Quantum search algorithm on weighted databases

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The Grover algorithm is a crucial solution for addressing unstructured search problems and has emerged as an essential quantum subroutine in various complex algorithms. This research extensively investigates Grover's search methodology within non-uniformly distributed databases, a scenario frequently encountered in practical applications. Our analysis reveals that the behavior of the Grover evolution differs significantly when applied to non-uniform databases compared to uniform or 'unstructured databases.' It is observed that the search process facilitated by this evolution does not consistently result in a speed-up, and we have identified specific criteria for such situations. Furthermore, we have extended this investigation to databases characterized by coherent states, confirming the speed-up achieved through Grover evolution via rigorous numerical verification. In conclusion, our study provides an enhancement to the original Grover algorithm, offering insights to optimize implementation strategies and broaden its range of applications.

I. INTRODUCTION

The Grover algorithm, conceived by L. K. Grover in 1997 [1], marked a significant advancement in the field of quantum computing [2], particularly in addressing the challenge of query complexity. In the classical paradigm, searching an unstructured database typically necessitates n steps, where n is the size of the database. Grover's groundbreaking algorithm, however, revolutionizes this approach by reducing the required steps to merely $\sqrt{n}$. This quantum search algorithm has emerged as a cornerstone in the development of quantum computational routines, celebrated for its ability to significantly amplify the amplitude of the quantum state that encodes the desired information. The versatility and applicative potential of the Grover algorithm have been demonstrated across a spectrum of challenging problems. For instance, it has provided innovative solutions to the satisfiability problem [3], as well as in the burgeoning field of quantum machine learning [4]. Further applications include tackling constrained polynomial binary optimization [5] and enhancing quantum amplitude estimation techniques [6], showcasing a clear computational superiority over traditional methods. Recent explorations have extended the utility of the Grover algorithm [7] to the domain of adiabatic quantum computing [8–10], underscoring its adaptability and relevance in the rapidly evolving landscape of quantum research. This paper specifically delves into the algorithm's seminal application in database searching, highlighting its transformative impact and ongoing significance in the quest for efficient quantum computing solutions. Through this focus, we aim to illuminate the enduring value and broad applicability of Grover's algorithm [1, 11, 12], from its initial proposal to its current and potential future contributions to quantum computing and beyond.

The search problem unfolds as follows: within a given database, each element is distinctly indexed. When the database is of finite size, locating a specific element necessitates iterative queries to its index. Typically, the query count scales with the database size. Grover's seminal work explored this quandary in the realm of quantum computing. Through specific evolution operators, the amplitude of the basis state housing the target data can be boosted to unity. The steps required for such enhancement scale proportionally to the square root of the database size, ensuring a guaranteed quadratic acceleration. This concept has been integrated into numerous platforms [13–15], with additional advancements showcased in recent proposals [16–19].

The initial discourse on the search dilemma predominantly centers on managing unstructured databases, following a conventional approach in theoretical computational discussions that remains detached from specific physical contexts. However, as we transcend the limits imposed by current computing platforms and strive for advancements, particularly in the evolution of novel computing architectures, data encoding states may not uniformly distribute. Thus, delving into the potential enhancements of the Grover search algorithm in such scenarios presents an opportunity to broaden its utility and applicability significantly.

Moving forward, we conduct an analysis of the aforementioned issue. The database under scrutiny is comprehensive, characterized by distributions spanning various types. We define the Grover evolution tailored to such a database and calculate the necessary steps for executing the search operation. By comparing our approach with classical methodologies, we methodically identify the prerequisites for achieving acceleration through Grover evolution. Subsequently, we showcase two illustrative examples to elucidate our observations: the first example validates the harmony between our theory and Grover's established results, while the second example exemplifies that employing the Grover search on a database governed by coherent state probabilities leads to acceleration compared to conventional methods. This is followed by an elaborate exposition of our overarching methodology.

II. GROVER SEARCH ON WEIGHTED DATABASES

Consider a database $\{x_1, \ldots, x_M\}$, with integer M. An arbitrary element x_n in the database is a real number, which represents a certain characteristic of objects. In the original version of search problems, all x_ms are distinct to each other. Here we assume that parts of the elements in the database are the same. This is also common for the real-world databases. Suppose that there are N distinguished types of elements in the database, denoted by $y_1, \ldots, y_N$. Therefore, the database $\{x_1, \ldots, x_M\}$ can be re-organized by $\{(y_1, p_1), \ldots, (y_N, p_N)\}$, where $p_1, \ldots, p_M$ represent the proportions of distinct characteristics $y_1, \ldots, y_N$ in the total database. An illustration of the search problem on the databases is given by Fig. 1.

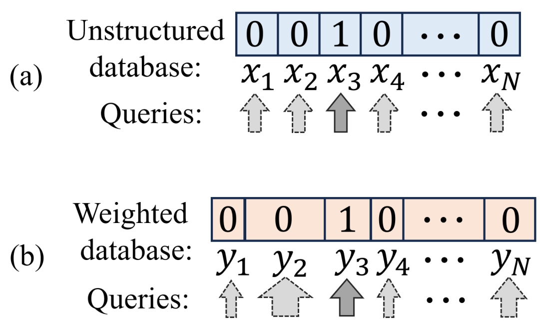

FIG. 1. An illustration of the search problem on unstructured database (a) and weighted database(b). "0" and "1" mark the ordinary and the target data sample respectively. The widths of the squares of the samples represent the proportions.

To search for a certain characteristics in $\{(y_1, p_1), \ldots, (y_N, p_N)\}$ by using classical algorithms, the required number of steps s is proportional to the reciprocal number of its proportion. Therefore, in general, s satisfies

$$\min_{j=1,\ldots,N}\left\{\frac{1}{p_j}\right\} \leqslant s \leqslant \max_{j=1,\ldots,N}\left\{\frac{1}{p_j}\right\}. \tag{1}$$

To perform the same task by using Grover evolution [20], one can consider the following state

$$|D\rangle = \sum_{n=0}^{N} P(n)|n\rangle. \tag{2}$$

$\{|1\rangle, |2\rangle, \cdots, |N\rangle\}$ is a set of orthonormal basis and $|D\rangle$ is a superposition of them. $P(n)$ is the complex amplitude of the basis state $|n\rangle$, yielding that $|P(n)|^2 = p_n$, and $\sum_{n=0}^{N}|P(n)|^2 = 1$. According to the idea of Grover search, the amplitude of the target state can be amplified by repetitive evolution so that the search can be completed by only one step. Then, the total step number of performing the search equals to the repeat number of the evolution operators. Suppose that the target state is $|k\rangle$, the basic two operators for evolution are defined by

$$U_D = 2|D\rangle\langle D| - 1,\ U_k = 1 - 2|k\rangle\langle k|. \tag{3}$$

The amplification operator required by Grover search is defined by $G \coloneqq U_D U_k$. Suppose that after performing G for t times on $|D\rangle$, the whole state evolves to $|k\rangle$. Then, the step number for searching $|k\rangle$ is given by t.

The next key problem is to compare the step numbers of the two methods, validating whether a speed-up exists. For such purpose, we analyze the above evolution under G as follows. Applying G once to the state $|D\rangle$, one has

$$G|D\rangle = (1 - 4|P(k)|^2)|\alpha\rangle - 2P^*(k)|k\rangle. \tag{4}$$

Furthermore, if G is applied for r times, a recurrence relation can be obtained,

$$G^r|D\rangle = a_r|D\rangle + b_r|k\rangle, \tag{5}$$

where

$$\begin{aligned} a_r &= [1 - 4|P(k)|^2]a_{r-1} - 2P^*(k)b_{r-1}, \\ b_r &= b_{r-1} + 2P(k)a_{r-1}. \end{aligned} \tag{6}$$

For sufficient large r, the amplification leads to that $a_r \to 0$ and $b_r \to 1$. This asymptotic behaviour can be seen by approximating a_r with a continue function $f_a(x)$ with real variable x, such that $f_a(r) = a_r$. Apply the approximation $a_r - a_{r-1} \sim \partial f_a/\partial x$, and the same for b_r. Thereafter, two partial differential equations can be obtained, shown by

$$\begin{aligned} \frac{\partial f_a}{\partial x} &= -4f_a|P(k)|^2 - 2f_b P^*(k), \\ \frac{\partial f_b}{\partial x} &= 2f_a P(k). \end{aligned} \tag{7}$$

Substitute the second equation to the first equation, one has

$$\frac{\partial^2 f_a}{\partial x^2} + 4|P(k)|^2\frac{\partial f_a}{\partial x} + 4|P(k)|^2 f_a = 0. \tag{8}$$

Notice that such equation is a standard second-order partial differential equation. Its solution has been discussed thoroughly. In general, the solution of can be given by

$$\begin{aligned} &f_a = C_1 e^{q_1 x} + C_2 e^{q_2 x}, && \Delta > 0 \\ &f_a = (C_1 + C_2 x)e^{q_1 x}, && \Delta = 0 \\ &f_a = e^{\gamma x}(C_1 \cos\beta x + C_2 \sin\beta x), && \Delta < 0 \end{aligned} \tag{9}$$

where $q_{1,2} = (-4|P(k)|^2 \pm \sqrt{\Delta})/2$ with $\Delta = 16|P(k)|^4 - 16|F(k)|^2$. C_1 and C_2 are constants depending on initial conditions. γ and β are the real and imaginary part of complex $q_{1,2}$ when $\Delta < 0$. In our case, $|P(k)| < 1$ so that $\Delta < 0$. The case when $|P(k)| = 1$ means that state $|k\rangle$

can be searched with one step, which is trivial and is not considered here. Thus, the solution to Eq. (8) is

$$f_a = e^{-2|P(k)|x}(C_1 \cos(2\tilde{\Delta}x) + C_2 \sin(2\tilde{\Delta}x)), \tag{10}$$

where $\tilde{\Delta} = \sqrt{|P(k)|^2 - |P(k)|^4}$. The dynamics given by Eq. (10) is a damping oscillation. The period of the oscillation is $T = \pi/\tilde{\Delta}$. It indicates that in the time of T, there is a moment when f_a takes its maximum, approaching to be one. Therefore, the steps number for the search is in the order of T. The speedup of the Grover search under the condition can be verified by comparing the order of T and s. More strictly, one has the condition

$$\min_{k=1,\ldots,N} \left\{\tilde{\Delta}^{-1}(k)\right\} < \min_{j=1,\ldots,N} \left\{\frac{1}{p_j}\right\}. \tag{11}$$

The condition given by Eq. (11) indicates a global speed up over the classical treatment. Notice that we omit the constant factor π because it does not affect the order. If one limits the problem to searching the kth element in the database, the condition can be loosen to

$$\tilde{\Delta}^{-1}(k) < \frac{1}{p_k} = \frac{1}{|P(k)|^2}. \tag{12}$$

Then, because $|P(k)|$ is not zero generally,

$$|P(k)| < \sqrt{1 - |P(k)|}. \tag{13}$$

Such a condition indicates a local speed up over the classical treatment, which is only effective for searching one element. Obviously, the inequality holds when $|P(k)| < 1/2$. It is easy to satisfy such condition when N is sufficiently large.

In what follows, we provide two specific examples of the above general analysis. In the first example, we show that the original unstructured search by Grover's idea can be obtained from our consideration. In the second, we show the results when the distribution of database is that of a coherent state.

III. TWO EXAMPLES

I. Back to unstructured search. The case of unstructured search can be easily obtained by setting $P(k) = 1/\sqrt{N}$. Then,

$$\tilde{\Delta} = \sqrt{\frac{1}{N} - \frac{1}{N^2}} = \sqrt{\frac{N-1}{N^2}}. \tag{14}$$

When N is big enough, one has $\sqrt{(N-1)/N^2} \approx 1/\sqrt{N}$. Therefore, the step number for Grover search is in the order of $\sqrt{N}$. It worth mentioning that, in such a case, because $|P(k)| = 1/\sqrt{N} \to 0$ for big N, the factor $e^{-2|P(k)|x}$ is close to one. It guarantees f_a finally approaches to one.

The classical search algorithm on the unstructured database is basically checking each elements in the database one by one. Because the probability of finding one element is $1/N$, the step number for the searching by classical treatment is in the order of N. Hence, a quadratic speedup can be observed by comparing the order of the two step numbers.

II. Grover search by using coherent state. In this part, we consider the case when the distribution of database $\{(y_1, p_1), \ldots, (y_N, p_N)\}$ satisfies (or partially satisfies) the distribution of the coherent state. The coherent state in the particle number basis can be expressed by

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{q=0}^{\infty} \frac{\alpha^q}{\sqrt{q!}} |q\rangle, \tag{15}$$

where α is a complex number. Such a state naturally

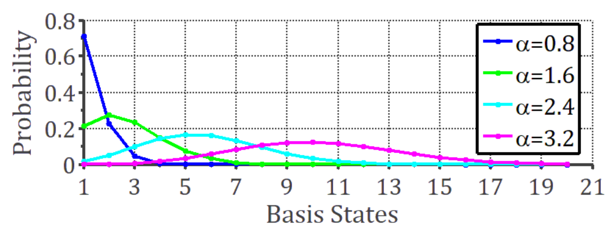

FIG. 2. The probability distribution of $|\alpha'\rangle$ when $|\alpha| = 0.8,\ 1.6,\ 2.4, \ldots,$ and 3.2. We take $q_1 = 1$ and $N = 20$. The cases of other q_1 and N are similar.

occurs in optical amplification cavity. Notice that there are infinite basis states in the coherent state. Therefore, for finite databases, one can consider encoding them into parts of the state (15). Define the N-dimensional database state $|\alpha'\rangle$,

$$|\alpha'\rangle = N_q \sum_{q=q_1}^{q_1+N} \frac{e^{-\frac{1}{2}|\alpha|^2}\alpha^q}{\sqrt{q!}} |q\rangle, \tag{16}$$

where N_q is the normalization factor, given by

$$N_q = \left[\sum_{q=q_1}^{q_1+N} \frac{e^{-|\alpha|^2}|\alpha|^{2q}}{q!}\right]^{-\frac{1}{2}}. \tag{17}$$

Thus, for a target state $|k\rangle$ in the database, one has,

$$\begin{aligned} |P(k)| &= \frac{e^{-\frac{1}{2}|\alpha|^2}|\alpha|^k}{\sqrt{k!}} \cdot N_q \\ &= \frac{|\alpha|^k}{\sqrt{k!}} \left[\sum_{q=q_1}^{q_1+N} \frac{|\alpha|^{2q}}{q!}\right]^{-\frac{1}{2}}. \quad (q_1 \leq k \leq q_1 + N) \end{aligned} \tag{18}$$

Notice that, when q_1 is large enough, $|\alpha|^k/\sqrt{k!}$ slowly varies with k. Thus, the case will go back to the unstructured database, as shown in the first part of section III. When q_1 is not large enough, the magnitude of $|P(k)|$ is given by α and q_1. We numerically provide several

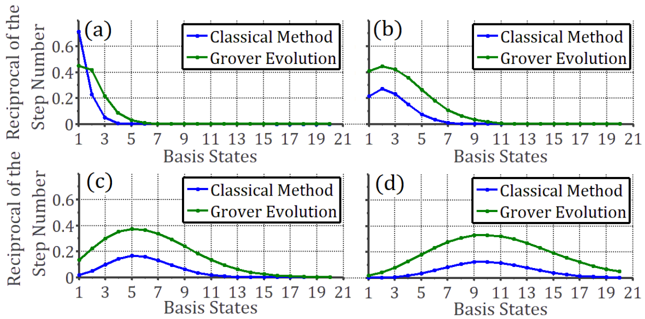

FIG. 3. The comparison of reciprocals of step numbers when searching a basis state $|k\rangle$ $(k = 1, ..., 21)$ by classical and Grover treatments. The y-axis represents the reciprocal of the step numbers. The value of α is 0.8 in (a), 1.6 in (b), 2.4 in (c), and 3.2 in (d).

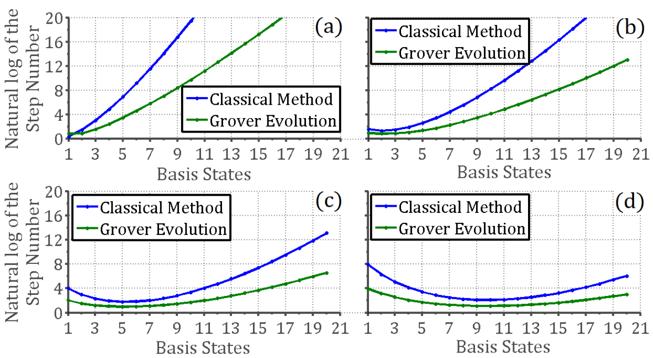

FIG. 4. The comparison of the natural logarithm of step numbers when searching a basis state $|k\rangle$ $(k = 1, ..., 21)$ by classical and Grover treatments. The y-axis represents the natural logarithm of the step numbers. The value of α is also 0.8 in (a), 1.6 in (b), 2.4 in (c), and 3.2 in (d).

cases shown in Fig. 2. By substituting the probability distribution to $\tilde{\Delta}$, the order of the step number can be estimated. The step number of the classical treatment is obtained by $1/p_k$ when searching for y_k. In order to show a clear comparison, we firstly compare the reciprocal of the step numbers of the two cases, and the results is shown in Fig. 3. From the results, we can see that in general, the Grover evolution is a better strategy over the classical treatment. An exception occurs in Fig. 3(a), when searching for the first element. This is because α is relatively small in such a case. We secondly compare the natural logarithm of the step numbers of the cases, and the results are shown in Fig. 4. By Fig. 4, a clear advance in steps number can be observed, and the exception also occurs in (a). The results in Fig. 3 and Fig. 4 indicate that the Grover search on a database distributed in the probability given by the coherent state is able to show an advance over the classical methods. According to our conditions in section II, such an advance belongs to the local speedup.

IV. CONCLUSION

We investigate the application of Grover's algorithm for weighted database searches, a prevalent scenario in practical settings. Utilizing Grover's evolution, we calculate the requisite steps for the search and contrast these calculations with classical methodologies. Through detailed analysis, we pinpoint the specific conditions conducive to acceleration through Grover's algorithm. To illustrate our discoveries, we showcase two compelling examples. The first example validates our theoretical framework by aligning closely with Grover's seminal outcomes. In the second example, we demonstrate how implementing Grover's search on a database governed by a probability distribution resembling a coherent state yields significant speed enhancements compared to traditional methods. These results represent a significant advancement of the original Grover algorithm, enriching its implementation strategies and broadening its scope of potential applications.

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