Predicting Optimal Depth in Quantum Approximate Optimization Algorithm

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Introduction: The quantum approximate optimization algorithm (QAOA) is designed to approximate solutions to combinatorial optimization problems [1]. With long enough circuits, QAOA can approximate the adiabatic evolution, which certifies success. Moreover, QAOA has been shown to be successful in approximating solutions to several combinatorial problems even with medium depths. Determining the optimal (critical) QAOA depth for a given combinatorial problem is, however, a non-trivial task and would typically require the algorithm to be repeated with increasing depths until the solution is attained. In this work we show that it is possible to predict the optimal QAOA depth in a more efficient manner: for n variable MAX-CUT problems on k-regular graphs one can predict the optimal QAOA depth by the so called saturation depth (depth at which effective quantum dimension saturates [2]) with a very high accuracy. We demonstrate this numerically for n up to 20 and k up to 7. Moreover for the special case of $k = 2$ we analytically prove that the optimal depth is upper bounded by $\lfloor \frac{n}{2} \rfloor$ (which coincides with the saturation depth) for all even values of n, thus partially proving the conjecture in [1].

Quantum Approximate Optimization Algorithm: Given a problem Hamiltonian H, whose ground state encodes the solution to a combinatorial optimization problem, QAOA searches for a solution $|g\rangle$ such that $\langle g|H|g\rangle = \min H = E_g$. A p depth QAOA ansatz is parameterized as:

$$|\psi_p(\boldsymbol{\gamma}, \boldsymbol{\beta})\rangle = \prod_{k=1}^{p} e^{-i\beta_k H_x} e^{-i\gamma_k H} |+\rangle^{\otimes n}. \tag{1}$$

Here $\gamma_k \in [0, 2\pi)$, $\beta_k \in [0, \pi)$ and $H_x = \sum_{j=1}^{n} X_j$. The cost function is given by the expectation of the problem Hamiltonian with respect to the ansatz state. The algorithm minimizes this cost function to output:

$$E_p^*(H) = \min_{\boldsymbol{\gamma}, \boldsymbol{\beta}} \langle \psi_p(\boldsymbol{\gamma}, \boldsymbol{\beta})| H |\psi_p(\boldsymbol{\gamma}, \boldsymbol{\beta})\rangle. \tag{2}$$

Here $E_p^*(H)$ is the estimated ground state energy of H. The quality of the estimation is determined via the performance metric $E_p^*(H) - E_g \geq 0$. It is known to be a monotonically decreasing function of p, until it reaches zero. The performance metric reaching zero implies that the corresponding optimization problem is deemed to be solved.

Definition 1 (Critical depth)**.** *p^* is said to be the critical depth of a QAOA ansatz for a problem Hamiltonian H iff $\forall p \geq p^*$, $E_p^*(H) - E_g = 0$.*

Effective Quantum Dimension: The ability of a variational quantum circuit to minimize a problem Hamiltonian is intrinsically linked to its expressive power. A quantification of the expressive power of a variational circuit can be given by effective quantum dimension [2].

Definition 2 (Effective quantum dimension [2])**.** *Given a p depth variational quantum circuit $U_p(\boldsymbol{\theta})$, the effective quantum dimension of the circuit $\mathcal{Q}(U_p)$ is defined as:*

$$\mathcal{Q}(U_p) = \max_{\boldsymbol{\theta}} \operatorname{rank}[\mathcal{F}(\boldsymbol{\theta})], \tag{3}$$

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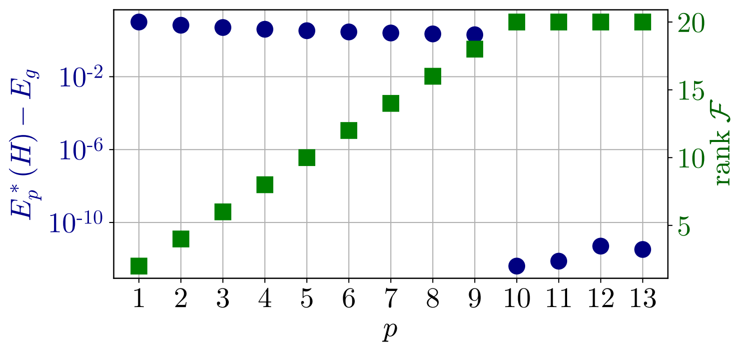

FIG. 1. Plot showing the variation of $E_p^*(H) - E_g$ (blue) and $\mathcal{Q}(U_p)$ (green) with QAOA depth. The problem Hamiltonian H is the 20 qubit MAX-CUT problem Hamiltonian on a 2-regular graph. Here $\mathcal{Q}(U_p)$ was obtained by maximising rank$[\mathcal{F}(\boldsymbol{\gamma}, \boldsymbol{\beta})]$ over 50 randomly sampled QAOA parameters for each p.

where $\mathcal{F}(\boldsymbol{\theta})$ is the quantum Fisher information (QFI) matrix.

In [3] over-parameterization of a variational circuit was defined in terms of effective quantum dimensions: a variational circuit is said to be over-parameterized if $\mathcal{Q}(U_p)$ saturates upon increasing the number of parameters past some critical value. A more convenient definition can be given in terms of circuit depth.

Definition 3 (Saturation depth). *p_{s} is said to be the saturation depth iff $\forall p \geq p_{\mathrm{s}}$, the effective quantum dimension $\mathcal{Q}(U_p) = \mathcal{Q}(U_{p_{\mathrm{s}}})const$.*

Thus, a variational circuit $U_p(\boldsymbol{\theta})$ is over-parameterized iff $p \geq p_{\mathrm{s}}$. Based on this definition one might argue that in the over-parameterized regime, $p \geq p_{\mathrm{s}}$, the expressive power of the ansatz (quantified by $\mathcal{Q}(U_p)$) stagnates. We therefore ask the following question: how does the saturation depth p_{s} relate to the critical depth required to minimize a given problem Hamiltonian.

Results: We investigate the interrelationship between the critical QAOA depth p^* and its saturation depth p_{s}. In particular we consider the MAX-CUT problem on k-regular graphs (V, E) with $k \in [2:7]$ and $|V|$ upto 20. Note that instances of a MAX-CUT problem can be encoded as an n qubit problem Hamiltonian:

$$H = \sum_{(i,j) \in E} Z_i Z_j, \tag{4}$$

where $n = |V|$. We minimize H with respect to ansatz (1), and numerically determine the corresponding p^*. As per Definition 1, p^* is the smallest QAOA depth for which the performance metric $E_p^*(H) - E_g = 0$. Attaining this condition in practice, however, depends on the precision of the numerical experiments, and one might choose arbitrary thresholds. Therefore, in order to avoid any peculiarity induced by an arbitrarily set threshold, we adopt a slightly modified criteria to determine p^*. We note that during the Hamiltonian minimization $E_p^*(H)$ experiences a sharp drop at a certain depth and does not improve any further in the presence of additional QAOA layers (see Fig. 1). We stipulate this depth to be p^*. Subsequently we compare p^* to the saturation depth p_{s} as obtained from the effective quantum dimension for the QAOA ansatz (1).

MAX-CUT on 2-regular graphs: The MAX-CUT problem Hamiltonian on a 2-regular graph (a.k.a. ring of disagrees) is a well studied case in the QAOA literature. It has been numerically observed in [1] that the critical QAOA depth for such Hamiltonians is $p^*(n) = \lfloor \frac{n}{2} \rfloor$. In this work we have analytically proved, by exploiting specific patters in the QAOA parameters, that $p = \frac{n}{2}$

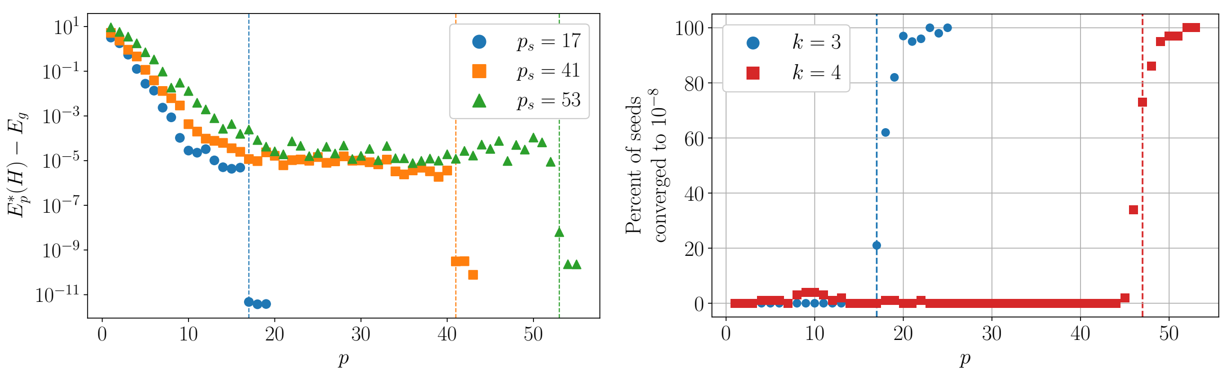

FIG. 2. (left) Variation of $E_p^*(H) - E_g$ with QAOA depth p. The problem Hamiltonians H are of type (4) embedding the MAX-CUT problem for 3-regular graphs with 10 qubits. With different colors and markers shown are the results for Hamiltonians with different p_s, which are indicated by vertical dashed lines. (right) the percentage of seeds for which a QAOA ansatz is able to minimize a MAX-CUT instance with 10 qubits and $k = 3, 4$. With different colors and markers shown are the results for Hamiltonians with different p_s, which are indicated by vertical dashed lines.

is sufficient to minimize a MAX-CUT Hamiltonian on a 2-regular graph for any even number of qubits. This establishes an upper limit on $p^*(n)$ for even values of n. Furthermore we have numerically verified for upto $n = 20$ qubits, that an exact estimation of the critical QAOA depth can be made from the saturation depth of the ansatz. That is, we observe that $p^*(n) = p_{\mathrm{s}}(n) = \lfloor \frac{n}{2} \rfloor$ for the MAX-CUT problem on two regular graphs (see Fig. 1).

MAX-CUT on k-regular graphs for $k > 2$: We implemented QAOA to solve the MAX-CUT problem on all k-regular graphs with $k \in [3 : 7]$, $n \in [2 : 10]$ and $p_{\mathrm{s}} \leq 55$. There are 56 such graphs in total. We calculate p^* for each of these cases and compare it with the corresponding saturation depth p_{s}. Firstly we observe that $p_{\mathrm{s}} - p^* \geq 0$ thus signifying that p_{s} can act as an upper bound on the critical depth for MAX-CUT problems on regular graphs. Moreover we observe that in 69.6% of the cases the critical depth could be exactly predicted by the saturation depth; $p^* = p_{\mathrm{s}}$, while in 91.1% of the considered cases $p_{\mathrm{s}} - p^* \leq 3$. Only in 3 out of the 56 cases we observed a significant difference between p^* and p_{s}. However after further analysis we observed that: while there exists such seeds for which a p depth QAOA ansatz ($p < p_{\mathrm{s}}$) is able to minimize a MAX-CUT instance, the relative proportion of seeds for which a QAOA ansatz is able to minimize a MAX-CUT instance, remains insignificant at $p = p^*$, but suddenly explodes at $p = p_{\mathrm{s}}$ (see Fig. 2).

Conclusion: Our results show that for n variable MAX-CUT problems on k-regular graphs the optimal QAOA depth can be inferred from a more easily computable quantity—the saturation depth—with a high accuracy. Moreover for the special case of $k = 2$ we have analytically proved that the optimal QAOA depth is upper bounded by $p_{\mathrm{s}}(n) = \lfloor \frac{n}{2} \rfloor$ for all even values of n thus confirming that such problems can indeed be solved at linear depths (with respect to n).

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