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Variational Learning of Grover's Search Algorithm with Partial Diffusion Operator

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ABSTRACT

This paper introduces a new approach to improve Grover's search algorithm by utilizing variational learning, with a specific focus on incorporating a partial diffusion operator. Grover's search algorithm is a well-known quantum algorithm that provides a quadratic speedup for searching an unsorted database. However, its performance can be further enhanced by modifying its diffusion operator. In this work, we aim to identify a parameterized quantum circuit that can effectively learn and optimize Grover's search algorithm, incorporating a partial diffusion operator. The key idea behind this approach is to use variational learning, a technique that employs parameterized quantum circuits to optimize the algorithm's performance. By adjusting the parameters of the quantum circuit, the algorithm can be tailored to better solve the search problem. Variational learning is employed to determine the optimal parameters for the partial diffusion operator, enabling the quantum circuit to adapt to different problem instances. Our experimental results demonstrate that the optimized quantum circuit outperforms the traditional Grover's algorithm that uses the standard partial diffusion operator. The results suggest that the proposed approach offers significant improvements in terms of algorithmic efficiency and performance. This advancement could have important implications for the development of quantum algorithms, particularly in applications related to database search and optimization problems. In conclusion, this paper presents a promising new method to enhance Grover's search algorithm, utilizing variational learning and a partial diffusion operator, with results showing improved performance over the original algorithm.

1. INTRODUCTION

Using quantum fourier transform, we can regain optimal query complexity of Grover algorithm without losing the freedom of using arbitrary diffusion operators for quantum searching, but the total number of operators required is still order of B times more than Grover algorithm [1]. This paper demonstrates that modifying Grover's algorithm allows access to a more general class of diffusion operators for fast quantum search, allowing for faster quantum evolution from known states to unknown targets [2]. The Grover partial search algorithm, originally suggested by

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Grover and Radhakrishnan, and modified by Korepin, is the optimal one for finding target items in databases faster than any classical algorithm [3]. The optimized Grover-Radhakrishnan partial search algorithm reduces the number of queries to the oracle, improving efficiency and running on the same hardware as the usual Grover algorithm [4]. The Partial Diffusion Operator in a quantum search algorithm improves reliability and performance in searching unstructured lists with multiple matches, even when the number of matches is unknown [5].

A neuronal version of Grover's quantum algorithm could enhance signal coincidence detection, synaptic plasticity, and other vital cell functions by rapidly selecting, ordering, and counting optional response regulation choices [6]. Quantum computing has witnessed significant advancements in recent years, with Grover's search algorithm standing out as a pivotal algorithm in the field. This paper delves into the exploration of variational learning applied to Grover's search algorithm, specifically incorporating a partial diffusion operator. The aim is to identify a parameterized quantum circuit with optimal parameters through variational learning, ultimately outperforming the traditional Grover's algorithm with partial diffusion. This research contributes to the ongoing efforts in enhancing quantum algorithms, leveraging variational techniques to augment the efficiency of Grover's search algorithm [7].

Parameterized quantum circuits have been utilized for problem-solving through variational learning. Grover's algorithm [8] stands out as a prominent quantum algorithm employed for database search tasks. The primary objective of this paper is to ascertain a model that exhibits superior reliability when compared to Grover's algorithm with partial diffusion. The enhanced performance of Grover's algorithm with partial diffusion becomes evident particularly when the number of matches exceeds $\frac{N}{2}$, where $N = 2^n$ represents the size of the list, and n denotes the number of qubits. Given that our proposed model outperforms Grover's algorithm with partial diffusion, it inherently surpasses Grover's algorithm as well with an increasing number of matches, denoted as M. The structure of this paper unfolds as follows: Firstly, we provide a description of Grover's algorithm with partial diffusion, highlighting its advantages over the traditional Grover's algorithm. Subsequently, we elucidate the variational learning approach applied to this method. Finally, we identify the optimal parameters using various optimizers and compare the accuracy of our model with that of Grover's algorithm with partial diffusion.

1.1. Computational methods

In this section, first we outline the problem, and then we explain Grover's with partial diffusion. Finally, we present our result: a proper model found through variational learning.

1.1.1 Problem statement

We have a list with N elements and a function f, where the value of f for M elements is 1 and is 0 for the rest. Our aim is to find all M elements.

1.1.2 Grover's algorithm with partial diffusion

We describe briefly the algorithm for n qubits here, however, for more details you can read [9]. The algorithm steps are as follows:

- Preparing n+1 quantum registers: We have n+1 quantum registers that one of them is used to store oracle value

$$|W_0\rangle = |0\rangle^{\otimes n} \otimes |0\rangle \tag{1}$$

- Initializing registers:
  We put a hadamard gate on each of the first qubits. So they contain 2N states:

$$|W_1\rangle = (H^{\otimes n} \otimes I)|W_0\rangle = (\frac{1}{\sqrt{N}}\sum_{i=0}^{N-1}|i\rangle) \otimes |0\rangle \tag{2}$$

- Adding oracle operator to system: The oracle maps each state to one or zero and stores the result in the N+1th register.

$$|W_2\rangle = \frac{1}{\sqrt{N}}(|i\rangle \otimes |0 \oplus f(i)\rangle) = \frac{1}{\sqrt{N}}\sum_{i=0}^{N-1}|i\rangle \otimes |f(i)\rangle \tag{3}$$

- Adding partial diffusion operator: The partial diffusion operator (Y) is like the diffusion operator in Grover's search algorithm but it performs the inversion about the subspace of the problem

$$Y = H^{\otimes n} \otimes I(2|0\rangle\langle 0| - I)H^{\otimes n} \otimes I \tag{4}$$

We can rewrite the system as follows:

$$\sum_{k=0}^{P-1}\delta_k|k\rangle = \sum_{j=0}^{N-1}\alpha_j\,(|j\rangle \otimes |0\rangle) + \sum_{j=0}^{N-1}\beta_j\,(|j\rangle \otimes |1\rangle) \tag{5}$$

So we have:

$$\begin{aligned} Y(\sum_{k=0}^{P-1}\delta_k|k\rangle) &= (H^{\otimes n} \otimes I(2|0\rangle\langle 0| - I)H^{\otimes n} \otimes I)\sum_{k}^{p-1}\delta_k|k\rangle \\ &= 2(H^{\otimes n} \otimes I|0\rangle\langle 0|H^{\otimes n} \otimes I)\sum_{k=0}^{P-1}\delta_k|k\rangle - \sum_{k=0}^{P-1}\delta_k|k\rangle \\ &= \sum_{j=0}^{N-1}(2\langle\alpha\rangle - \alpha_j)(|j\rangle \otimes |0\rangle) - \sum_{j=0}^{N-1}\beta_j(|j\rangle \otimes |1\rangle \end{aligned} \tag{6}$$

And $\langle\alpha\rangle = \frac{1}{N}\sum_{j=0}^{N-1}\alpha_j$

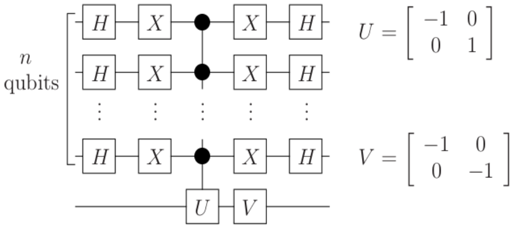

Fig. 1. Diffusion operator for n qubits system

The primary concept behind employing partial diffusion is to execute inversion about the mean of a subsystem that encompasses all elements, denoted as x, where f(x) equals zero, and half of the elements, denoted as t, where f(t) equals one. Let M represent the number of matches for which the oracle's output is equal to 1. We denote the sum of these elements as $\sum_i{}'$ and the sum of others with $\sum_i{}''$.

So:

$$|W_2\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1}{}' |i\rangle \otimes |1\rangle + \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1}{}'' |i\rangle \otimes |0\rangle \tag{7}$$

And after applying diffusion operator:

$$|W_3\rangle = c_1 \sum_{i=0}^{N-1}{}' |i\rangle \otimes |1\rangle + b_1 \sum_{i=0}^{N-1}{}' |i\rangle \otimes |0\rangle + a_1 \sum_{i=0}^{N-1}{}'' |i\rangle \otimes |0\rangle \tag{8}$$

And the mean in the diffusion operator is:

$$\langle\alpha_1\rangle = (\frac{N-M}{N\sqrt{N}}) \tag{9}$$

And:

$$a_1 = 2\langle\alpha_1\rangle - \frac{1}{\sqrt{N}};\ \ b1 = 2\langle\alpha_1\rangle;\ \ c_1 = -\frac{1}{\sqrt{N}} \tag{10}$$

- Measurement: If we measure the first n qubits, we will find the answer with following probability:

  i) probability to find a match of M possible matches:

$$P_s^{(1)} = M(b_1^2 + c_1^2) = M(\left(\frac{2N-M}{N\sqrt{N}}\right)^2 + \left(-\frac{1}{\sqrt{N}}\right)^2) = 5\left(\frac{M}{N}\right) - 8\left(\frac{M}{N}\right)^2 + 4\left(\frac{M}{N}\right)^3 \tag{11}$$

  ii) probability to find undesired result:

$$P_{ns}^{(1)} = (N-M)a_1^2 \tag{12}$$

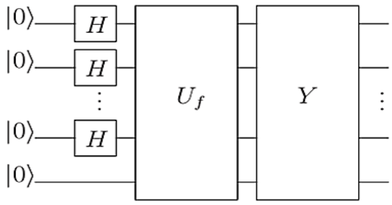

Fig. 2. Quantum circuit for Grover's algorithm with partial diffusion operator

We can compare the result of Grover with partial diffusion with the result of Grover.

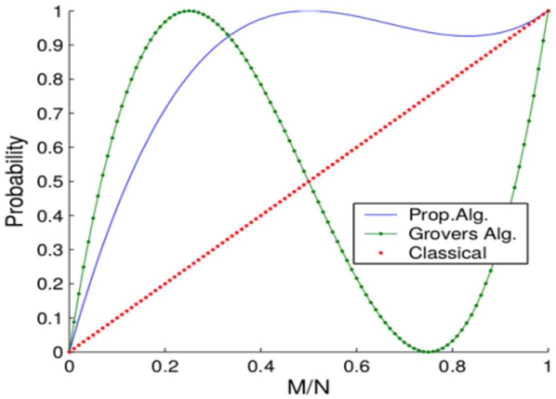

Fig. 3. A plot of comparison of probability of success in the first iteration

1.2. Variational method

In the quest to develop a model capable of learning Grover's algorithm with partial diffusion, we draw inspiration from [10]. To commence, we construct the oracle utilizing the following algorithm:

```
1- $U_f = 0$ $the\ dimesion\ of\ U_f\ is\ 2^{n+1}$

2- $For\ w = 0\ to\ w = 2^n$
      $if\ f(w) == 1$:
         $U_f += e^{i\alpha}|w\rangle|1\rangle\langle w|\langle 0| = e^{i\alpha}|w1\rangle\langle w0|$
      else:
         $U_f += e^{i\beta}|w\rangle|1\rangle\langle w|\langle 0| = e^{i\beta}|w1\rangle\langle w0|$
3- c=0
4- $For\ i = 0\ to\ 2^{n+1}$:
       if all the elements of the ith row are equal to zero:
          $U_f += |i\rangle\langle 2c+1|$
          c+=1
     $i$ is the number of row
```

To construct a diffusion operator (Y) resembling Grover with partial diffusion, we employ the circuit in Figure 1, but with $U = \begin{bmatrix} e^{i\theta} & 0 \\ 0 & 1 \end{bmatrix}$. Subsequently, using the newly defined U, we generate the new (Y) as illustrated in Figure 2. In multiple scenarios, we endeavor to identify optimal angles for the model, employing different variational forms. An essential clarification regarding the angles is that they are contingent on the number of matches and the number of qubits, remaining independent of the solution to the problem. In other words, different matches with the same size share the same angles.

i. Variational forms:

Standard Oracle Variational Diffusion: In this scenario, we consider the angle of the diffusion operator as a variable, while setting the angle of the oracle operator to zero.

Restricted Variational Oracle and Diffusion: Here, we assume that the angles of both the diffusion and oracle operators are variables and are constrained to be equal.

Variational Oracle Standard Diffusion: In this case, we take the angle of the oracle operator as a variable, while fixing the angle of the diffusion operator to π.

Variational Oracle and Diffusion: This encompasses both the oracle and diffusion angles as variables.

To determine optimal angles for these variational forms, various optimizers are employed, and an exhaustive search across the entire problem space is conducted. The results obtained from different approaches are subsequently compared.

2. CONCLUSION

The optimal results are derived from the 4th variational form, showcasing superior performance compared to the non-variational method. The comparative analysis is presented in Table 1.

Table 1. Optimizers comparison

Optimizer	1 Match	2 Matches	3 Matches
COBYLA	0.2562	0.5131	0.7436
CG	0.2631	0.5156	0.7572
AQGD	0.2577	0.5139	0.755
Searching whole space	0.8521	1	0.963

Figure 4 shows the accuracy of the variational method and the grover algorithm with partial diffusion.

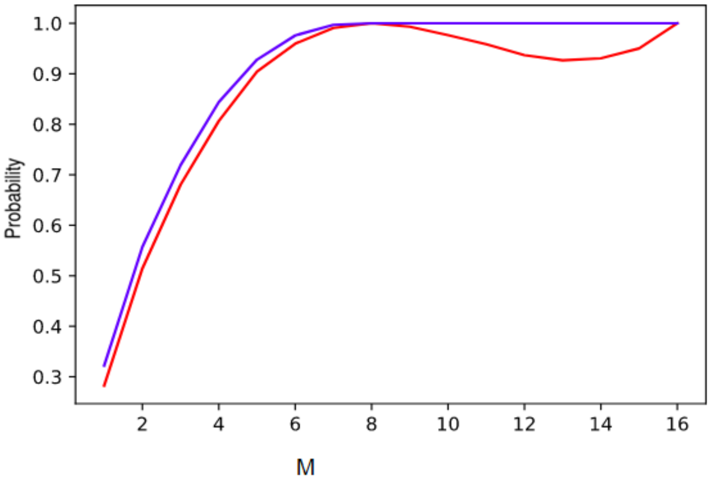

Fig. 4. The blue line presents the accuracy of variational method, and the red line presents the accuracy of Grover's algorithm with partial diffusion

Transparency Statement

The data supporting this study are available upon reasonable request to the corresponding author, subject to ethical and confidentiality considerations.

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Declaration of Interest

The authors declare that they have no competing interests.

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