Reachability Deficits in Quantum Approximate Optimization

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The quantum approximate optimization algorithm (QAOA) has rapidly become a cornerstone of contemporary quantum algorithm development. Despite a growing range of applications, only a few results have been developed towards understanding the algorithms ultimate limitations. Here we report that QAOA exhibits a strong dependence on a problem instances constraint to variable ratio—this problem density places a limiting restriction on the algorithms capacity to minimize a corresponding objective function (and hence solve optimization problems). Such *reachability deficits* persist even in the absence of barren plateaus [1] and are outside of the recently reported level-1 QAOA limitations [2]. Building on general numerical experiments, we compare the presence of reachability deficits with analytic solutions of the variational model of Grover's search algorithm. Comparing QAOA's performance between random 3-SAT (NP-hard) and 2-SAT (efficiently solved) instances, reachability deficits increased with problem density.

Introduction. Variational hybrid quantum/classical algorithms have become an area of significant interest [3]. These algorithms minimize an objective functions which can be largely agnostic to systematic errors. This increases their potential in current Noisy Intermediate-Scale Quantum devices (NISQ) [4–6]. These hybrid algorithms involve parameterized quantum circuits trained in a classical learning loop. Particular interest is the Quantum Approximate Optimization Algorithm (or QAOA) designed for realizing approximate solutions to combinatorial optimization problems [7]. Although QAOA has been shown to approximate solutions to problems such as MAX-CUT [8] and realize Grover's search algorithm [9, 10], not much is known about its limitations.

Recent findings suggest that randomly parameterized quantum circuits in the large scale will suffer from *barren plateaus* resulting in an exponentially low probability to find correct solutions [1]. Recent results also show that classical algorithms in a certain restrictive (single depth) setting can outperform level-1 QAOA [2]. Can higher depth versions achieve supremacy over classical algorithms?

QAOA performance has an evident dependence on the circuit-depth and it is observed that increasing depth improves the quality of the possible approximation (at the cost of increasing the parameter search space). We show that circuit depth is not the only limiting restriction. Indeed, we found that finding appropriate solutions has strong dependence on the ratio of a problems constraint to variables (problem density). Hence, QAOA exhibits a strong dependence on a problems density and for any fixed ansatz, there exists a problem instances of high-density that appear not to be accessible. This feature persists as a fundamental limitation exhibited by QAOA.

As a tool to study the performance of QAOA, we turn to constraint satifiability problems, which have a successful history. Such problems are expressed in terms of n variables and m clauses or constraints. The density of such problem instances is the clause to variable ratio, the clause density $\alpha = m/n$. k-SAT clauses are randomly generated to form random instances by uniformly selecting unique k-tupels from the union of a variable set (cardinality $n > k$) and its element wise negation. We consider both random instances of the NP-complete problem 3-SAT, as well as random instances of 2-SAT which is efficiently solvable. QAOA's limiting performance exhibits strong dependence on the problem density in both cases.

We call the QAOA problem general when considering random 3-SAT and 2-SAT instances with the standard one-body driver Hamiltonian [7]. In both cases we found strong limiting dependence of QAOA for clause densities above ~ 1. Moreover, the deference between the two problems (i.e. 2- vs 3-SAT) seemed negligible where the density played the dominate role. We further consider this same scenario, replacing the driver Hamiltonian with a n-body projector $(|+\rangle\langle+|)^n$. While problem density dependence is still strongly exhibited, we found a decrease in the error of best-possible-approximation. Finally, by considering a single projector onto a solution space and the same driver as above, the variational version of Grover's search algorithm is recovered. While the clause density is fixed for a given n (and actually exhibits inverse dependence on n), the analytical solutions of this model provide a test bed to ascertain that energy approximation is critically dependent on circuit depth at each fixed density.

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Quantum Approximate Optimization. The usual procedure in implementing QAOA is as follows [7]:

1. Create ansatz states, $|\psi(\boldsymbol{\alpha},\boldsymbol{\beta})\rangle$ on a quantum computer where, $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, ..., \alpha_p)$ and $\boldsymbol{\beta} = (\beta_1, \beta_2, ..., \beta_p)$ are tunable parameters. The state is prepared by applying a sequence of $2p$ gates acting on the reference state, $|+\rangle^{\otimes n}$ as,

$$|\psi(\boldsymbol{\alpha},\boldsymbol{\beta})\rangle = \prod_{i=1}^{p} \mathcal{U}(\alpha_i, \beta_i) \, |+\rangle^{\otimes n} . \tag{1}$$

2. Measurement of this state is done to compute the expected value of the objective function of interest, $\langle \mathcal{V} \rangle$. For QAOA, the objective function is the optimization problem.

3. Classical optimization algorithms are used to assign set of parameters, $\boldsymbol{\alpha}^*$ and $\boldsymbol{\beta}^*$ that minimize $\langle \psi(\boldsymbol{\alpha},\boldsymbol{\beta})| \, \mathcal{V} \, |\psi(\boldsymbol{\alpha},\boldsymbol{\beta})\rangle$.

4. Steps 1 and 2 are repeated by adjusting parameters to approximately minimize $\mathcal{V}$, $\langle \psi(\boldsymbol{\alpha}^*,\boldsymbol{\beta}^*)| \, \mathcal{V} \, |\psi(\boldsymbol{\alpha}^*,\boldsymbol{\beta}^*)\rangle \approx \min(\mathcal{V})$.

The variational ansatz states created by QAOA take inspiration from the quantum adiabatic algorithm, where a system is initialized in an easy to prepare ground state of a local Hamiltonian $\mathcal{H}_x = \sum_i \sigma_x^{(i)}$, the driver Hamiltonian, which is then slowly transformed to the problem Hamiltonian $\mathcal{H}$ [12]. Trotterization of this procedure gives a long QAOA sequence as can be understood from equation (1) where,

$$\mathcal{U}(\alpha_k, \beta_k) = \exp\{-i\beta_k \mathcal{H}_x\}.\exp\{-i\alpha_k \mathcal{H}\}. \tag{2}$$

However, the Trotter approximation is evidently violated for a typical sequence. Outside of this understanding, the performance of QAOA seems rather remarkable.

Quantum Approximation in Boolean Satisfiability. Boolean satisfiability is the problem of determining satisfiability of a Boolean expression written in conjunctive normal form (CNF). It is possible to map any Boolean satisfiability problem into 3-SAT; conjunction of clauses restricted to 3 literals, via Karp Reduction. It is well known that 3-SAT is NP-Complete [11]. 2-SAT, is the problem restricted to clauses limited to 2 literals. This problem can be solved in polynomial-time [13]. 2-SAT exhibits an algorithmic phase transition at a critical clause to variable ratio, $\alpha_c = 1$ [14]. The transition is emperically exhibited in 3-SAT numerics, but a critical clause to variable ratio is yet to be proven. At $\alpha_c \approx 4.27$, a sharp transition can be observed in the probability of satisfiability for randomly generated 3-SAT instances [15]. This implies that for $\alpha < \alpha_c$ almost all instances are satisfiable and for $\alpha > \alpha_c$, almost all instances are not.

Known algorithms exhibit a slow-down around the phase transition, suggesting that most of the hard-instances are concentrated near this point.

In order to approximate solutions of 3-SAT and 2-SAT, an embedding scheme must be made that maps SAT-instances into Hamiltonians. We use the techniques described in [16–18] to form an Ising Hamiltonian from a given SAT instance as

$$\mathcal{H}_{\text{SAT}} = \sum_l \mathcal{P}(l), \tag{3}$$

where l indexes each clause in the SAT instance and $\mathcal{P}(l)$ are rank-one projectors that penalize each unsatisfiable assignments with at-least 1 unit of energy. By this construction, we embed solutions to the 3-SAT or 2-SAT instances into the ground state space of $\mathcal{H}_{\text{SAT}}$. 2-SAT requires only quadratic interactions whereas 3-SAT requires 3-body ones. Satisfiable instances are characterized by a zero ground state energy, $E_g = 0$ and unsatisfiable instances with $E_g \geq 1$.

QAOA with standard settings, $\mathcal{H}_x = \sum_i \sigma_x^{(i)}$ and $\mathcal{H} = \mathcal{H}_{\text{SAT}}$, can now be used to calculate the energy approximation E_g^{QAOA}, where

$$E_g^{\text{QAOA}} = \min_{\boldsymbol{\alpha},\boldsymbol{\beta}} \langle \psi(\boldsymbol{\alpha},\boldsymbol{\beta})| \, \mathcal{H}_{\text{SAT}} \, |\psi(\boldsymbol{\alpha},\boldsymbol{\beta})\rangle . \tag{4}$$

We numerically study E_g^{QAOA} as a function of clause density α, for p-depth QAOA circuit on randomly generated 3-SAT and 2-SAT instances (See Fig. 1). For some critical depth p^*, QAOA returns the exact ground state energies for both 3-SAT and 2-SAT instances up-to a set tolerance. We fix the tolerance as a condition on the overlap between the QAOA generated state and the exact ground state which can be calculated as follows:

Let $\{|\text{gs}_i\rangle\}$ be the d degenerate ground states of $\mathcal{H}_{\text{SAT}}$ then the overlap,

$$\eta = \sum_{i=1}^{d} |\langle \psi_p(\boldsymbol{\alpha},\boldsymbol{\beta}) | \text{gs}_i \rangle|^2. \tag{5}$$

The critical depth is then defined as the minimum circuit depth for which the algorithm attains $\eta > 0.99$. Numerical investigation illustrates that the critical depth depends on the problem instance non-trivially. We observe

instances to the left of the phase transition, $\alpha < \alpha_c$ require a QAOA circuit with depth p^* which depends on α to recover exact ground state energies. For instances, $\alpha > \alpha_c$, critical depth p^* does not depend on α and we instead find that QAOA converges to the exact ground state energies simultaneously for all instances to the right side of the transition. Note in particular that this does not coincide with the algorithmic phase transition point exhibited in 3-SAT, although the critical depth of exhibited reachability deficits is closer for 2-SAT.

Reachability Deficits. QAOA on 3-SAT and 2-SAT instances exhibit poor recovery of ground state energies past a critical circuit depth p^*, whereas p^* has a strong dependence on the problem density. For $p < p^*$ optimization in equation (4) cannot recover exact energies due to the deficiency of states that QAOA can reach. This deficiency arises from the structure of QAOA anzats (1) and (2). Since the ansatz are created according to the problem Hamiltonian $\mathcal{H}$, and the driver Hamiltonian $\mathcal{H}_x$, the circuit depth needed for QAOA to recover exact ground state energies depends on both $\mathcal{H}$ and $\mathcal{H}_x$. With the standard QAOA driver we observe the critical depth to depend on the clause density of SAT instances. A similar dependence is also observed when we modify QAOA with a new driver $\mathcal{H}_x = |+\rangle\langle+|^{\otimes n}$ (see Fig. 2). The modified version requires lower circuit depths for achieving similar performance as standard QAOA but still exhibits reachability deficits. Based on these findings, QAOA suffers from reachability deficits for circuit depths $p < p^*$ where p^* is dependent on the problem density.

Reachability deficits are different from barren plateaus [1], where randomly parameterised quantum circuits for large problem sizes have exponentially low success in finding states that minimize the objective function. In the case of barren plateaus the state that achieves global minima of the objective function is accessible but choosing initial parameters randomly have greater probability to set the initial guess on a plateau of states where evaluation of gradients concentrates to zero. In contrast, irrespective of the initial parameter setting, QAOA with depth $p < p^*$ cannot reach optimal values as the corresponding state that achieves it becomes inaccessible.

Variational Grover Search. As expected we recover the critical-depth when restricting QAOA to fixed problem densities. One such example is the variational Grover Search model described in [10, 19]. This model can be solved analytically to recover the critical depth needed for QAOA to return exact ground state energies.

Variational Grover search can be thought of as QAOA with the following setting,

$$\mathcal{H} = |\omega\rangle\langle\omega|$$

and

$$\mathcal{H}_x = |+\rangle\langle+|^{\otimes n},$$

where $|\omega\rangle \in \mathbb{C}_2^{\otimes n}$ is the objective state we are searching for. Hence the objective function of interest here is the minimization of the expected value of the Hamiltonian $\mathcal{H} = \mathbb{1} - |\omega\rangle\langle\omega|$ over the QAOA ansatz state $|\psi(\boldsymbol{\alpha}, \boldsymbol{\beta})\rangle$ or,

$$\min_{\boldsymbol{\alpha},\boldsymbol{\beta}} \langle(\mathbb{1} - |\omega\rangle\langle\omega|)\rangle_{|\psi(\boldsymbol{\alpha},\boldsymbol{\beta})\rangle} = \min_{\boldsymbol{\alpha},\boldsymbol{\beta}} \left(1 - |\langle\omega|\psi(\boldsymbol{\alpha}, \boldsymbol{\beta})\rangle|^2\right). \tag{6}$$

The unitary gates that appear in equation (2) can be simplified into the following expressions;

$$\begin{aligned} \exp\{-i\alpha_k \mathcal{H}\} &= \exp\{-i\alpha_k |\omega\rangle\langle\omega|\} \\ &= \mathbb{1} + \left(e^{-i\alpha_k} - 1\right) |\omega\rangle\langle\omega|, \end{aligned} \tag{7}$$

similarly,

$$\begin{aligned} \exp\{-i\beta_k \mathcal{H}_x\} &= \exp\left\{-i\beta_k |+\rangle\langle+|^{\otimes n}\right\} \\ &= \mathbb{1} + \left(e^{-i\beta_k} - 1\right) |+\rangle\langle+|^{\otimes n}. \end{aligned} \tag{8}$$

We can then write the prepared ansatz state from a p-depth QAOA circuit as,

$$|\psi_p(\boldsymbol{\alpha}, \boldsymbol{\beta})\rangle = \mathrm{A}_p \frac{1}{\sqrt{\mathrm{N} - 1}} \sum_{x \neq \omega} |x\rangle + \mathrm{B}_p |\omega\rangle, \tag{9}$$

where, the amplitudes of one step can be related to the amplitudes of the next step via the recursive application of the matrix,

$$M_p = \begin{pmatrix} 1 + \frac{a(\mathrm{N}-1)}{N} & -a\,(b+1)\,\frac{\sqrt{\mathrm{N}-1}}{N} \\ -a\frac{\sqrt{\mathrm{N}-1}}{N} & (b+1)\left(1 + \frac{a}{\mathrm{N}}\right) \end{pmatrix}. \tag{10}$$

Here, $a = e^{-i\alpha_p} - 1$, $b = e^{-i\beta_p} - 1$ and $\mathrm{N} = 2^n$. Substituting equation (9) in equation (6) we obtain the approximated energy as

$$E_g^{\mathrm{QAOA}} = 1 - |B_p|^2. \tag{11}$$

Minimization in equation (6) is done numerically and the approximated energy as a function of circuit-depth is computed (see Fig. 3). For each problem size it is observed that approximated energy converges to the exact ground state energy $E_g = 0$, when the circuit-depth reaches the critical value, p^*. At this depth, QAOA is able to exactly recover $|\psi_{p^*}(\boldsymbol{\alpha^*}, \boldsymbol{\beta^*})\rangle = |\omega\rangle$ for some set of parameters $\boldsymbol{\alpha^*}$ and $\boldsymbol{\beta^*}$.

If we set $p < p^*$, the minimization in equation (6) terminates with $E_g^{QAOA} > 0$. This implies that in equation

(9) $|A_p|^2 \neq 0$. It is evident that in such a case, QAOA cannot reach the state $|\omega\rangle$. The reachability deficit is removed only when the QAOA circuit is set with $p \geq p^*$. To establish the dependence of p^* on the problem density, we increase n, the size of the search space and recover a Grover scaling, $\mathcal{O}(\sqrt{N})$ for p^*.

Discussion. QAOA has been applied many times throughout the literature, with many findings that reporting its surprising success. However, findings todate appear to be implicitly constrained to instances of low-problem density (the ratio of an instances constraints to variables). Hence, considered instances are not representative of the full range of statistical likely examples, and are at best only representative of the low-density subset. It is precisely this low-density subset which appears not to exhibit reachability deficits.

Interestingly, we found little dependence of QAOA's ability to approximate the ground state energy between 3-SAT (NP-hard to minimize) and 2-SAT (efficiently minimized) instances. Instead, both 3-SAT and 2-SAT appear to exhibit strong dependence of the algorithms performance on the instances problem density.

We observe that instances with $\alpha < \alpha_c$ require low depth QAOA circuits when compared to instances $\alpha > \alpha_c$ which require higher depths to approximate the minimum of an objective function up-to a given accuracy. This is rather different than the computational phase transition in Boolean satisfiability. Indeed, traditional classical algorithms exhibit fleeting resources (computational time) at the phase transition and it is commonly believed that most hard instances of SAT are concentrated near this transition. Although instances to the right ($\alpha > \alpha_c$) are considered easy classically and hence require less computational resources, the same is not observed in QAOA.

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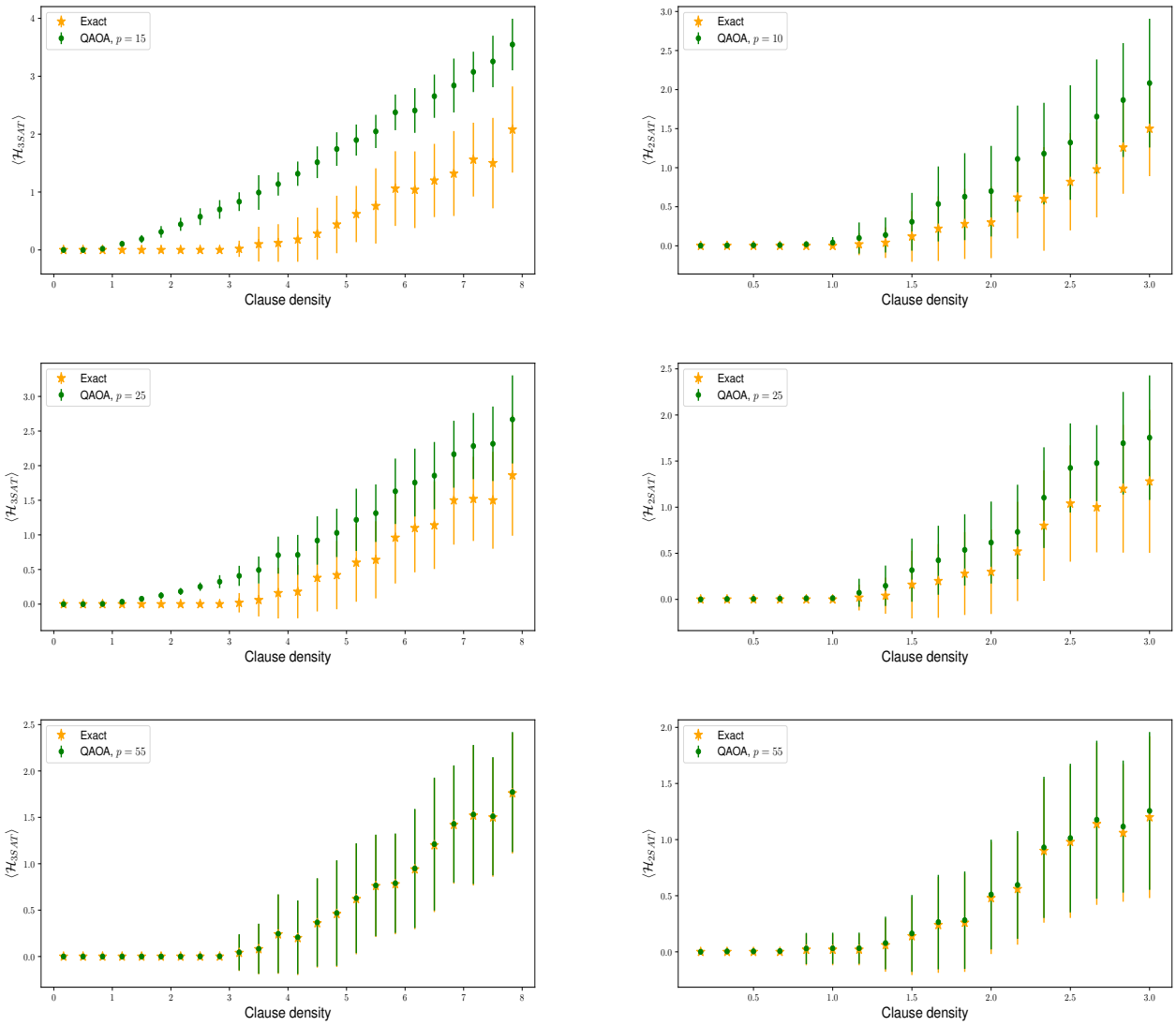

Figure 1. Energy versus clause density for 3-SAT (Left) and 2-SAT (Right). Dots show the averaged energies obtained from QAOA and stars show the exact values averaged on 50 randomly generated SAT instances for $n = 6$. Plots also show convergence to exact values for increasing depth.

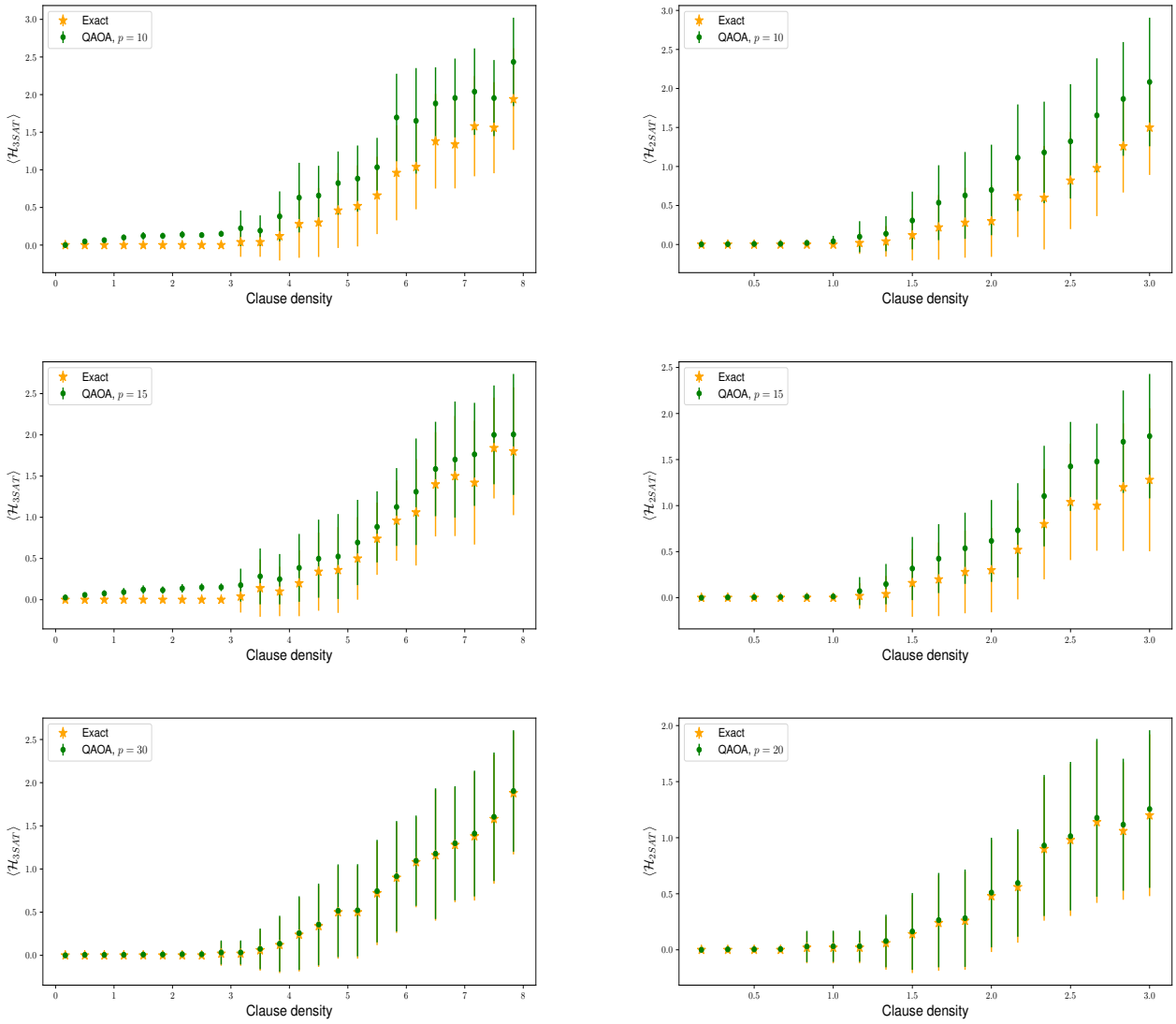

Figure 2. Energy versus clause density for 3-SAT (Left) and 2-SAT (Right) for QAOA with driver Hamiltonian, $\mathcal{H}_x = |+\rangle\langle+|^{\otimes n}$. Dots show the averaged energies obtained from QAOA and stars show the exact values averaged on 50 randomly generated SAT instances for $n = 6$. Plots also show convergence to exact values for increasing depth.

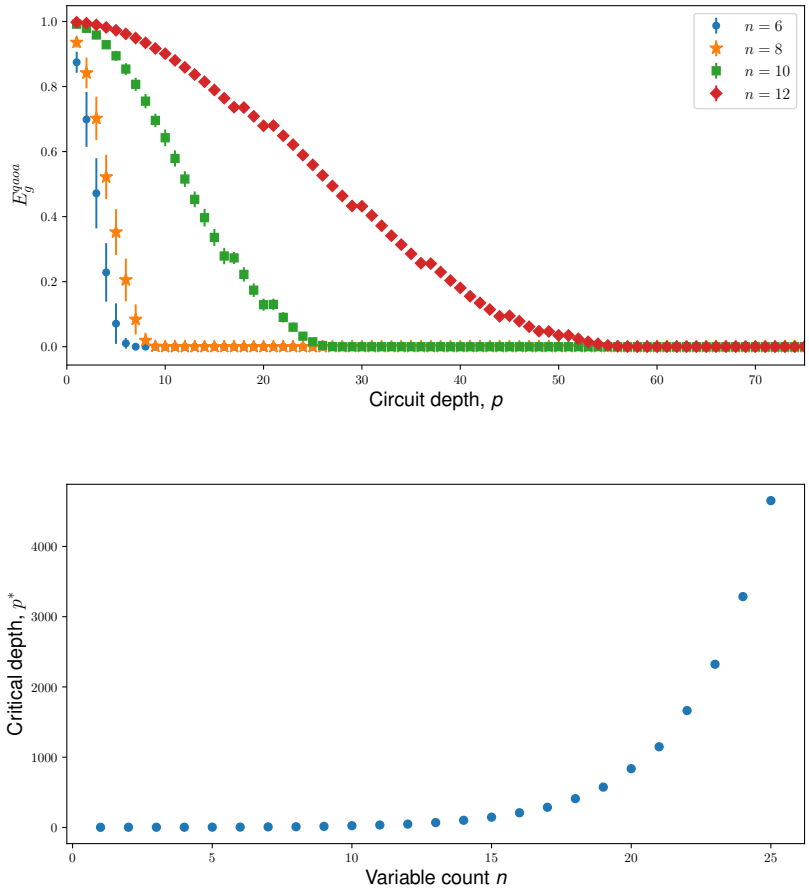

Figure 3. Top: Convergence to exact ground state energy as a function of QAOA circuit depth for the variational Grover search model on search space size, $n = 6, 8, 10$ and 12. Bottom: Scaling of critical depth p^* with variable count, n.