we introduce this problem to the quantum optimization domain.

Specifically, we study the problem of detecting those problem instances of where QAOA is most likely to yield an advantage over a conventional algorithm. As our case study, we compare QAOA against the well-understood approximation algorithm of Goemans and Williamson (GW) on the Max-Cut problem. As exactly predicting the performance of algorithms can be intractable, we utilize machine learning to identify when to resort to the quantum algorithm. We achieve cross-validated accuracy well over 96%, which would yield a substantial practical advantage. In the process, we highlight a number of features of instances rendering them better suited for QAOA. While we work with simulated idealised algorithms, the flexibility of ML methods we employed provides confidence that our methods will be equally applicable to broader classes of classical heuristics, and to QAOA running on real-world noisy devices.

I. INTRODUCTION

Quantum computing in the near-to-mid term – the so-called NISQ era [20] – is likely to be limited in many ways, including size (qubit numbers), gate fidelities, architecture (qubit connectivity) and qubit life-times (coherence times). Consequently, much effort is dedicated to the development of algorithms that can work around some of these constraints. Approaches based on parameterized quantum circuits – such as variational quantum eigensolvers [22], the quantum approximate optimization algorithm (QAOA) [10], and some flavours of quantum machine learning [4], stand out as some of the most likely NISQ-suited algorithm families. They are suitable in part because the quantum computational depth, dictating required coherence times, can be treated as a tunable “hyper-parameter”, and made to fit the device constraints. In this work, we specifically focus on the QAOA algorithm, which consists of a quantum circuit of a user-specified depth $d$, inducing $2p$ QAOA parameters which are tweaked to solve a combinatorial optimization problem. QAOA is interesting from the perspectives of approximation, and heuristic optimization.

Approximation with QAOA - Initially, the QAOA algorithm was designed as an approximation algorithm, i.e., an algorithm intended to provide an efficient, but approximate solution to an otherwise intractable problem. Approximation algorithms differ from heuristic methods in that they provide mathematically provable a-priori guarantees on the quality of the solution, whereas heuristics utilize expert knowledge, and domain-specific operators to achieve good performance in practice, with less concern regarding theoretical worst case bounds. For instance, one of the most natural applications of the QAOA algorithm is to solve so called MaxCut problems, where the task is to identify a bipartition of a given graph, which maximizes the number of edges (the cut) crossing the two sets. Finding the actual maximum of the cut $C_{\text{max}}$ is NP-hard [1] but the problem allows non-trivial polynomial-time approximation. The best known classical approximation algorithm, of Goemans and Williamson (GW) [12], guarantees an approximation ratio of $\alpha \approx 0.878$ (referred to as the GW bound). In the case of randomized algorithms like GW, this means that the value of the output cut is at least $\alpha C_{\text{max}}$ with high probability. Under which conditions better efficient approximations can be achieved is a hard open question, and depends on details. For instance, it is known that achieving an approximation ratio above $16/17 \approx 0.94$ for general graphs is NP-hard [13] (so as hard as finding the exact solution), and it is possible that the actual NP-hard bound may be $\alpha$. For more special graphs the GW can do better, e.g. for 3-regular graphs, the ratio of 0.932 is achieved. To use QAOA for optimization, a critical step is finding the optimal classical circuit parameters for a given depth. For a constant depth, this can be done in polynomial time, yielding a poly-time approximation algorithm [2]. The question of whether QAOA can improve over GW for any constant depth was open for a number of years, and has been resolved very recently, in the negative [6]. However, already at depth $d = 1$ it achieves the ratio of 0.6924. While falling short of the GW bound, this is a highly non-trivial result, as prior to GW, the best algorithms achieved only $1/2 + O(1/k)$ even after decades of efforts. This makes QAOA an interesting algorithm, and allows the possibility that QAOA performs better than

¹ Technically, the decision variant of the problem, deciding whether the cut is larger than some integer $k$, is NP-complete.
² Without constant depth limits, it is known that QAOA can achieve exact solutions, but the classical parameter optimization then can take exponential time.
³ In other words, the achieved approximation ratio is below $1/2 + \varepsilon$ for any constant $\varepsilon > 0$. 
GW (or some other classical algorithm) on some classes of instances. Setting the theoretical approximation aspects aside, this suggests the substantial practical potential of QAOA as a heuristic optimizer.

**Heuristic optimization with QAOA** - The above-mentioned theoretical results motivate studying how to best use QAOA for practical optimization problems via numerical (and real-device) experiments. As mentioned previously, to actually use QAOA one needs to find the optimal classical parameters. Although finding exact optima for any constant depth can be done in polynomial time \[10\], the actual overheads are prohibitive, requiring billions of evaluations already for small graphs and depth in low single digits. Almost as much research has been dedicated to developing heuristics and analytical techniques to find good circuit parameter values for QAOA \[5, 27, 29, 31\], as has been to actual evaluation of the performance of QAOA \[8\]. This is justified as any evaluation of QAOA will be in part limited by the limitations of the classical optimizer. The early studies are promising, showing, e.g., that QAOA with depth \(p = 8\) significantly outperforms GW on a set of Erdős-Rényi random graphs (with edge probability 0.5) \[8\]. A somewhat related theoretical study identifies that there exist instances where QAOA will outperform quantum and simulated annealing methods \[28\].

Perhaps the first main issue with QAOA is that many open questions still remain, e.g., regarding the comparison of QAOA with other heuristic optimization methods, on other graphs, with different optimizers, and with varying levels of experimental (or simulated) noise – in part as simulating, or actually running it on a real device QAOA is computationally costly, for larger graphs, preventing large-scale analyses. We note that the issue of noise was addressed e.g. in \[1, 13, 30\].

The second issue is more subtle and pertains to the importance of predicting when to use QAOA, on an instance-to-instance basis (on a more practical importance). Note that despite these early successes of QAOA on, realistically speaking, very small instances, QAOA cannot beat even the bare GW algorithm on all instances at any constant depth \[6, 16\]. This holds even when assuming ideal parameters and zero noise. We note that this result was not unexpected, as previously known results imply that, under the so-called unique games conjecture (UGC \[17, 18\]), QAOA could not beat GW unless BQP contains NP.

QAOA should thus not be expected to universally win even against GW, let alone all standard heuristic methods, optimized for certain classes of problems. Further, given the expected substantially higher expenses of running actual quantum hardware, in practice we will need to leverage this additional cost against the actual improvement (potentially) offered by QAOA over less costly classical algorithms. Thus one should tackle the challenge of algorithm selection in quantum optimization, which in the classical realm is mostly concerned with using the fastest algorithm for a given instance \[19\]. As we clarify presently, detecting which instances are “quantum-suitable” is likely itself a hard problem, requiring a heuristic treatment.

**Contributions** - In this work we contribute to these two issues, as follows:

- we compare the performance of QAOA with GW on a different family of graphs, namely 4-regular graphs;
- we specify two pragmatically motivated criteria specifying when QAOA should be used over GW;
- we design a machine learning model which achieves over 96% and over 82% balanced accuracy in predicting which MaxCut instances satisfy the above criteria, respectively, which can be used for algorithm selection;
- we highlight a number of graph properties which are strongly correlated with a QAOA advantage, which may help guide further theoretical analyses.

The structure of the paper is as follows. Section II provides the necessary background on GW and QAOA. In section III we detail the simulation performed, comparing QAOA and GW, and which we used to fix the criteria when one algorithm should be chosen over another, and to generate the datasets needed for machine-learning-based algorithm selection. In section IV we describe the algorithm selection model, and discuss the critical features (characteristics) of MaxCut instances which influence which algorithm does better. We conclude our paper with a discussion in section V.

### II. BACKGROUND

The MaxCut problem is one of the famous 21 NP-complete problems identified by Karp, and it naturally occurs in computer science and physics. Consider a graph \(G\) over a vertex set \(V\), and edge set \(E\), with \(N\) vertices. The problem is to find a subset \(S \subseteq V\) such that the number of edges between \(S\) and \(V \setminus S\) is maximized. The set of edges between \(S\) and \(V \setminus S\) is called a cut, and we will denote the size of the maximal cut with \(C_{\text{max}}\). The problem naturally extends to weighted graphs, where the objective is to maximize the total weight of the edges of the cut. A common phrasing of the MaxCut problem is as follows. Let \(w_{ij}\) be the weight associated to the edge \((i, j) \in E\) (1 in the case of an unweighted graph), then the MaxCut problem is to identify the bitstring \(z = (z_1, \ldots, z_N) \in \{-1, 1\}^N\) where \(z_i = 1 \iff i \in S\) maximizing the cost function

\[
C(z) = \sum_{(i,j) \in E} w_{ij}(1 - z_i z_j)/2. \tag{1}
\]

This quadratic binary optimization (QUBO) formulation connects the MaxCut problem with the task of finding ground states of classical spin Hamiltonians. As phrased, the MaxCut problem is to identify the set \(S(z) = \{i | z_i = 1\}\) s.t. \(C(z) = C_{\text{max}}\), but, even the problem of identifying the cut size (distinguishing the \(\text{max}\) versus the \(\text{argmax}\) problem for \(C(z)\)) is computationally difficult. The MaxCut problem is in the APX class \[24\], the set of NP optimization problems that allow polynomial-time approximation algorithms with approximation ratio bounded by a constant).
A. Goemans-Williamson Algorithm for MaxCut

The best classical approximation algorithm for MaxCut is that of Goemans and Williamson [12] (GW). It is based on solving a related relaxation of the problem – intuitively, we solve an optimization problem in the continuous domain \([-1, 1]^N\) as a semi-definite program, giving a real-valued solution with the associated cost \(C_{\gamma,\beta}\). Then a sampling process which depends on the probabilities specified by the entries in the real-valued solution (a random projection routine) generates a feasible bitstring solution. Note that the cost of the found bitstring is upper bounded by \(C_{\gamma,\beta}\), and in fact it can happen that \(C_{\gamma,\beta} < C_{\gamma,\beta}\).

Nonetheless, the expected value attained by the cost function using this procedure is provably lower bounded by \(\alpha C_{\max}\) with \(\alpha \approx 0.878\), for all input graphs - in other words, it is an \(\alpha\)-approximation algorithm.

While better approximation bounds are possible for special graphs (e.g., for 3-regular graphs [15], or for graphs with large cuts [12]), assuming the UGC [17], GW provides the best possible polynomial-time approximation, unless \(\mathbb{P} = \mathbb{NP}\).

B. Quantum Approximate Optimization Algorithm for MaxCut

The QAOA approach is inspired by adiabatic quantum computing, and as the first step, the classical cost function is encoded in a quantum Hamiltonian defined on \(N\) qubits by replacing each variable \(z_i\) in eq. [4] by the single-qubit operator \(\sigma_i^z\), and omitting the constant shift:

\[
H_C = \sum_{(i,j) \in E} \frac{w_{ij}}{2} \sigma_i^z \sigma_j^z, \tag{2}
\]

Note that this corresponds to a diagonal operator w.r.t. the computational basis, with \(\langle \psi | H_C | \psi \rangle = w - C(\psi)\), where \(w = \frac{1}{2} \sum_{(i,j) \in E} w_{ij}\) is half of the total weight of the graph. The second ingredient is the so-called mixer Hamiltonian \(H_B = \sum_{j=1}^N \sigma_j^x\) corresponding to the typical initial Hamiltonian in an adiabatic quantum computing protocol, whereas \(H_C\) corresponds to the target Hamiltonian, and the bitstring corresponding to the ground state of \(H_C\) also maximizes \(C(\psi)\).

Instead of resorting to an adiabatic method, in QAOA we implement the (time-independent) time-evolution interchanges using \(H_B\) and \(H_C\), yielding a quantum circuit of depth \(O(p)\) for constant-degree graphs, so critically independent of the graph size (see e.g. [14]). This circuit is then applied to a fixed initial state, generating:

\[
|\gamma, \beta\rangle = e^{-i\beta_1 H_B} e^{-i\gamma_1 H_C} \cdots e^{-i\beta_p H_B} e^{-i\gamma_1 H_C} |\psi\rangle \otimes N,
\]

defined by the 2p parameters \(\gamma_i, \beta_i, i = 1 \ldots p\) (corresponding to the number of times of evolution of the individual Hamiltonians). We will refer to these parameters also as the QAOA angles as they map onto the angles in parameterized gates of the corresponding quantum circuit.

Such a quantum state when measured yields a probability distribution over all possible bitstrings.\(^4\) The classical optimization challenge of QAOA is to identify the sequence of parameters \(\gamma\) and \(\beta\) so as to maximize the expected value of the cost function from the measurement outcome, i.e. the quantity \(r = F_p(\gamma, \beta) = w - \langle \gamma, \beta | H_C | \gamma, \beta \rangle\).

If we denote the optimal parameters maximizing \(F_p\) with \(\gamma^*, \beta^*\), the approximation ratio of QAOA achieved on the given instance is given by:

\[
r^* = \frac{F_p(\gamma^*, \beta^*)}{C_{\max}}. \tag{3}
\]

For this value to be computable, \(C_{\max}\) for the given graph must be known. Note that it is known that if \(p \to \infty\), then we have \(r^* \to 1\) [10]. This quantity – the expected achieved approximation ratio – is equally defined for the GW and for the QAOA algorithm, and we use it as our central figure of merit regarding the performance of the two algorithms on MaxCut instances. In the next section, we analyze the performance of both algorithms on a new domain – that of 4-regular graphs, complementing previous analyses done on 3-regular graphs and Erds-Renyi random graphs. The obtained dataset will be used to define reasonable criteria when to consider QAOA to have done “significantly better”, and also to train a machine learning classifier to predict this criterion.

III. PERFORMANCES ON 4-REGULAR GRAPHS

In order to systematically compare QAOA against other algorithms, certain choices regarding the QAOA set-up (hyperparameters), the problem test set, and regarding the exact notion of “better performance” need to be made.

Regarding the problem test set, as mentioned earlier, we chose to focus on 4-regular graphs, in part because they are relatively easy to generate, yet have not been considered in the literature in the context of comparison to GW.

Important choices to be made are regarding the QAOA algorithm details, specifically the depth of the circuit we will allow, and the optimizer used. The basis of our optimization is the Nelder-Mead (NM) algorithm, with some QAOA-specific tweaks, detailed shortly. NM is a common choice due to the relatively small dimensionality of the parameter space. For instance, NM was used in [19] to give a computational time cost for running QAOA against a classical heuristic. Perhaps the most important choice, the allowed circuit depth, is non-trivial. Note that it is known that if the circuit is deep enough, relative to the instance size, we will find true optima (given that the QAOA circuit parameters themselves are chosen optimally). The exact functional scaling of the depth required for this is not known, but as clarified, having the depth depend on the instance size would lead to intractable optimization demands regarding the QAOA parameters – and defeat the idea of NISQ-friendly constant-depth constructions. However, since we are bounded to relatively small instances due to the cost of quantum simulation, already depths 7-9 may allow us to achieve better performance than what is asymptotically possible for any constant depth\(^5\). On

\(^4\) In the limit of infinite depth, the distribution will converge to a distribution with full support in the optima.

\(^5\) More precisely, since QAOA finds the exact optimum in the
the other hand, keeping the depth too low may prevent any advantage in the upper range of the graph sizes and test-set sizes that we could tackle. To help us with the choice here, we analyzed the performance of QAOA on a range of depths, as described next.

Finally, this brings us to the choice of the appropriate definition of “better performance”. Relating to previous works, in [8] (although the objective was not to formally define such a criterion), an average improvement of the approximation ratio of 2% was considered a significant improvement. Our choice specified in the next section is also guided by the data acquisition stage, i.e., the performance analysis on our graph test sets.

A. Simulation methods

We built a set of randomly generated 4-regular graphs from where we varied the number of nodes $N = 11, \ldots, 24$, with 20 instances generated per size, i.e., in total 280 instances. For each graph, the $C_{\text{max}}$ value was found by brute-force so that approximation ratios can be computed. We evaluated both the GW and QAOA algorithm on each instance. Regarding GW, we ran the standard algorithm and computed the effective performance by dividing the expected cost (estimated using 1000 projections) by the actual $C_{\text{max}}$.

Regarding our evaluation of QAOA, more details are warranted. We run QAOA on a quantum simulator, starting from $p = 1$ and increasing the depth up to $p = 10$. The algorithm we use for the QAOA parameter optimization is based on the Nelder-Mead (NM) method, whose performance dramatically depends on the choice of initial values/angles. We embed the NM algorithm in an optimization procedure outlined in [5] for finding good near-optimal angles for maximizing $F_C(\vec{\gamma}, \vec{\beta})$. The procedure is based on the observation that the evaluation of the QAOA objective function for fixed parameters on graphs generated from a “reasonable” distribution concentrates with little fluctuation. This suggests that optimal angles for QAOA from one instance can be used as a starting point for other instances, which is then improved via local search. Specifically, for a given depth, we find candidates for optimal angles starting from random “seed” positions. The newly found angles are then used as starting points for NM on the next instance. After passing through all graphs in the set, we attempt improving the best achieved ratios for a given $p$. This is done by trying out all angles found for each graph as seeds for further optimisation with NM, but only in the case that the achieved performance was not already better than what GW achieves. This is motivated by the fact that we are predominantly interested in the performance of QAOA assuming the capacity to achieve optimal parameters/angles, and identifying when that performance surpasses GW.

In those cases where QAOA still underperformed relative to GW, we also ran also QAOA with depth 11 and 12, but ultimately, even this did not improve the performance. In the following subsection we present the results obtained using the method above.

B. Results

We used simulations to first identify the depth of QAOA we wish to focus on. Intuitively we looked for a depth when using QAOA is obviously interesting relative to the performance of GW. Such a decision will also depend on the choice of the criterion of what makes an algorithm heuristically better than another. In our case, we looked at three figures of merit: minimum and median of the performance ratio, and overall percentage of instances where QAOA outperformed GW. Additionally, we address the more practically motivated criteria where we aim to identify settings where QAOA does not just outperform GW, but does so with a significant margin, and in the regime where the performance is already much better than the GW lower bounds. Here we selected the threshold of 98% for practical and pragmatic reasons: it may be high enough that no poly-time approximation algorithm can do better even on our restricted family of graphs (regardless of the UGC conjecture). This would make it a “genuinely heuristic” feature. Yet, it is low enough that we have

| Depth | Minimal ratio | Median ratio |
|-------|---------------|--------------|
| 1     | 0.7312        | 0.7979       |
| 2     | 0.8026        | 0.8641       |
| 3     | 0.8488        | 0.9050       |
| 4     | 0.8777        | 0.9302       |
| 5     | 0.8993        | 0.9446       |
| 6     | 0.9031        | 0.9523       |
| 7     | 0.9209        | 0.9607       |
| 8     | 0.9195        | 0.9622       |
| 9     | 0.9259        | 0.9737       |
| 10    | 0.9390        | 0.9800       |
| GW    | 0.9265        | 0.9658       |

6 As we explain shortly, we will investigate another, more stringent criterion which requires an objectively higher performance quality, and a larger gap over GW. In principle, we could have forced further optimizations on all instances that failed that criterion (but were already better than GW). We opted not to do so, because such a process would not be feasible in practice. Note that we can guide our optimizations of QAOA relative to the performance of GW (as we can run GW in polynomial time), but we cannot do the same in practice for any criteria which evaluate the actual achieved ratio of QAOA, as this would require computing $C_{\text{max}}$. |
FIG. 1. Boxplot of ratios for $p = 1, 2, 3$ and $8, 9, 10$ as well as the ratio of GW.

sufficiently many YES and NO instances for a meaningful analysis.

Fig. 1 shows boxplots, representing the quartiles of achieved ratios, presented according to depths from 1 to 10. Interesting depths for QAOA start at $p = 8$. Indeed, for $p = 8, 9, 10$, QAOA yields a better expected cost than GW on respectively 57.5%, 67.8% and 92.14% of the instances. Table I displays the obtained minimum and median ratios (averages yield similar conclusions but are generally more sensitive to outliers) on the generated set. At depth 10, we see a clear advantage of QAOA with respect to the minimal ratio criterion.

In addition to the expected cost, we also investigated the standard deviation of the output of the algorithms. This quantity is particularly relevant when randomized algorithms are used as subroutines in other algorithms (e.g. as steps in local search), in which cases more stable performance (with a worse mean) may be preferred over on-average-better, but much less reliable performance. We took the optimal angles obtained at depths 9 and 10, from which we sample the circuit 1000 times and compute the MaxCut cost. For GW, we use the 1000 random projections obtained for computing the expected ratios. From Fig. 2 we observe that the QAOA output is more spread out around the average than GW, and would require higher circuit depth to decrease it. In [10] it was shown that the upper bound on the spread (specifically, the variance) of the output distribution is dictated by a term of the form $(v - 1)^2p^2$, where $v$ is the constant degree of the graph (and $p$ is the depth). Due to this form, we applied a logarithmic fitting to the found variances, to estimate at which depths QAOA spread is guaranteed to concentrate more than GW. Numerically, we estimate this to occur after depth 20. However going to these higher depths did not yield better expected ratios (and did make optimisation significantly more costly and unstable), so we restricted the depths to $p \leq 10$ in the subsequent steps of our study.

Last but not least, we are interested in defining when QAOA is a good heuristic. In [8], the average approximation ratio (given on graph instances of similar size) at depth 8 was between 0.98 and 0.96, with an improvement close to 2% against GW. We then choose arbitrarily to define QAOA as a significantly good heuristic when QAOA yields a ratio higher than 0.98 and an improvement against GW by at least 2%. This occurred on 24 instances (8.5%) and gives rise to potentially good situations when QAOA is more suited to be advantageous. Having defined labels for our generated set of instances, we inferred when QAOA is more suited for applications.

IV. CHARACTERIZING QAOA ADVANTAGE

As indicated in the previous section, we identify two basic regimes of interest. The first criterion (1) – the GW vs. QAOA criterion, is the basic question: can we identify those instances where the ratio achieved by GW is surpassed by that of QAOA at all. The second is a question whether QAOA performs remarkably well in a more general sense – whether it is a "good heuristic", so to say. Note that what values an algorithm has to attain to be considered a "good heuristic" is of course arbitrary, and our decision of setting this threshold at 0.98 is motivated by three main factors: this is the highest value where we obtain non-trivial sample sizes where QAOA also outperforms GW by a substantial margin (2%); this is also likely in the NP-hard regime (if the performance could be attained for all graphs), even when restricted to 4-regular graphs. Finally, achieving objectively high performance values intuitively reduces the chances that other heuristic algorithms will generically be better at those instances.

Thus our second criterion (2) – the good heuristic criterion is: does QAOA attain performance above 0.98 with an advantage margin of at least 0.02 over GW?

Note that deciding the first criterion is trivial if we are allowed to actually run QAOA. The second criterion may be more problematic since it implies we can guess whether QAOA will do better than 0.98. Since we are interested in developing a methodology which helps us decide whether to run QAOA at all, we are only interested in detection methods which can be run efficiently on a classical device. So one may wonder whether characterizing instances with respect to the two criteria can be done algorithmically in polynomial time on a classical computer.

Regarding the two criteria, although we do not make any hard claims specifically for our choices, we point out that it is not difficult to see that finding exact predictors...
we can conclude that there exists a cut with value \( \alpha \), QAOA is an algorithms and criteria as well. For instance, assuming the output is YES, we have a cut value above this, and to the cut value under the UGC \( \alpha < \beta \). This is significantly lower than the plausible bound of 5/6 \[8\]. Thus, unless QAOA is weaker than a 0.77-approximation algorithm for all constant depths, deciding whether it beats the GW bound on a given instance would imply \( BQP \subseteq NP \), under the UGC.

In the more general case when we compare QAOA against more complicated heuristics, for which bounds may be unknown, proving formal claims may be even more difficult, and as we explain shortly, arguably less useful.

### A. Machine learning for performance prediction

The reasons above are an important factor why we resort to a machine learning (ML) approach, specifically supervised learning, to decide our criteria (1) and (2). Another one is because machine learning methods are also more robust, and flexible. We note that exactly the same method we employ here for characterising the performance of the idealized QAOA relative to GW can be used with any other classical heuristic, and with real-world, noisy QAOA implementations.

Our method is inspired by the approach in \[9\] where the authors inferred a ranking between different classical MaxCut heuristics, gathering instances from many MaxCut and QUBO libraries. However, due to the needs of quantum simulation, we could only provide more modest sample set and instance sizes.

In essence, we prepare a dataset of instances for which we compute the criterion value (NO/YES, or 0/1 for each criterion) – in supervised learning this is called a label. We then train a ML model to fit this value, using a subset of data – the training set; the performance reported is obtained by applying the model on the testing set. Using 4-fold cross-validation in our case gives an idea of generalisation and robustness of the model.

When relying on machine learning, a key step is the identification of the features, that is, the pieces of information (i.e. properties of the instance) based on which we will be training the model and making a decision. While the graph itself is a feature implicitly containing all the information we may care about, it is almost always useful to pre-compute many other derived properties (e.g. the graph density, or some property of the spectrum of the graph adjacency matrix) and use them directly in training the ML classifier. Note that in principle the performance itself could be a feature, however, we limit ourselves only to use features which can be computed classically, and efficiently relative to the running of the QAOA algorithm – the entire idea is to decide whether to employ the quantum device at all.

In general, our approach incorporates the 3 standard phases when employing ML: preparing the dataset (incl. pre-computation of the features, the running of the QAOA to compute the true criterion value, etc.), the training of the ML model, and evaluation. This process was iterated a number of times before the most informative features were identified. In our analysis we also discuss which
features contributed the most to prediction accuracy; this may also be informative for theoretical analyses of QAOA performance.

The learning model - In our study we have initially considered a number of models to perform prediction. We have experimented with decision trees – which are simple and would have high interpretability (meaning we can infer something about why the model makes certain decisions), and significantly more complex models, which were more successful, but less interpretable. As we are predominantly interested in high accuracy for these computationally hard predicates, vital for a practical advantage, we opted to deal with relatively complex models, the hyper-parameters of which were optimised using automated (auto-ML) techniques. Specifically, we built our models using the TPOT library [23], which builds the models using an evolutionary strategy. A clear advantage of such auto-ML methods is that they offer a significantly enhanced level of flexibility for the user, as much of the vital hyper-parameter optimization is taken care of automatically. This suggests that, with very little interventions from the user, the same techniques we provide could be used for noisy QAOA, or comparisons against very different types of heuristics. Such flexibility is a key desired feature of automated algorithm selection.

Features utilized for prediction - In our analysis we do not employ the raw graph description as a feature as it carries a lot of irrelevant information (e.g. both algorithms are invariant under graph isomorphisms). We used some of the features proposed in [7], while generating others for our results via a trial and error process. In the final analysis, we investigated the potential 20 features, listed in appendix B. These are grouped in three classes: (i) graph spectral properties, (ii) subgraph characteristics (e.g., maximum independent set size), and (iii) certain GW performance features (e.g., normalized value of the relaxed problem). This third class of features is of course GW-specific, but it should not be surprising that the performance of GW itself carries a lot of information about whether QAOA will do better. We note that some of the features in group (ii) are actually NP-hard to compute, so we cannot expect their exact values to be used in practice to guide our decisions. While we nonetheless investigated their value as predictors (we show they are absolutely unnecessary), the best results we report only utilize efficiently computable features. Criterion (1) is tackled before (2) as insights from (1) could be used to perform better for criterion (2).

B. Predicting Criterion (1): QAOA vs. GW

We computed the features for each of our 280 graph instances, and set the label to 1 when GW outperforms QAOA (at depth 10) in terms of the approximation ratio, and 0 otherwise. Note that to compute this particular label, the computation of the actual optimum is not necessary, but the running of QAOA is.

We then built a classifier by 4-fold stratified cross-validation and optimizing the average balanced accuracy over the validation sets; the data was split into 4 subsets, and the model is trained on 3 of them while being tested on a fourth. Stratified sampling is used in order to maintain the ratios of the labels in the sets. This procedure is performed 4 times and performances are averaged. k-fold cross-validation is a commonly used method to build ML models on small datasets while still giving a robust idea of performance and generalisation features.

Since our data is highly biased (QAOA outperforms GW significantly, more than half of the time), the relevant measure of performance is the so-called balanced accuracy [7], which uniformly averages the performances for YES and NO instances.

In our analysis, we initially used all 20 features, and then proceeded to prune out a smaller number with the highest impact on accuracy. In the end, we have identified two features which alone enable the same balanced accuracy, as all features combined, and these are:

- expected_costGW_over_sdp_cost: the expected cost over the 1000 random projections per instance divided by $C_{rlx}$.
- std_costGW_over_sdp_cost: the standard deviation of the cost approximated using 1000 random projections divided by $C_{rlx}$.

In other words, to achieve the +96% accuracy we report, we only need to use these two features. The model is described in appendix C.

A few comments are in order; first, note that both of these features exclusively characterise the output of GW – this is not too surprising as the criterion “better than GW” strongly depends on GW performance. For instance, the first of these two features is likely closely correlated to the actual performance of GW in terms of the approximation ratio (it is the exact value when $C_{rlx} = C_{max}$). However, we can also understand the performance analysis of GW as a feature extraction mechanism, which identifies the properties of graphs which also make them suitable for QAOA. This is indeed the case, as our classification algorithm correctly predicts QAOA advantage even in many instances where GW did exceptionally well, and also, correctly predicts that QAOA underperformed also when GW did “badly” as well – in other words, we capture more than the quality of performance of GW. Also importantly, this shows that NP-hard features are really unnecessary to decide criterion (1).

![FIG. 3. Partial dependence plot for the classifier built on two features. The contour lines from left to right represent probabilities thresholds: 0.67, 0.62, 0.56, 0.5, 0.45, 0.39.](image)
probabilities evolve according to those two features. In more details, our classification model outputs probabilities of assignments, and not the labels themselves. The closer the probability is to 1, the more likely the output label will be a 1. From the plot, we observe that the smaller the standard deviation of the cost applied on the random projections, and the closer the expected cost to $C_{rlx}$ is, the higher is the probability that GW outperforms QAOA. But this also means that the GW performance is not far from an actual optimum since $C_{rlx}$ upper bounds $C_{max}$. In order to understand the importance/impact of these features, we also performed a so-called permutation importance analysis, in essence based on permuting the values of one feature, and measuring the impact on the overall classifier performance. When this measure was applied to the two features above, we noted that performances decrease by $0.4283 \pm 0.1843$ for the standard deviation feature and $0.0533 \pm 0.0743$ for the expected cost, indicating the prior is more informative.

While showing that GW performance influences whether QAOA outperforms it is unsurprising, it opens the obvious question of whether it is possible to find other sufficiently informative features. We would especially be interested in finding features to be used in place of the standard deviation feature, which requires the costly random projection evaluations.

To this end, we have rerun the analysis from scratch, running through a new cycle of automated hyperparameter optimization, trying to match the performance without using these two GW-specific features – including using the NP-hard features. However, we have failed to achieve performance close to when those features were available. To understand this further, we have applied a regression approach, trying to predict the values of the expensive feature $\text{std}_\text{costGW}/\text{over_sdp}_\text{cost}$ from the other features. Note that if this were possible, then the other features indeed did contain sufficient information, even without these expensive features being explicitly present. We analyzed the explained variance of the constructed regressor, and obtained a low value of 0.7693. With this result, it became apparent that we should not expect to be able to recover the same levels of accuracy without these costly (but still efficiently computable) features, using our machine learning model. In principle, of course all features should be distillable from raw graph data, and in future work it will be valuable to achieve as good or better performance relying on better tuned models, and cheaper features.

To summarize the results of this section, we can report that the prediction performance for criterion (1), which can be achieved when many NP-hard graph-theoretical features are available, along with the less costly features, can easily be matched using just properties derived from the tractable GW performance. It is worth to note that the generation of the datasets for this prediction is also tractable (albeit, expensive), as it requires only the running of QAOA and of GW.

C. Predicting Criterion (2): QAOA as a High-Performing Heuristic

For this analysis, we considered the same dataset but the label was changed. We labeled with 1 the instances where the QAOA ratio exceeded 0.98 and where the gain was at least 2% over the performance of GW. Note that to generate this label, we did need the true $C_{max}$ values which we computed by brute-force. We will discuss this issue presently. We built a classifier which utilized all the features we discussed previously, including the features relying on the random projections and the NP-hard graph-theoretical features, which lead to 0.8255 in balanced accuracy. The analysis was done again using 4-fold cross validation. This performance provides a benchmark which we would ideally like to achieve using only those features which can be computed in polynomial time.

To do so, we performed importance analyses of the features and built a classifier (described in appendix C.2) using a subset of the features, first disregarding the GW-dependent features. With this collection of features, the obtained accuracy was essentially as good: 0.8236 and with a recall (intuitively the ability of the classifier to find all the class 1 instances) of 0.7917. We analyzed the feature importance shown in Figure C.2 which shows that not only the GW-specific features can be dropped, but also that the NP-hard graph-theoretic features are unnecessary. So we can discard features (ii) and (iii) in the second regime, keeping the green-highlighted ones – and these are all computationally efficiently computable features, yielding an efficient classifier. For completeness, we did train and test the classifier using only these features, resulting in the accuracy of 0.8236, as expected.

Further, we note that the reported performance is very good from a ML/classification point of perspective (in an absence of other well-established benchmarks).

In more detail, we report that the density and the ratio between the largest eigenvalues of the adjacency matrix of the graph seem to be most important for deciding criterion (2), while it seems that demanding the gap of 2% between GW and QAOA significantly diminished the explicit dependence on the GW features, which was so prominent for criterion (1). To further investigate this, we constructed a partial dependence plot, which revealed that regular graphs with more nodes are overrepresented in the high-performance regime.

Further, those cases correspond to the case when the largest eigenvalue of the Laplacian matrix is at least 1.05% times the second largest eigenvalue.

In summary, from our 82% accurate ML model, we found interesting graph properties which influence whether a QAOA approach will result in a high-performing heuristic. This is mainly dependent on the Laplacian spectrum and the density. Using ML explainability, we quantified best significantly handled graph instances. Specifically, the density and the ratio between the largest eigenvalues of the adjacency matrix of the graph were the most informative features in this regime. This highlights a possible direction for further analytic and experimental investigations of QAOA performances.
Finally, to our knowledge, the use of ML techniques to analyze the performance of quantum methods has only previously been employed in [21] (albeit for a different purpose); yet, we believe ML will play an ever increasing role in helping us identify interesting quantum heuristics, so we hope our work may motivate more studies in this direction. For instance, machine learning methods of the type we propose could conceivably be used to identify and characterise what types of datasets are best suitable for quantum-variational-circuit-based classification, which is arguably one of the key questions in NISQ-oriented quantum-enhanced machine learning domain.

In the process of analysing QAOA and GW performance, we found further evidence that QAOA can provide genuine advantages over the GW algorithm—specifically, we have shown that at that at depth \( p = 10 \), QAOA outperforms GW on most instances of 4-regular graphs up to size 24. With respect to predicting advantages, we constructed a model yielding an accuracy of 96% for the first regime—the key features here depend on the output of GW, and other features were less significant. For the second regime, we achieved a model with 82% balanced accuracy, and further used explainability methods to elucidate which graph features influence QAOA performance the most. In this regime, spectral properties of the graph, and basic graph density were most influential. We note that already the accuracy of 82% (4-fold cross-validated) would yield substantial optimizations in the use of quantum resources in any larger-scale optimization effort, of the type we may expect in, e.g., industrial applications.

We see numerous possibilities for future work. First, it would be interesting to perform a similar analysis on different graph families and identify when to use QAOA. Second, we could consider using Graph Sparsification [2], that converts a weighted graph into a sparser one preserving all cuts up to multiplicative error. This can be done classically in near-linear time, and quantumly even in sublinear time. We would then study if performances of both GW and QAOA are improved on the sparser instance. Third, an obvious limitation to this type of study is the size of the graph we can handle; to this end it would be interesting if divide-and-conquer type methods explored in [11] can be utilized to increase the size of datasets we can consider. Additionally, in our work, we did not tackle the important question of how the choice of QAOA optimization procedures influences the advantage gained. It is also important to consider how realistic, or real, noise effects affect performance. Note that since we employ quite general machine learning methods, we expect that a similar level of results could be obtained. Finally, more recent contributions also provide new modifications of QAOA to make it more suitable for standard real-world optimization objectives [3, 20]. We believe our methods can equally be applied in those settings.

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[1] Alam, M., Ash-Saki, A., and Ghosh, S. Analysis of quantum approximate optimization algorithm under realistic noise in superconducting qubits, 2019. arXiv:1907.09631
[2] Apers, S. and de Wolf, R. Quantum Speedup for Graph Sparsification, Cut Approximation and Laplacian Solving, 2019.
[3] Barkoutsos, P. K., Nannicini, G., Robert, A., Tavernelli, I., and Woerner, S. Improving variational quantum optimization using cvaR, 2019. arXiv:1907.04769
[4] Benedetti, M., Lloyd, E., Sack, S., and Fiorentini, M. Parameterized quantum circuits as machine learning models. 2019. doi:10.1088/2058-9565/ab4eb5 arXiv:1906.07682
[5] Brando, F. G. S. L., Broughton, M., Farhi, E., Gutfreund, S., and Neven, H. For fixed control parameters the quantum approximate optimization algorithm’s objective function value concentrates for typical instances, 2018. arXiv:1812.04170
[6] Bravyi, S., Kliesch, A., Koenig, R., and Tang, E. Obstacles to State Preparation and Variational Optimization from Symmetry Protection, 2019. arXiv:1910.08980
[7] Brodersen, K. H., Ong, C. S., Stephan, K. E., and Buhmann, J. M. The balanced accuracy and its posterior distribution. In 2010 20th International Conference on Pattern Recognition, pp. 3121–3124, Aug 2010. doi:10.1109/ICPR.2010.764
[8] Crow, R. A. Performance of the quantum approximate optimization algorithm on the maximum cut problem. 2018. https://arxiv.org/abs/1811.08419
[9] Dunning, I., Gupta, S., and Silberholz, J. What works best when? a framework for systematic heuristic evaluation. 2015. URL http://www.optimization-online.org/DB_FILE/2015/05/4895.pdf
[10] Farhi, E., Goldstone, J., and Gutfreund, S. A quantum approximate optimization algorithm, 2014. arXiv:1411.4028.
[11] Ge, Y. and Dunjko, V. A hybrid algorithm framework for small quantum computers with application to finding hamiltonian cycles. Journal of Mathematical Physics, 61 (1):12201, Jan 2020. doi:10.1063/1.5119235 URL http://dx.doi.org/10.1063/1.5119235
[12] Goemans, M. X. and Williamson, D. P. Improved approximation algorithms for maximum cut and satisfiability problems using semidefinite programming. J. ACM, 42 (6):1115–1145, November 1995. ISSN 0004-5411. doi:10.1145/227683.227684 URL http://doi.acm.org/10.1145/227683.227684
[13] Guerreiro, G. G. and Matsuura, A. Y. QAOA for Max-cut requires hundreds of qubits for quantum speed-up. Scientific Reports, 9(1):6903, 2019. ISSN 2045-2322. doi:10.1038/s41598-019-43176-9 URL http://doi.org/10.1038/s41598-019-43176-9
[14] Hadfield, S. Quantum algorithms for scientific computing and approximate optimization, 2018. arXiv:1805.03265
[15] Håstad, J. Some optimal inapproximability results. J. ACM, 48(4):798–859, July 2001. ISSN 0004-5411. doi:10.1145/502095.502098 URL http://doi.acm.org/10.1145/502095.502098
[16] Hastings, M. B. Classical and quantum bounded depth approximation algorithms, 2019. arXiv:1905.07047
[17] Khot, S. On the power of unique 2-prover 1-round games. In Proceedings of the Thirty-fourth Annual ACM Symposium on Theory of Computing, STOC ’02, pp. 767–775, New York, NY, USA, 2002. ACM. ISBN 1-58113-495-9. doi:10.1145/509907.510017 URL http://doi.acm.org/10.1145/509907.510017
[18] Khot, S., Kindler, G., Mossel, E., and O’Donnell, R. Optimal inapproximability results for MAX-CUT and other 2-Variable CSPs? SIAM J. Comput., 37(1):319–357, April 2007. ISSN 0097-5397. doi:10.1137/S0097539704447827 URL http://dx.doi.org/10.1137/S0097539704447827
[19] Kotthoff, L. Algorithm Selection for Combinatorial Search Problems: A Survey, pp. 149–190. Springer International Publishing, Cham, 2016. ISBN 978-3-319-50137-6. doi:10.1007/978-3-319-50137-6_6 URL https://doi.org/10.1007/978-3-319-50137-6_6
[20] Li, L., Fan, M., Coram, M., Riley, P., and Leichnauer, S. Quantum Optimization with a Novel Gibbs Objective Function and Ansatz Architecture Search, 2019. arXiv:1909.07621.
[21] Melnikov, A. A., Fedichkin, L. I., and Aldodjants, A. Predicting quantum advantage by quantum walk with convolutional neural networks, 2019. doi:10.1088/1367-2630/ab5c5e arXiv:1901.10632.
[22] Moll, N., Barkoutsos, P., Bishop, L. S., Chow, J. M., Cross, A., Egger, D. J., Filipp, S., Fuhrer, A., Gambetta, J. M., Ganzhorn, M., Kandala, A., Mezzacapo, A., Miller, P., Riess, W., Salis, G., Smolin, J., Tavernelli, I., and Temme, K. Quantum optimization using variational algorithms on near-term quantum devices. 2017. doi:10.1088/2058-9565/aab822 arXiv:1710.01022.
[23] Olson, R. S., Bartley, N., Urbanowicz, R. J., and Moore, J. H. Evaluation of a tree-based pipeline optimization tool for automating data science. In Proceedings of the Genetic and Evolutionary Computation Conference 2016, GECCO ’16, pp. 485–492. New York, NY, USA, 2016. ACM. ISBN 978-1-4503-4206-3. doi:10.1145/2908812.2908819 URL http://doi.acm.org/10.1145/2908812.2908819.
[24] Papadimitriou, C. H. and Yannakakis, M. Optimization, approximation, and complexity classes. Journal of Computer and System Sciences, 43(3):425 – 440, 1991. ISSN 0022-0000. doi:https://doi.org/10.1016/0022-0000(91)90023-X URL http://www.sciencedirect.com/science/article/pii/002200009190023X.
[25] Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, M., and Duchesnay, E. Scikit-learn: Machine learning in Python. Journal of Machine Learning Research, 12:2827–2830, 2011.
[26] Preskill, J. Quantum Computing in the NISQ era and beyond. Quantum, 2:79, August 2018. ISSN 2521-327X. doi:10.22331/q-2018-08-06-79 URL https://doi.org/10.22331/q-2018-08-06-79.
[27] Shadyulin, R., Safro, I., and Larson, J. Multistart methods for quantum approximate optimization, 2019. arXiv:1905.08768.
[28] Streif, M. and Leib, M. Comparison of qaoa with quantum and simulated annealing, 2019. arXiv:1901.01903.
[29] Verdon, G., Broughton, M., McClean, J. R., Sung, K. J., Babbush, R., Jiang, Z., Neven, H., and Mohseni, M. Learning to learn with quantum neural networks via classical neural networks, 2019. arXiv:1907.05415.
[30] Xue, C., Chen, Z.-Y., Wu, Y.-C., and Guo, G.-P. Effects of quantum noise on quantum approximate optimization
Algorithm, 2019. [31] Zhou, L., Wang, S.-T., Choi, S., Pichler, H., and Lukin, M. D. Quantum approximate optimization algorithm: Performance, mechanism, and implementation on near-term devices, 2018. 

Appendix A: Simulations

Generated graphs The following code reproduces the instances:
```python
from networkx import random_regular_graph
gs = []
for n in range(11, 25):
    for i in range(10):
        gs.append(random_regular_graph(4, n, i * 10))
        gs.append(random_regular_graph(4, n, (i + 1) * 11))
```

Appendix B: Features

Common features related to regular graphs and the spectrum of the Laplacian matrix:
- density: percentage of the number of edges in a complete graph with the same number of vertices. For regular graphs, this is strongly correlated to the number of vertices.
- log_norm_laplacian_ev1: logarithm of largest eigenvalue of the laplacian normalized by the degree.
- log_norm_laplacian_ev2: logarithm of the second largest eigenvalue of the laplacian normalized by the degree.
- the same for the third, fourth and fifth largest eigenvalues.
- log_laplacian_ev_ratio: logarithm of the ratio between the two largest eigenvalues.
- spectral_gap: the second smallest eigenvalue of the laplacian.

Set numbers for graphs:
- independence_number_over_number_edges: cardinality of a largest independent set of nodes in the graph normalized by the number of edges.
- matching_number_over_number_edges: cardinality of a maximum matching (size of a maximum independent edge set) normalized by the number of edges.
- diameter_over_number_edges: diameter is the maximum eccentricity normalized by the number of edges.
- domination_number_over_number_nodes: number of vertices in a smallest dominating set divided by number of nodes.
- zero_forcing_number_over_number_nodes: minimum cardinality of a zero forcing set divided by number of nodes.
- power_domination_over_number_edges: minimum cardinality of a power dominating set divided by number of nodes.

Features related to the relaxed solution of the semi-definite program in GW:
- percent_cut: ratio between $C_{rlx}$ and the number of edges.
- percent_positive_lower_part_relaxation_solution: percentage of elements that are positive in the relaxed solution after Cholesky factorization.
- percent_close1_lower_part_relaxation_solution: percentage of elements that are less than .1 in absolute value in the relaxed solution after Cholesky factorization.
- percent_close3_lower_part_relaxation_solution: percentage of elements that are less than .001 in absolute value in the relaxed solution after Cholesky factorization.

Appendix C: Models

We give below the code of the pipeline constructed by TPOT for the two Criteria. Each algorithm name (either data transformer or classifier) can be found in the Scikit-learn library [25]. Names ending in NB are Naive-Bayes classifiers.

1. Criterion (1)
```python
exported_pipeline = make_pipeline(
    make_union(
        Normalizer(norm="l2"),
        FunctionTransformer(copy)
    ),
    StackingEstimator(estimator=\KNeighborsClassifier(n_neighbors=41,\p=1,\weights="uniform")),
    MultinomialNB(alpha=0.1, fit_prior=False)
)
```

2. Criterion (2)
```python
exported_pipeline = make_pipeline(
    SelectPercentile(score_func=f_classif,\percentile=95),
    StackingEstimator(estimator=\DecisionTreeClassifier(criterion="entropy",\max_depth=2,\min_samples_leaf=13,\min_samples_split=9)),
    Binarizer(threshold=0.25),
    StackingEstimator(estimator=\KNeighborsClassifier(n_neighbors=8,\p=1,\weights="uniform")),
    StackingEstimator(estimator=\BernoulliNB(alpha=10.0, fit_prior=False)),
    StackingEstimator(estimator=GaussianNB()),
    MultinomialNB(alpha=0.001, fit_prior=False)
)```