# QAS-BO : Quantum Architecture Search Based on Bayesian Optimization Applied to Variational Quantum Algorithms

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***Abstract*— In the era of Noisy Intermediate-Scale Quantum (NISQ) computing, traditional quantum algorithms face the challenges of limited number of qubits, noise and decoherence. In order to address these issues, we propose a Quantum Architecture Search (QAS) method driven by Bayesian Optimization (BO), which is applied to variational quantum algorithms. In this work, QAS is regarded as a fixed-scale sampling problem. We innovatively propose a quantum gate pool and use a parameterized probabilistic model to dynamically determine the optimal quantum gate for each position in the quantum circuit, thus optimizing the circuit structure. Through using a gradient-free BO method based on radial basis function, we adaptively design end-to-end quantum circuits, significantly reducing circuit depths and improving computational accuracy. We conducted experiments on ground state energy estimation in quantum chemistry and combinatorial optimization problem. The experimental results show that our method is significantly superior to traditional methods and other meta-heuristic search methods in accuracy and efficiency. Our method not only reduces the depth of quantum circuits by up to 85% under a certain accuracy, but also improves the accuracy rate to nearly 100% in combinatorial optimization problem. This provides a powerful and efficient tool for designing optimal quantum circuits and promotes the practical application of quantum algorithms in the NISQ era.**

## I. INTRODUCTION

The arrival of Noisy Intermediate-Scale Quantum (NISQ) era brings opportunities and challenges to quantum computing. Traditional quantum algorithms like Quantum Phase Estimation (QPE) [1] demand numerous quantum gates and impose stringent demands on hardware. In the NISQ era, limited qubits and decoherence hinder long-term state maintenance and complex sequences. This causes QPE circuit depth to exceed NISQ hardware capabilities, restricting practical application.

In order to solve this problem, Peruzzo et al. proposed the Variational Quantum Eigensolver (VQE), which greatly reduced the required circuit depth [2]. However, VQE still faces the Barren Plateau (BP) problem [3], where the cost function gradients become extremely small when optimizing large Parameterized Quantum Circuits (PQCs), making the optimization process difficult and inefficient.

In this paper, we propose a novel method to optimize PQCs by using Bayesian Optimization (BO) driven Quantum Architecture Search (QAS) (called QAS-BO) (Figure 1). This is a powerful global optimization strategy without gradient, which can alleviate the BP problem. The whole algorithm aims at automatically designing end-to-end quantum circuits and dynamically adjusting the quantum architecture. Through heuristic search circuit and gaussian distribution to adjust the probability of quantum gate selection, our method does not need special domain knowledge, thus realizing the high automation of quantum circuit design process and the optimization of resource use and calculation efficiency.

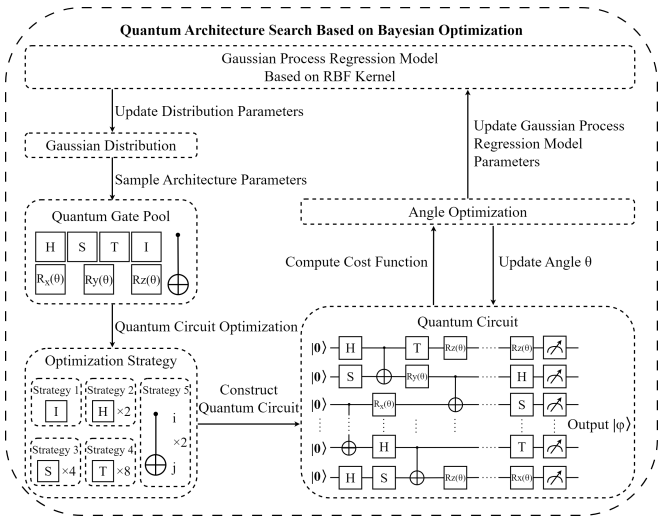


Fig. 1. QAS-BO method flow chart

Experimental results show that our QAS framework can effectively find the optimal quantum circuit for a specific quantum computing task, which further promotes the development of quantum computing technology.

## II. RELATED WORKS

### A. Quantum Architecture Search

The purpose of QAS is to automatically design PQCs to optimize and accelerate the performance of VQAs, reducing manual workload and discovering task-specific architectures.

Recently, research progress in QAS has focused on machine learning techniques: Reinforcement Learning (RL) [4] and Generative Adversarial Networks (GANs) [5] have shown promising results, while heuristic methods such as Particle Swarm Optimization (PSO) [6], and Simulated Annealing (SA) [7] have also been widely used. These methods integrate the advantages of classical and quantum computing, while taking into account hardware characteristics and noise environments.

Zhang et al. proposed a Differentiable Quantum Architecture Search (DQAS) method based on the Gumbel-Softmax

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techniques [8]. By transforming the discrete design problem of quantum circuits into a differentiable continuous optimization problem, the automatic design of quantum circuit is realized.

The above method is improved and expanded to be the Q-DARTS [9]. The extended algorithm includes two versions: macro search and micro search. And the setting of the parameter sharing pool is cancelled.

In our work, we regard the QAS as a fixed-scale sampling problem, in which each position only corresponds to a single parameter. Compared with the DQAS and Q-DARTS, this method significantly reduces the complexity of QAS, which needs to optimize two parameters for each position.

### *B. Bayesian Optimization for Quantum Computing*

In recent years, the application of BO in quantum computing has made remarkable progress. Many works have demonstrated the potential and effect of this optimization method in improving quantum algorithm and quantum circuit design.

Duong et al. improved the performance of BO in the search of Quantum Neural Network (QNN) architectures by introducing a quantum gate distance metric [10]. Nicoli et al. put forward a BO method driven by physical information in their research [11]. They combined the intrinsic physical characteristics of VQE, introduced a new VQE kernel function and a new acquisition function named EMICoRe, and proposed an angle optimization method, which effectively reduced the posterior uncertainty.

Our method is different from [10], and aims at optimizing quantum circuits themselves directly. Optimizing a circuit instead of its matrix representation can avoid the complexity of matrix calculation, especially in high-dimensional space, which can significantly reduce the computational overhead. The optimization results can be directly mapped to the actual quantum hardware for verification and execution.

## III. OUR FRAMEWORK

We regard QAS as a fixed-scale sampling problem. We use the BO method to fine-tune the quantum architecture to optimize the circuit architecture. Then, combining with the prior knowledge in the quantum field, we further optimize the circuit design and effectively reduce the circuit depth to resist the influence of quantum decoherence. Finally, we use the COBYLA algorithm [12] to optimize the angle parameters in order to achieve higher efficiency and stability.

### *A. Quantum Gate Pool Setting and Mapping of Quantum Circuits*

We propose an innovative framework for the selection and layout of quantum gates, aiming at automating the design process of quantum circuits. This framework uses parameterized probabilistic model to dynamically determine the optimal quantum gate for each position in the quantum circuit, thus optimizing the circuit structure.

Our method integrates a quantum gate pool given in (1). It is complete, which means that any unitary circuit

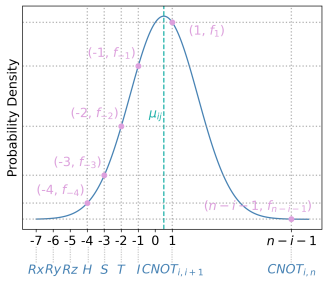


Fig. 2. Sampling of $C_{ij}$ from the Gaussian distribution

can be represented only by the gates in the quantum gate pool. The quantum gate pool $\mathcal{G}$ is composed of a universal quantum gate set $\mathcal{G}_1$, commonly used rotation gate set $\mathcal{G}_2$ and the $I$ gate to ensure the flexibility and robustness of the architecture.

$$\begin{aligned} \mathcal{G}_1 &= \{H, S, T, CNOT\}, \\ \mathcal{G}_2 &= \{Rx(\theta), Ry(\theta), Rz(\theta)\} \\ \mathcal{G} &= \mathcal{G}_1 \cup \mathcal{G}_2 \cup \{I\} \end{aligned} \tag{1}$$

For a quantum circuit with $n$ qubits and $m$ layers, any unitary operation $U$ can be represented by Equation (2). The unitary matrix $U_{ij}$ in the $i$-th qubit and $j$-th layer of the circuit is determined by the corresponding quantum gate $C_{ij}$.

$$\begin{aligned} U &= \prod_{j=1}^{m} \bigotimes_{i=1}^{n} U_{ij}, \quad U_{ij} = \begin{cases} C_{ij}, & \text{if } C_{ij} \in \mathcal{G}_i \\ I, & \text{otherwise.} \end{cases} \\ \mathcal{G}_i &= \{R_x(\theta), R_y(\theta), R_z(\theta), H, S, T, I\} \\ &\quad \cup \{CNOT_{i,i+1}, \ldots, CNOT_{i,n}\} \end{aligned} \tag{2}$$

The quantum gate $C_{ij}$ for the $i$-th qubit and the $j$-th layer position is derived from the probability density function of the Gaussian distribution in (3) (see also Figure 2).

$$\begin{aligned} p(C_{ij} = \mathcal{G}_i^{(k)}) &= \max_k f(k|\mu_{ij}, \sigma^2) \\ f(k|\mu_{ij}, \sigma^2) &= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(k-\mu_{ij})^2}{2\sigma^2}} \end{aligned} \tag{3}$$

where $\mathcal{G}_i^{(k)}$ is the $k$-th quantum gate in $\mathcal{G}_i$. $\mu_{ij}$ is the mean corresponding to the $i$-th qubit and the $j$-th layer position. $\sigma$ is the standard deviation.

### *B. Quantum Architecture Search Based on Bayesian Optimization*

Bayesian optimization (BO) is an efficient global optimization method, especially suitable for optimizing complex black-box functions with high cost and noise. The detailed algorithm workflow can be found in Algorithm 1.

In our work, we comprehensively consider a variety of noise sources, including quantum decoherence, environmental noise, control error and the error of precise adjustment of pulse amplitude and duration due to the limitation of practical operations [13]. The representative model for these noise sources is $f_{NOISE} \sim \mathcal{GP}(0, \sigma^2_{NOISE})$.

**Algorithm 1** Bayesian Optimization Algorithm with Noise

**Input:** Black box function $E(\mu)$, search space $\mu \in \mathbb{D}^{mn} \subset \mathbb{R}^{mn}$

**Output:** $E_m = \min_\mu E(\mu)$

1: Set the prior for $E(\mu)$ following the GPR model based on the RBF kernel.
2: **for** $i = 1$ to $N_C$ **do**
3: Sample initial points $\mu_i \in \mathbb{D}^{mn}$ randomly.
4: Initial training set $\Gamma \leftarrow \Gamma \cup \{\mu_i, E(\mu_i)\}$.
5: **end for**
6: Set $E_m = \min_j \left[\{E(\mu_i)\}_{i=1}^{N_C}\right]$.
7: Optimize hyperparameters $\ell, \sigma^2$ and $\sigma^2_{NOISE}$ according to $\Gamma$.
8: **for** $n = 1$ to $N_{BO}$ **do**
9: Update the posterior distribution of $E(\mu)$ by using the hyperparameters $\ell, \sigma^2$ and $\sigma^2_{NOISE}$.
10: Select the best sampling point $\widetilde{\mu}$ by using the acquisition function based on posterior distribution.
11: **if** $E(\widetilde{\mu}) < E_m$ **then**
12: $E_m \leftarrow E(\widetilde{\mu})$.
13: **end if**
14: Update training set $\Gamma \leftarrow \Gamma \cup \{\widetilde{\mu}, E(\widetilde{\mu})\}$.
15: Optimize hyperparameters $\ell, \sigma^2$ and $\sigma^2_{NOISE}$ according to $\Gamma$.
16: **end for**

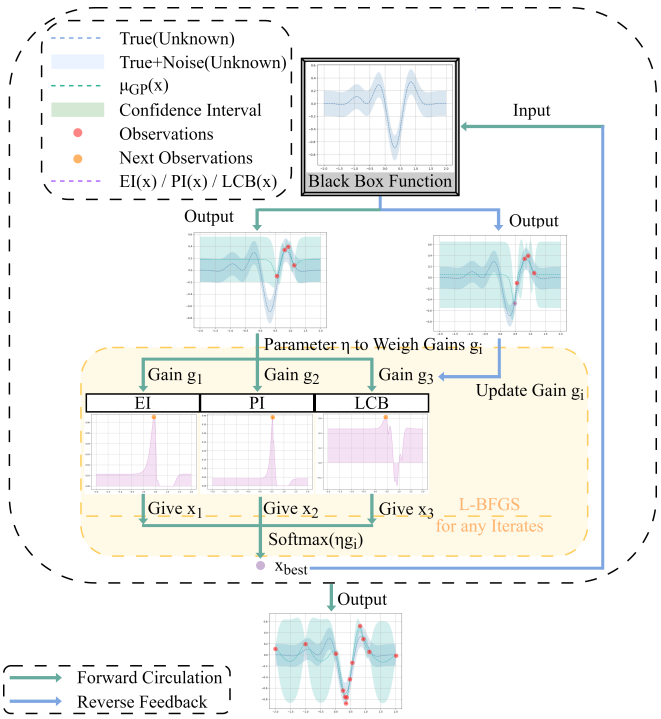


Fig. 3. Implementation of the adaptive acquisition function strategy based on MAB principle.The figure shows a one-dimensional special case, which is only used to clearly show the working principle of this strategy.

The optimization process revolves around adjusting the Gaussian distribution parameters representing the circuit architecture.

We establish the GPR model based on the Radial Basis Function (RBF) kernel (4) as a proxy model to approximate the unknown objective function. The model is used to predict and update the optimization process of quantum circuit parameters in order to minimize the objective function.

$$\begin{aligned} f(x) &\sim \mathcal{GP}(m(x), k(x, x')) \\ k(x, x') &= \sigma^2 \exp\left(-\frac{\|x - x'\|^2}{2l^2}\right) + \sigma^2_{NOISE} I \end{aligned} \tag{4}$$

where $x, x'$ are elements in the input space, and $m(x)$ is a mean function, which provides the expected output value for the input point $x$. Here $\sigma^2$ represents the fluctuation of the function between different node values, and $l$ represents the degree of correlation between nodes. Note that $\sigma^2_{NOISE}$ represents the variance of the noise model, which describes the fluctuation of the observed values around the real values.

For the given training set $\Gamma = \{(\mu_i, E(\mu_i))\}_{i=1}^z$, the Log Marginal Likelihood (LML) of the GPR model is defined as:

$$\begin{aligned} &\log p(\mathbf{E}(\mathbf{N}) \mid \mathbf{N}, \ell, \sigma^2, \sigma^2_{NOISE}) \\ &= -\frac{1}{2}\mathbf{E}(\mathbf{N})^T \mathbf{K}^{-1} \mathbf{E}(\mathbf{N}) - \frac{1}{2}\log|\mathbf{K}| - \frac{z}{2}\log 2\pi \end{aligned} \tag{5}$$

where $\mathbf{N} = (\mu_1, \ldots, \mu_z)$ represents the matrix of input data, $\mathbf{E}(\mathbf{N}) = (E(\mu_1), \ldots, E(\mu_z))^T$ represents the vector of the target output, $\mathbf{K} = (k(\mu_i, \mu_j))^{z \times z}$ represents the covariance matrix.

The optimization of the key hyperparameters $\ell, \sigma^2, \sigma^2_{NOISE}$ in the GPR model aims to find the parameter set that maximizes the LML, achieved via the Limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) algorithm. L-BFGS updates parameters by computing gradients of LML with respect to hyperparameters, enabling the kernel function to capture data correlations and naturally integrate noise handling. This approach simplifies model representation and enhances computational efficiency.

The new sampling point $\widetilde{\mu}$ is selected by maximizing the acquisition function. There are three main acquisition functions: Expected Improvement (EI), Probability Improvement (PI) and Lower Confidence Bound (LCB) [14]. EI (6) tends to search carefully around the known optimal value.

$$\begin{aligned} EI(\mu) &= \mathbb{E}\left[\max\left(E(\mu) - E(\widetilde{\mu}), 0\right)\right] \\ &= \left(m(\mu) - E(\widetilde{\mu}) - \xi\right)\Phi(Z) + \sigma(\mu)\phi(Z) \end{aligned} \tag{6}$$

PI (7) tends to explore potential areas that have not been fully tested.

$$PI(\mu) = \Phi\left(\frac{m(\mu) - E(\widetilde{\mu}) - \xi}{\sigma(\mu)}\right) \tag{7}$$

And LCB (8) provides a trade-off between exploration and utilization.

$$LCB(\mu) = m(\mu) - \kappa\sigma(\mu) \tag{8}$$

where $m(\mu)$ represents the predicted mean at point $\mu$. $\sigma(\mu)$ represents the predicted standard deviation at point $\mu$, and $Z = \frac{m(\mu) - E(\widetilde{\mu})}{\sigma(\mu)}$. The term $\xi$ is a small exploration parameter. $\Phi(\cdot)$ and $\phi(\cdot)$ are the cumulative distribution function and

the probability density function of the standard normal distribution. $\kappa$ is a coefficient that balances exploration and exploitation, dynamically adjusted based on the number of optimization iterations.

Our research adopts the adaptive acquisition function strategy based on Multi-Armed Bandit (MAB) principle (Figure 3) [15]. By maintaining the historical performance log of each strategy, and using the softmax function (9) to calculate the selection probability, the strategy with better performance has a higher selection probability, but all strategies have the possibility of being selected.

$$softmax\left(\eta g_i\right) = \frac{e^{\eta g_i}}{\sum_j e^{\eta g_j}} \tag{9}$$

where $g_i$ is the gain weight of the $i$-th acquisition function, which represents the gain values of different acquisition functions (EI, PI, LCB). $\eta$ is an adjustment parameter to adjust the influence of different acquisition function weights. This method ensures the diversity and comprehensiveness of the selection of acquisition points by the acquisition function. The randomness is introduced to avoid over-reliance on the deterministic selection, which is helpful to explore the optimal solution and reduce the risk caused by single strategy deviation.

The whole optimization framework not only pursues the efficiency of parameter optimization, but also aims to improve the robustness and reliability of the algorithm in the face of complex practical environment. In addition, we use multi-core parallel computing to accelerate the optimization process and improve the overall computing efficiency. All experiments were conducted on a server with an Intel Xeon Silver 4210R CPU at 2.40 GHz, 40 cores, and 512 GB RAM.

## IV. APPLICATIONS

### A. Ground State Energy Estimation in Quantum Chemistry

VQE provides a new method for quantum chemistry to estimate the ground state energy of molecules efficiently. It approached the ground state solution of Schrodinger equation by simulating the quantum mechanical behavior of molecules on a quantum computer, thus providing a key theoretical basis for determining the most stable geometric configuration of molecules.

The main goal of VQE is to find the minimal energy state of a quantum system, named the energy of the ground state $E_{min}$. In this method, the system's total energy is described with the Hermitian operator Hamiltonian $H$, whose minimal eigenvalue corresponds to the ground state of the system. In VQE, the PQC performs the unitary transformation $U(\theta)$, known as $ansatz$ [16]. Then, it uses the ansatz to prepare the parametrized quantum state $|\psi(\theta)\rangle = U(\theta)|\psi_0\rangle$, where $|\psi_0\rangle$ is the initial quantum state. The parameters $\theta$ of the quantum circuit are iteratively adapted by the classical optimization algorithm to reach a minimum of the energy expectation value $E_{min}$ (10), which, in turn, corresponds to the energy

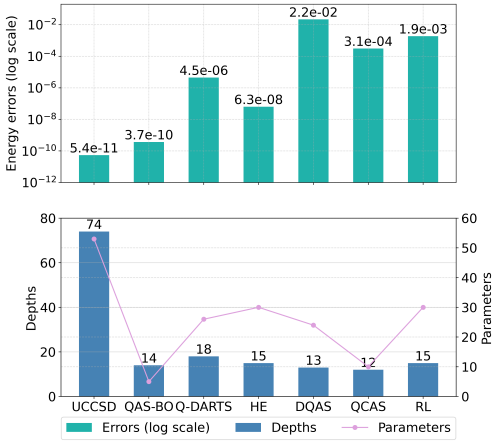


Fig. 4. $H_2$ Estimation: Energy error, depth, and parameters comparison

of the system's ground state.

$$\begin{aligned} E(\boldsymbol{\theta}) &= \langle\psi(\boldsymbol{\theta})|H|\psi(\boldsymbol{\theta})\rangle \\ E_{min} &\leq \min_{\theta} E\left(\theta\right) \end{aligned} \tag{10}$$

Our algorithm is compared with the Unitary Coupled Cluster Singles and Doubles (UCCSD) [17] method and the Hardware-Efficient (HE) [18] method in detail, with part of the results shown in Table I. As we can see, our algorithm is significantly superior to HE in energy calculation accuracy. Compared with the UCCSD, our algorithm is only one order of magnitude worse in energy accuracy, and the results of each experiment are within the range of chemical accuracy (That is, the error is less than 0.0016 Å). And when the simulation object becomes ions, especially systems with strong electron correlation or asymmetric electron distribution, the UCCSD ansatz shows obvious shortcomings.

In terms of quantum circuit depth, our algorithm shows a significant resource efficiency advantage. Compared with the depth required by the UCCSD, our algorithm greatly reduces the number of quantum gates required. This optimization makes the algorithm more feasible when dealing with large-scale molecular systems, especially under the existing quantum hardware conditions, as the number and depth of gate operations directly affect the practical application of the algorithm.

In addition, we made a deep comparative research on the $H_2$ molecule, and compared our method with other heuristic search methods, including Q-DARTS, DQAS, QCAS [19] and RL (Figure 4). The results show that our method can find quantum circuits with higher accuracy and shallower circuit depth than these known methods. In quantum computing, the deeper the circuit is, the more susceptible it is to noise, which will accelerate the process of quantum decoherence [20] and affect the accuracy and reliability of calculation. Our research results confirm that the optimized shallow circuit can effectively alleviate this problem and enhance the practicability of quantum computing.

TABLE I

COMPARISON OF ESTIMATION RESULTS FOR VARIOUS MOLECULES ACROSS DIFFERENT RANDOM SEEDS AND METHODS

| | **QAS-BO** | | | | UCCSD | | HE | |
|---|---|---|---|---|---|---|---|---|
| | Energy Error (Seed 0) | Energy Error (Seed 1) | Energy Error (Seed 2) | Avg depth | Energy Error | Depth | Energy Error | Depth |
| $HeH^+$ | $9.1 \times 10^{-10}$ | $7.6 \times 10^{-10}$ | $7.7 \times 10^{-10}$ | 9 | $6.5 \times 10^{-8}$ | 11 | $2.1 \times 10^{-7}$ | 17 |
| $H_2^+$ | $1.2 \times 10^{-9}$ | $2.9 \times 10^{-9}$ | $4.5 \times 10^{-9}$ | 21 | $6.1 \times 10^{-1}$ | 9 | $2.1 \times 10^{-6}$ | 23 |
| $H_2$ | $3.6 \times 10^{-10}$ | $3.7 \times 10^{-10}$ | $7.7 \times 10^{-10}$ | 17 | $5.4 \times 10^{-11}$ | 74 | $8.4 \times 10^{-6}$ | 15 |
| LiH-4 | $4.5 \times 10^{-6}$ | $5.3 \times 10^{-5}$ | $4.7 \times 10^{-6}$ | 33 | $2.3 \times 10^{-7}$ | 222 | $6.6 \times 10^{-4}$ | 19 |
| LiH-6 | $3.1 \times 10^{-4}$ | $2.5 \times 10^{-4}$ | $2.1 \times 10^{-4}$ | 46 | $2.3 \times 10^{-7}$ | 317 | $1.7 \times 10^{-3}$ | 21 |

TABLE II

EXPERIMENTAL RESULTS OF COMBINATORIAL OPTIMIZATION PROBLEM: COMPARATIVE ANALYSIS OF CIRCUIT DEPTH AND ACCURACY RATE, WHERE QAOA-$p$ REPRESENTS ANSATZ COMPOSED OF $p$ LAYERS OF $H_C$ AND $H_M$.

| | Unweighted Max-Cut-4 nodes | | | Unweighted Max-Cut-6 nodes | | | Unweighted Max-Cut-8 nodes | | |
|---|---|---|---|---|---|---|---|---|---|
| | **QAS-BO** | QAOA-3 | QAOA-4 | **QAS-BO** | QAOA-4 | QAOA-5 | **QAS-BO** | QAOA-4 | QAOA-5 |
| Depth | 24 | 44 | 57 | 27 | 87 | 106 | 40 | 63 | 76 |
| Accuracy | 100.00% | 87.50% | 100.00% | 100.00% | 29.30% | 46.38% | 100.00% | 90.43% | 89.45% |
| | Weighted Max-Cut-4 nodes | | | Weighted Max-Cut-6 nodes | | | Weighted Max-Cut-8 nodes | | |
| | **QAS-BO** | QAOA-6 | QAOA-7 | **QAS-BO** | QAOA-7 | QAOA-8 | **QAS-BO** | QAOA-8 | QAOA-10 |
| Depth | 27 | 47 | 54 | 30 | 144 | 163 | 46 | 94 | 114 |
| Accuracy | 100.00% | 94.82% | 98.54% | 100.00% | 52.25% | 27.25% | 96.19% | 20.41% | 41.89% |
| | NAE 3-SAT-4 literals | | | NAE 3-SAT-6 literals | | | NAE 3-SAT-8 literals | | |
| | **QAS-BO** | QAOA-4 | QAOA-5 | **QAS-BO** | QAOA-2 | QAOA-3 | **QAS-BO** | QAOA-4 | QAOA-5 |
| Depth | 10 | 30 | 37 | 19 | 46 | 57 | 50 | 68 | 81 |
| Accuracy | 100.00% | 98.73% | 100.00% | 100.00% | 8.92% | 12.32% | 100.00% | 4.59% | 10.21% |

### *B. Combinatorial Optimization Problem*

Combinatorial optimization problem is an important field in mathematical optimization, which mainly involves finding the optimal solution in the set of discrete objects that meet specific constraints. This problem is widely used in many practical fields, such as network design, scheduling, routing, planning and so on. As the problem size increases, the size of the solution space typically grows exponentially. Therefore, such problems are classified as classic NP-hard problems.

The Quantum Approximate Optimization Algorithm (QAOA) is an approximate optimization algorithm with polynomial time, which is used to solve combinatorial optimization problems [21]. For graphs with $n$ nodes, QAOA transforms a combinatorial optimization problem into a large sparse diagonal matrix $H_C$ (11), and its goal is to find the minimum eigenvalue of $H_C$. Classically, its time complexity is $O(2^n)$. From the view of quantum computing, these steps are realized by quantum circuits.

$$H_C = -\sum_{(i,j)\in E} \frac{I - Z_i Z_j}{2} \tag{11}$$

QAOA's quantum circuit has a fixed architecture, and its initial state is generally a uniform superposition state (12).

$$|+\rangle = \frac{1}{\sqrt{2^n}} \sum_{z=0}^{2^n-1} |z\rangle \tag{12}$$

The quantum circuit is formed by the cost Hamiltonian $H_C$ and the mixed Hamiltonian $H_M$ (13) which interact repeatedly. The former contains graph information, while the latter explores $2^n$ different combinations.

$$H_M = \sum_i X_i \tag{13}$$

By minimizing the quantum circuit energy (14), the optimal solution of the target problem can be solved.

$$\begin{aligned} |\psi(\theta)\rangle &= \prod_{l=1}^{p} e^{-i\beta_l H_M} e^{-i\gamma_l H_C} |+\rangle \\ E(\theta) &= \langle\psi(\theta)|H_C|\psi(\theta)\rangle, \theta = (\beta, \gamma) \\ \beta &= (\beta_1, \beta_2, \ldots, \beta_p), \gamma = (\gamma_1, \gamma_2, \ldots, \gamma_p) \end{aligned} \tag{14}$$

where $\beta_l$ and $\gamma_l$ denote the rotation parameters for $H_M$ and $H_C$ in the $l$-th layer, respectively.

By utilizing our algorithm to adaptively search for quantum circuits for unweighted Max-Cut problem, weighted Max-Cut problem and Not-All-Equal 3-Satisfiability (NAE 3-SAT), we have successfully designed quantum circuits with lower depth and higher accuracy. In 4-node, 6-node and 8-node problems (Table II), the accuracy of our method reaches 100%, and the required circuit depth is obviously lower than the QAOA algorithm. QAOA performs better on the unweighted Max-Cut problem under the same dimensions. However, its accuracy drops sharply for the weighted Max-Cut problem and the NAE-3SAT problem. This is because its ansatz fails to effectively capture critical information when the weights have large disparities or include negative values.

In the 10-node unweighted Max-Cut problem (Figure 5), the accuracy reaches 98.93%, far exceeding that of QAOA-4 (13.57%) and QAOA-5 (6.05%), while the depth is only 41, significantly lower than that of 93 and 112 of QAOA-4 and QAOA-5.

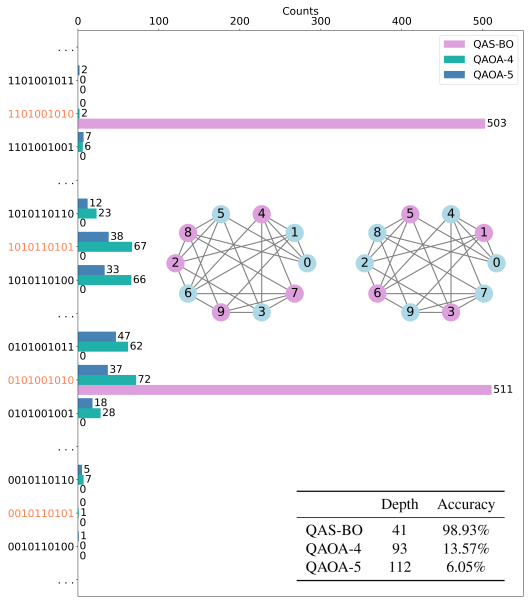


Fig. 5. The unweighted Max-Cut problem (10 nodes): Distribution of quantum states for different algorithms with 1024 measurements

We only need a few measurements to get the correct results. Of course, our method can make the accuracy reach 100% under the condition of increasing the circuit depth. The lower circuit depth enhances the anti-noise ability of the circuit and makes it more robust in the actual quantum computing environment. And the dimension of the search space accepted by our algorithm can be higher.

## V. DISCUSSION

The QAS method based on Bayesian Optimization proposed in this work shows excellent performance in dealing with complex quantum circuit design problems. The experimental results show that our method is significantly superior to benchmark methods in computational accuracy and circuit depth, especially when dealing with molecular ion systems with strong electron correlation or asymmetric electron distribution. In addition, our method also shows high accuracy and resource efficiency on the combinatorial optimization problem. And compared with ground state energy estimation in quantum chemistry, the acceptable search space dimension of the combinatorial optimization problem can be higher. The full paper and code can be found at https://github.com/igfbslwff1/QAS-BO.

Future work will focus on optimizing the search strategy in BO based on the characteristics of quantum computing problems, aiming to improve search efficiency and result accuracy.

## ACKNOWLEDGMENT

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