Enhancing QAOA Ansatz via Multi-Parameterized Layer and Blockwise Optimization

Francesca De Falco, Simone Piperno, Leonardo Lavagna,
Andrea Ceschini, Antonello Rosato, and Massimo Panella

Department of Information Engineering, Electronics and Telecommunications,
University of Rome "La Sapienza", 00184 Rome, Italy
Email: {francesca.defalco, simone.piperno, leonardo.lavagna, andrea.ceschini,
antonello.rosato, massimo.panella}@uniroma1.it

1 Introduction and Scope

Recently, the Quantum Approximate Optimization Algorithm (QAOA) has emerged as a powerful tool for addressing complex combinatorial problems [1]. QAOA leverages the inherent parallelism of quantum systems to efficiently find approximate solutions, showing great promise in real-world applications [2]. In particular, quantum advantage is proved in specific problem instances, highlighting the practical viability of QAOA along with its potential to outperform classical algorithms [3], [4]

Although QAOA has stood out as a leading candidate for near-term Noisy Intermediate-Scale Quantum (NISQ) applications [5], maximizing the performance of QAOA still remains a challenge, particularly in scenarios with long circuit depths and complex optimization landscapes [3]. Furthermore, QAOA optimization is characterized by a multitude of factors, including the topology of the optimization problem, the number of involved qubits, and the chosen parameterization of the quantum circuit. These factors collectively contribute to the landscape's ruggedness, with several local minima and saddle points that impede efficient parameters' exploration [6]. As a result, finding the global optimum by QAOA is increasingly challenging, especially as the size of the problem grows [7].

In this paper, we present a novel approach to enhance the performance of QAOA through a blockwise optimization strategy and the addition of a suitable layered ansatz after the last layer of the QAOA circuit; we will refer to this approach as Enhanced QAOA (EQAOA). Specifically, we introduce a method that iteratively optimizes both the standard QAOA circuit and the custom ansatz, culminating in a joint optimization phase. The intuitive rationale behind this algorithm is to leverage the strengths of both the QAOA's structured optimization, over problem-specific Hamiltonians, and the flexibility of a parameterized ansatz in order to explore a more extensive solution space. This mixed strategy aims at significantly improving both the convergence rate and quality of the final solution, particularly for the Maximum Cut (MaxCut) problem.

The effectiveness of the proposed methodology is proved through several experiments on complete, Erdős-Rényi and random 3-regular graphs. By employing custom ansatz layers alongside standard QAOA components and blockwise optimization, we achieve success probabilities exceeding 90% even on random graphs with up to 12 nodes. Notably, denoting with p the number of QAOA cost and mixer operator layers, our approach with $p = 1$ and enough ansatz layers outperforms the vanilla QAOA methodology with higher p values and no ansatz layers, yielding improvements over 10% in success probability on random graphs even when compared to QAOA circuits with large values of p.

2 Enhanced QAOA

Our EQAOA approach involves a blockwise optimization of the QAOA with a custom ansatz placed after the last layer of the QAOA. Using a blockwise optimization enables an iterative refinement process that aims at fine tuning the quantum circuit for improved performance.

First, we begin by optimizing the parameters of the standard QAOA circuit, in order to find optimal weights that maximize its performance for a given optimization problem. Next, we introduce a custom ansatz into the QAOA framework while keeping the previously optimized QAOA weights fixed; we expect this additional trainable layer to enhance the expressiveness of the quantum circuit, although further investigations will be necessary in this regard. Finally, we optimize the whole circuit by using a joint optimization that will ensure the coherence between the QAOA layers and the added ansatz. A detailed pseudocode description of the EQAOA procedure is summarized in Algorithm 1.

The proposed EQAOA method empirically demonstrates several advantages over traditional QAOA. Firstly, it seems to provide a systematic way to incorporate additional expressiveness into the quantum circuit through the introduction of an extra trainable component. Secondly, the complexity of the parameter space is reduced thanks to the blockwise optimization, making the overall optimization process more efficient and less prone to local minima.

ALGORITHM 1: Pseudocode of the EQAOA Procedure.

input: hyperparameters related to the optimization (i.e. 'maxiter', etc.) and to the EQAOA circuit (p, number of layers, etc.)

setup: experiments can be performed by varying input data and test conditions.

loop for m runs:

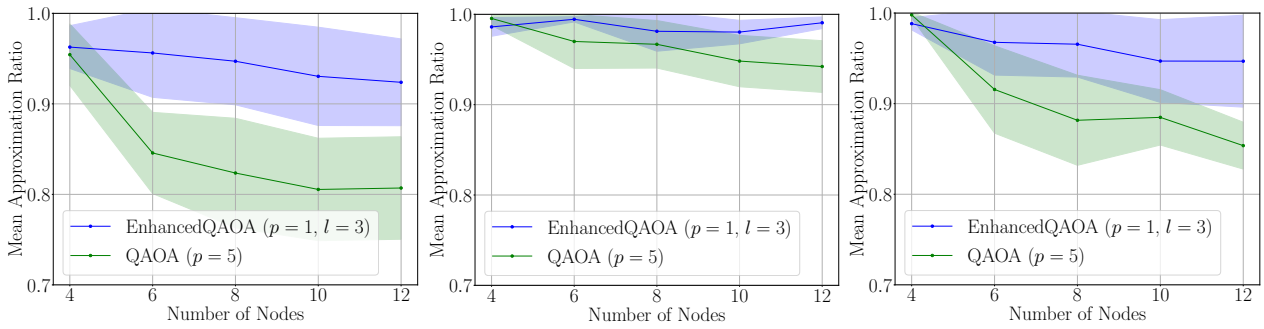
1. **QAOA circuit preparation:** Preparation of the initial state as a uniform superposition using Hadamard gates (H):
$$|\psi_0\rangle := H^{\otimes n}|0\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_z |z\rangle \,.$$
2. **Computation** of cost operator $U_{g_\Gamma}(\gamma_k) = e^{-i\gamma_k g_\Gamma}$ and a mixer operation $U(\beta_k) = e^{-i\beta_k \sum_{j=1}^n \sigma_x^{(j)}}$, where $\gamma_k \in [0, 2\pi)$ and $\beta_k \in [0, \pi)$ are randomly chosen angles.
3. **Vanilla QAOA optimization:** Update the set of of parameters $\gamma^* = (\gamma_1^*, \ldots, \gamma_p^*)$ and $\beta^* = (\beta_1^*, \ldots, \beta_p^*)$ from the optimization of the vanilla QAOA.
4. **Custom ansatz optimization:** optimization of the ansatz parameters $\theta^* = (\theta_1^*, \ldots, \theta_l^*)$, keeping the previously optimized QAOA parameters fixed and with the introduction of a custom ansatz after the last layer of the QAOA circuit.
5. **Entire EQAOA final optimization:** obtain the final parameters $\gamma^{**} = (\gamma_1^{**}, \ldots, \gamma_p^{**})$, $\beta^{**} = (\beta_1^{**}, \ldots, \beta_p^{**})$, and $\theta^{**} = (\theta_1^{**}, \ldots, \theta_l^{**})$ via optimization of the entire EQAOA.

3 Experiments and Discussion

We focus on the MaxCut problem as the paradigmatic problem for QAOA. Our study encompasses complete graphs, random graphs with 50% edge probability and random 3-regular graphs with node sizes ranging from 4 to 12. For each graph type, we generate 10 different instances per node count, but for complete graphs (only one per node count) and 4-node 3-regular graphs (only one), ensuring a diverse range of graph structures for comprehensive analysis.

In this experimental setup, we perform 10 independent runs for each graph instance. The optimization is conducted using the Constrained Optimization By Linear Approximation (COBYLA) optimizer, setting 10000 as the maximum number of function evaluations ('maxiter'), 2 as the reasonable initial changes to the variables ('rhobeg'), 0.0002 as the final accuracy in the optimization ('tol'). The additional ansatz in the EQAOA is made up of l layers of Matchgate circuit [8], and a final layer of parametrized R_y gates on each qubit. Both the vanilla QAOA and the EQAOA are tested by varying the QAOA level p from 1 to 5; the depth l of the ansatz used in the EQAOA ranges from 1 to 3.

The results in Fig. 1 show the worthiness of the proposed approach. Across the different types of graphs, EQAOA achieves up to a 10% higher approximation ratio than the vanilla QAOA. Remarkably, EQAOA yields better results with $p = 1$ and $l = 3$ than the standard QAOA does with $p = 5$.



(a) Random Erdos-Rényi Graphs (b) Complete Graphs (c) Random 3-Regular Graphs

Figure 1: Mean Approximation Ratio versus the number of nodes for the different types of graphs: proposed EAQOA (blue); standard QAOA (green). The colored area is the standard deviation across different runs and graph instances.

Our findings underscore the potential of blockwise optimization strategies in overcoming the limitations of standard QAOA methodologies. This is further proved in Fig. 2, where a comparison of probability distributions between the proposed EQAOA and the vanilla QAOA for MaxCut states is reported. Future works will explore the implementation of EQAOA on near-term quantum hardware and its application to a broader range of optimization tasks.

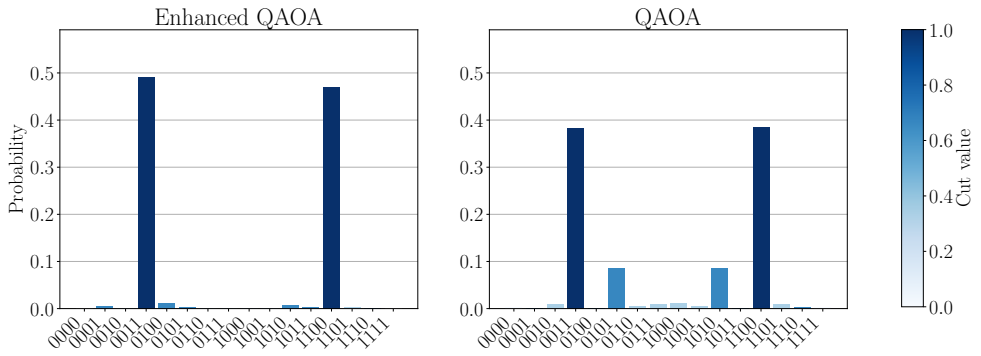


Figure 2: Comparison of probability distributions between our EQAOA (left) and the vanilla QAOA (right) for MaxCut states.

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