An initial condition robust outer-loop optimization strategy for a Quantum Approximate Optimization Algorithm

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Outer-loop optimization for a QAOA [1]

We will use the P5 Ising problem [2] as an ongoing example. The goal is to maximize H given a planar graph $G = (V, E)$.

$$H = -\sum_{(i,j)\in E} \sigma_i^z \sigma_j^z - \sum_{i\in V} \sigma_i^z$$

Using a p^{th} level QAOA, the goal then is to find

$$\max_{\beta,\gamma} C(\beta,\gamma)$$

where

$$C(\beta,\gamma) = \langle +^{\otimes n} | U_H^\dagger(\gamma_1) U_D^\dagger(\beta_1) \dots U_H^\dagger(\gamma_p) U_D^\dagger(\beta_p)\, H\, U_D(\beta_p) U_H(\gamma_p) \dots U_D(\beta_1) U_H(\gamma_1) | +^{\otimes n} \rangle$$

with

$$U_H(\gamma) = e^{-i\gamma H/2}$$
$$U_D(\beta) = \prod_{i=1}^{n} e^{-i\beta\sigma_i^x/2}$$

The landscape of C has many local optima, making it difficult to optimize and highly dependent on the initial choice of angles. One of the reasons that C is so hard to optimize is because of the difficulty of computing gradients and hessians of QAOA circuits, restricting us to gradient-free minimization methods that have slower convergence rates and worse overall performance. Most gradient-free minimization methods have only heuristic tendencies rather than performance guarantees. Consider, for example, the many local optima that various optimizers find in Fig 1. As system size increases, the spectral landscape becomes increasingly complex. As shown to the right, finding the global optima at $p = 1$ tends to give good results for larger p, thus a heuristic that avoids local optima at small p is needed.

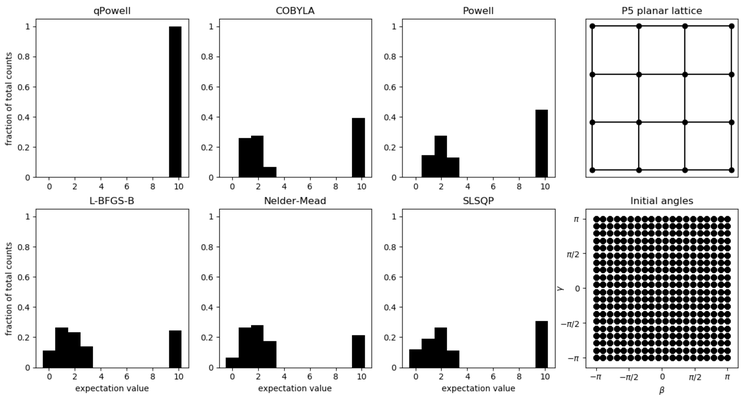

Fig: 1. Dependence of maximation on initial angles, for $p = 1$.

qPowell method

Often SciPy [3] minimization methods are used for the outer-loop parameter optimization for a QAOA. We have found their performance to vary dramatically depending on the initial angles provided, even at $p = 1$. We introduce a minimization method called *qPowell* that is a bounded variant of the Powell method [4]. We have found in all cases we tested that qPowell will converge to the global optima regardless of the initial angles provided for QAOA at $p = 1$. We tested all other SciPy minimization methods and found that none of them had this property. Fig 1 shows the distribution of the QAOA expectation value for the P5 Ising problem on a 4x4 planar graph when sweeping through parameter space for the initial conditions for various SciPy methods as well as qPowell. Notice that qPowell find the global optima every time.

The qPowell method is a conjugate direction method in which angles are restricted to be inside the hypercube in parameter space with side length 2π. At each iteration, there is a set of directions in parameter space. The minimizer will perform a line search along each direction individually to locate the optima along that direction. After each iteration, the directions are updated based on the previous update steps.

Fig 2 shows the path that the angle parameters take through an example P5 Ising $p = 1$ QAOA landscape when starting from the same initial conditions. Notice that qPowell does not get caught in the same local optima that COBYLA finds because the bounded line search is able to find a better optima.

A possible extension to qPowell is restricting the bounding hypercube more by using information about optimal angle tendencies as a function of index and p.

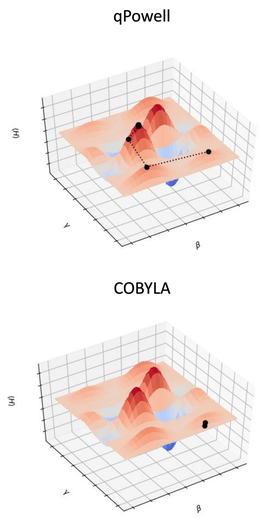

Fig: 2. Example qPowell vs COBYLA parameter path

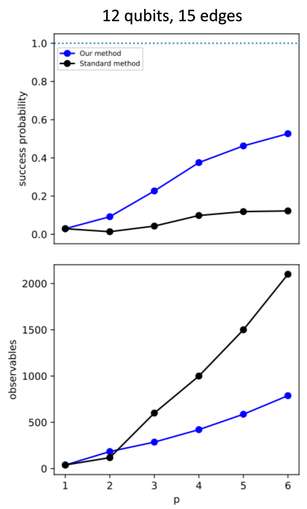

Fig: 3. Note that our method is consistent, but this is just one of many possible outcomes for the standard method.

Interpolation method [5]

The standard method for a QAOA is initializing $2p$ random angles and optimizing with a gradient-free minimization method. However, this method is highly dependent on the chosen initial angles and therefore returns inconsistent results as the number of qubits increases. Recently, an initialization strategy has been proposed in [5] that gives a heuristically good guess for the angles for QAOA at level p given an optimized QAOA circuit at level p-1. It is based on the observation that the angles tend to be smooth functions of their index, and therefore interpolating $2p - 2$ angles to $2p$ tends to be a good starting point. By using qPowell at level $p = 1$, and then initializing the starting angles at each subsequent level with the interpolation method, we find consistent results that are independent of the two initial chosen angles.

Figs 3 and 4 show this method versus the standard method for various P5 Ising instances, and Fig 4 includes elementary noise simulation using the noise model shown In Fig 5.

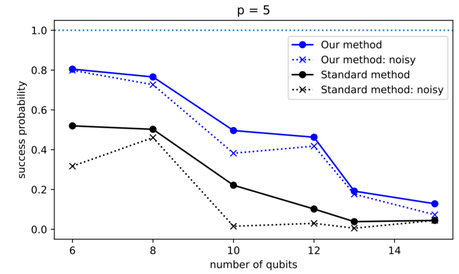

Fig: 4. Success probability as a function of qubits for $p = 5$ QAOA. The probabilities are averaged over many graph instances.

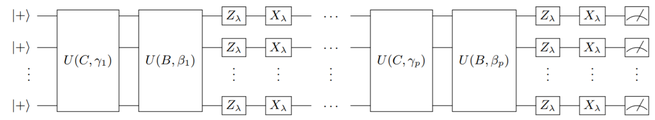

Fig: 5. The QAOA circuit with a noise model used in our simulations. Z_λ and X_λ corresponds to applying a Z or X gate respectively with probability λ. Throughout the report, we use $\lambda = 0.005$.

References

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