Data Search Algorithms based on Quantum Walk

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Abstract—For searching any item in an unsorted database with N items, a classical computer takes O(N) steps but Grover’s quantum searching algorithm takes only O(√N) steps. However, it is also known that Grover’s algorithm is effective only in the case where the initial amplitude distribution of dataset is uniform, but is not always effective in the non-uniform case. In this paper, we propose some quantum search algorithms. First, we propose an algorithm in analog time based on quantum walk by solving the schrodinger equation. The proposed algorithm shows best performance in optimum time. Next, we will apply the result to Grover search algorithm. It is shown that the proposed algorithm shows better performance than the conventional one. Further, we propose the improved algorithm by introducing the idea of the phase rotation. The algorithm shows best performance compared with the conventional ones.

Index Terms—quantum search algorithm; Grover search algorithm; initial amplitude distributions of dataset; observed probability

I. INTRODUCTION

With quantum computation, many studies have been made. Shor’s prime factoring and Grover’s data search algorithms are well known[1], [2], [4]. Further, Ventura has proposed quantum associative memory by improving Grover’s algorithm [3], [5]. Data search problem is to find any data efficiently from unsorted dataset. For searching any item in an unsorted database with N items, a classical computer takes O(N) steps but Grover’s algorithm takes only O(√N) steps. However, it is also known that Grover’s algorithm is effective only in the case where the initial amplitude distribution of dataset is uniform, but is not always effective in the non-uniform case[3]. Further, Ventura has proposed the quantum searching algorithm but it is effective only in the special case for the initial amplitude distribution[6], [7]. Therefore, it is necessary to find effective algorithms even in the case where the initial amplitude distribution of dataset is not uniform. For example, associative memory needs non-uniform initial data distribution [3]. In this paper, we propose some quantum search algorithms. First, we propose an algorithm in analog time based on quantum walk by solving the schrodinger equation. The proposed algorithm shows best performance in optimum time. Next, we will apply the result to Grover search algorithm. It is shown that the improved algorithm shows better performance than the conventional one. Further, we propose the algorithm by introducing the idea of the phase rotation[8]. The proposed algorithm shows best performance compared with the conventional ones.

This work is supported by Grant-in-Aid for Scientific Research (C) (No.22500207) of Ministry of Education, Culture, Sports, Science and Technology of Japan.

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II. PRELIMINARY

The basic unit in quantum computation is a qubit c₀|0⟩ + c₁|1⟩, which is a superposition of two independent states |0⟩ and |1⟩ corresponding to the states 0 and 1 in a classical computer, where c₀ and c₁ are complex numbers such that |c₀|² + |c₁|² = 1. We use the Dirac bracket notation, where the ket |i⟩ is analogous to a column vector. Let a be a positive integer and N = 2ᵃ. A system with n qubits is described using N independent state |i⟩ (0 ≤ i ≤ N − 1) as follows:

\[ |i⟩ = \sum_{i=0}^{N-1} c_i |i⟩ \]  

where cᵢ is a complex number, \[\sum_{i=0}^{N-1} |c_i|^2 = 1 \text{ and } |c_i|^2 \text{ is the probability of state } |i⟩\]. The direction of cᵢ in the complex plane is called the phase of state |i⟩ and the absolute value |cᵢ| is called the amplitude of state |i⟩. In quantum system, starting from any quantum state, the desired state is formed by multiplying column vector of the quantum state by unitary matrix. Finally, we can obtain the desired state with high probability through observation[2]. The problem is how we can find unitary matrix. Grover has proposed the fast data search algorithm. Let us explain the Grover’s algorithm shown in Fig.1. Grover has proposed an algorithm for finding one item in an unsorted database. In the conventional computation, if there are N items in the database, it would require O(N) queries to the database. However, Grover has shown how to perform this using the quantum computation with only O(√N) queries[2]. Let Z_N = {0, 1, ⋯, N − 1}. Let us define the following operators.

\[ I_0 = \text{Identity matrix except for} \]  
\[ I(a + 1, a + 1) = -1, a \in Z_N \]  

which inverts any state |ψ⟩ and

\[ W(x, y) = \frac{1}{\sqrt{N}} (-1)^{x_0y_0 + ⋯ + x_{N-1}y_{N-1}} \]  

for \[x = \sum_{i=0}^{N-1} x_i 2^i, y = \sum_{i=0}^{N-1} y_i 2^i\], which is called the Walsh or Hadamard transform and performs a special case of discrete Fourier transform. We begin with the |0⟩ state and apply W operator to it, where |0⟩ means that all states are 0 and the number of 0’s for 0 is N. As a result, all the states have the same amplitude \[1/\sqrt{N}\]. Next, we apply the I₀ operator, where |τ⟩ is the searching state. Further, we apply the operator

\[ G = -WI₀W \]  

Followed by the I₀ operator \[T = (\pi/4)\sqrt{N}\] times and observe the system[2]. G operator has been described as inverting each of the state’s amplitudes around the average

\[ I_0 = \text{Identity matrix except for} \]  
\[ I(a + 1, a + 1) = -1, a \in Z_N \]  

which inverts any state |ψ⟩ and

\[ W(x, y) = \frac{1}{\sqrt{N}} (-1)^{x_0y_0 + ⋯ + x_{N-1}y_{N-1}} \]  

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one of all states.

**Example 1** [6]:
Let \( n = 4 \) and \( N = 16 \). Let searching data \( |\tau\rangle = |6\rangle = |0110\rangle \) and the number of stored (memorized) data \( l = 16 \). Then, the desired data \( 0110 \) is obtained with the probability 0.96 by using Grover’s algorithm. We can get the searching data with high probability.

Next, assuming that stored data are \( |0\rangle, |3\rangle, |6\rangle, |9\rangle, |12\rangle, \) and \( |15\rangle \), and searching data is \( |6\rangle \), that is \( l = 6 \). The initial state \( |\psi\rangle \) is as follows:

\[
|\psi\rangle_i = \begin{cases} 
1 & \text{for any } i \text{ of stored data} \\
0 & \text{otherwise,}
\end{cases}
\]  

Then, the desired data \( 0110 \) is obtained with the probability 0.44. It shows that Grover’s algorithm does not always give a good result in the case where \( N \neq l \).

Therefore, it is needed to find effective algorithms even in the case where the initial amplitude distribution of dataset is not uniform.

### III. Quantum Search in Analog Model Based on Quantum Walk

![Fig. 2. Description of data search problem](image)

In the following, we introduce a quantum search algorithm using analog model of quantum walk. In order to clarify the problem, we will explain the Fig.2. It is assumed that \( l \) pieces of data are memorized (stored) in the system of \( N \) pieces of data. Now we want to find any data in \( m \) pieces of data (marked) with high probability. Grover has shown the effective algorithm in the case of \( N = l, m = 1 \) (see Fig.1).

#### A. Schroedinger equation and quantum walk

In this chapter, we propose an algorithm based on quantum walk in analog time model. As the state of system in quantum model is determined by the Schroedinger equation, we can obtain the result by solving the Schroedinger equation under the special condition[9],[10].

The Schroedinger equation for the state of system is represented as follows[9]:

\[
\frac{ih}{\Delta t}|\psi\rangle = H|\psi\rangle,
\]  

where \( h \) is Plank constant and \( H \) is Hamiltonian which means all the energy of the system. Then \( H = H^\dagger \) holds, where \( H^\dagger \) is the transposed matrix of complex conjugate for \( H \).

Then the solution is represented by

\[
|\psi(t)\rangle = U(t)|\psi(0)\rangle,
\]  

where

\[
U(t) = \exp(-itH)
\]  

and \( U(t) \) is called time expansion operation of the state and \( |\psi(0)\rangle \) is the initial state of system. Therefore, the state of system is determined by Hamiltonian \( H \). Let \( P_w(t) \) be defined as the observed probability of system at time \( t \) as follows:

\[
P_w(t) = |\langle w|U(t)|\psi(0)\rangle|^2.
\]  

The state of system to search is called the marked one and the other is called the unmarked state. The number of marked states is \( m \)(see Fig.2). Hamiltonian \( H_p \) corresponding to the potential energy is represented by an identity matrix except for

\[
H_p(j_i, j_i) = -1,
\]  

where \( i \in Z_m \).

Let \( L \) be the state assignment over the graph. Then the Hamiltonian \( H \) of the system is defined using the mobility \( r \) as follows[9]:

\[
H = -\gamma L + H_p
\]  

Let \( G = (V, E) \) be the perfect graph to act for system, where \( V \) is the set of vertexes and \( E \) is the set of edges. Then \( L \) is represented as follows:

\[
L = -NI + \begin{pmatrix} 
1 & 1 & \cdots & 1 \\
1 & 1 & \cdots & 1 \\
\vdots & \vdots & \ddots & \vdots \\
1 & 1 & \cdots & 1 
\end{pmatrix}
\]  

\[
= -NI + \sum_{x} \sum_{y} |x\rangle \langle y|
= -NI + N|s\rangle \langle s|,
\]  

where

\[
|s\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle
\]

Finally, Hamiltonian \( H \) is represented as follows:

\[
H = \gamma NI - \gamma N|s\rangle \langle s| + H_p
\]  

It is known that any quantum arrives at any place (state) in \( O(\sqrt{N}) \) steps by using quantum walk. Assuming that the potential energy of the place to arrive is low, the high probability of the state is performed.

Then, let \( U \) be defined as follows:

\[
U = \exp(-\frac{1}{2}i\gamma NI) \exp(iA),
\]  

where

\[
A = \gamma NI|s\rangle \langle s| - H_p - \frac{1}{2}\gamma NI
\]
B. Derivation of the time expansion operator \( U \)

Let us compute the Eq.(15).

Let \( C \) be any matrix. Then the following relation holds:

\[
\exp(C) = \sum_{r=0}^{\infty} \frac{1}{r!} C^r.
\]  

(17)

In order to compute the Eq.(15), \( A^r \) must be computed.

Here, in order to understand the computation of \( A^r \) easily, we will consider the case of \( N = 8 \).

\[
A^r = \begin{pmatrix}
\zeta(r) & \delta(r) & \alpha(r) & \alpha(r) & \delta(r) & \delta(r) & \alpha(r) & \alpha(r) \\
\beta(r) & \epsilon(r) & \beta(r) & \beta(r) & \eta(r) & \eta(r) & \beta(r) & \beta(r) \\
\alpha(r) & \delta(r) & \zeta(r) & \alpha(r) & \delta(r) & \delta(r) & \alpha(r) & \alpha(r) \\
\beta(r) & \eta(r) & \beta(r) & \beta(r) & \epsilon(r) & \eta(r) & \beta(r) & \beta(r) \\
\beta(r) & \eta(r) & \beta(r) & \beta(r) & \eta(r) & \epsilon(r) & \beta(r) & \beta(r) \\
\alpha(r) & \delta(r) & \alpha(r) & \alpha(r) & \delta(r) & \delta(r) & \alpha(r) & \alpha(r) \\
\alpha(r) & \delta(r) & \alpha(r) & \alpha(r) & \delta(r) & \delta(r) & \alpha(r) & \alpha(r) \\
\alpha(r) & \delta(r) & \alpha(r) & \alpha(r) & \delta(r) & \delta(r) & \alpha(r) & \alpha(r)
\end{pmatrix}
\]

(18)

From the relation that \( A^{r+1} = A^r A \) and \( A^1 \) is known, the following recursion formula are obtained:

\[
\beta(r+1) = \left\{ (N-m)\gamma \right\} - \frac{1}{2} \beta(r) + (m-1)\gamma, \quad \gamma(r+1) = (N-m)\gamma(\beta(r) + \left\{ (m-1)\gamma \right\}) \quad \eta(r+1) = (N-m)\gamma(\beta(r) + (m-1)\gamma), \quad \epsilon(r+1) = (N-m)\gamma(\beta(r) + (m-1)\gamma), \quad \alpha(r+1) = (N-m)\gamma(\beta(r) + (m-1)\gamma), \quad \delta(r+1) = (N-m)\gamma(\alpha(r) + (m-1)\gamma) \quad \delta(r+1) = (N-m)\gamma(\alpha(r) + (m-1)\gamma) \quad \delta(r+1) = (N-m)\gamma(\alpha(r) + (m-1)\gamma)
\]

(19, 20, 21, 22, 23, 24)

Now, let \( v_1(r), v_2(r), K_1 \) and \( K_2 \) be defined as follows:

\[
v_1(r) = \begin{pmatrix}
\beta(r) \\
\eta(r) \\
\epsilon(r)
\end{pmatrix} \quad v_2(r) = \begin{pmatrix}
\alpha(r) \\
\delta(r) \\
\zeta(r)
\end{pmatrix}
\]

(25, 26)

Then, the following relation hold:

\[
v_1(r+1) = K_1 v_1(r) \quad v_2(r+1) = K_2 v_2(r)
\]

(29, 30)

By diagonalizing the matrices \( K_1 \) and \( K_2 \), \( v_1 \) and \( v_2 \) are obtained. As a result, the operator \( U \) is obtained as follows:

\[
U = \begin{pmatrix}
\zeta & \delta & \alpha & \alpha & \delta & \delta & \alpha & \alpha \\
\beta & \beta & \beta & \eta & \eta & \beta & \beta & \beta \\
\alpha & \delta & \alpha & \delta & \delta & \alpha & \alpha & \alpha \\
\alpha & \delta & \zeta & \delta & \delta & \alpha & \alpha & \alpha \\
\alpha & \delta & \beta & \delta & \delta & \alpha & \alpha & \alpha \\
\alpha & \delta & \beta & \delta & \delta & \alpha & \alpha & \alpha \\
\alpha & \delta & \alpha & \delta & \delta & \alpha & \alpha & \alpha \\
\alpha & \delta & \alpha & \delta & \delta & \alpha & \alpha & \alpha
\end{pmatrix}
\]

(31)

IV. SEARCH ALGORITHMS BASED ON QUANTUM WALK

A. Application to quantum search problem in analog time

The result of the chapter III is applied to quantum search problem. Remark that \( t \) is in analog time. The method is
called the method 1 (in analog time)[9]. The probability \( P_w(t) \) is computed by the Eq.(9). Then the initial amplitudes \( \psi_a(0) \) and \( \psi_b(0) \) of memorized and non-memorized data of time 0 is as follows:

\[
\psi_a(0) = \frac{1}{\sqrt{l}}
\]

\[
\psi_b(0) = 0
\]

From the Eq.(7), the following result is obtained

\[
\psi_a(t) = \frac{1}{\sqrt{l}} [(l - m)\alpha_m + (m - 1)\beta_m + \delta_m]
\]

\[
\psi_b(t) = \frac{1}{\sqrt{l}} \cos \sqrt{\gamma} m t + \frac{i}{\sqrt{l}} \sqrt{\gamma} \sin \sqrt{\gamma} m t
\]  \hspace{1cm} (42)

As a result, the observed probability of search data \( P_w(t) \) is obtained from the Eq.(9) as follow:

\[
P_w(t) = \frac{1}{l} \cos^2 \frac{m}{N} t + l \frac{m}{N} \sin^2 \frac{m}{N} t
\]  \hspace{1cm} (43)

Let us show the example of four cases, (1) \( m = 1, l = N \), (2) \( m = 2, l = N \), (3) \( m = 1, l = N/2 \), (4) \( m = 2, l = N/2 \) for \( N = 1024 \). The result shows \( P_w((\pi/2)\sqrt{N/m}) = 1/(mN) \), where \( t = (\pi/2)\sqrt{N/m} \) is the optimum time. If \( l = N \), then \( P_w(t) = 1/m \) and \( P_w(t) = 1 \) for \( m = 1 \). Fig.3 shows the simulation result. The case1 and case2 for \( N = l \) shows high probability.

B. Improved search algorithm in analog time

The state \( \psi_a(t_1) \) of memorized data after \( t_1 \) step and the state \( \psi_b(t_1) \) of non-memorized data after \( t_1 \) step are represented as follows:

\[
\psi_a(t_1) = \frac{1}{\sqrt{N}} \cos \sqrt{N} t_1 + \frac{i}{\sqrt{N}} \sin \sqrt{N} t_1
\]

\[
\psi_b(t_1) = \frac{i}{\sqrt{N}} \sin \sqrt{N} t_1
\]  \hspace{1cm} (44)

When \( t_1 = (\pi/2)\sqrt{N/l} \), it holds \( \psi_a(t_1) = \psi_b(t_1) \). Therefore, the states except for marked data at the step \( t_1 \) are identical, so the method 1 is possible to apply at the time \( t = t_1 \). The use of the method 1 for the time interval \( t_2 \) leads to the following probability:

\[
\psi_w(t_2 + t_1) = \frac{i}{\sqrt{N}} [(N - m)\alpha_m + (m - 1)\beta_m + \delta_m]
\]

\[
= \frac{1}{\sqrt{N}} \cos \sqrt{N} t_2 - \frac{1}{\sqrt{m}} \sin \sqrt{N} t_2
\]  \hspace{1cm} (46)

\[
P_a(t_2 + t_1) = \frac{1}{N} \cos^2 \sqrt{N} t_2 + \frac{1}{m} \sin^2 \sqrt{N} t_2
\]  \hspace{1cm} (47)

By taking \( t_2 = (\pi/2)\sqrt{N/m} \), it holds \( P_a(t_1 + t_2) = 1/m \). The method is called the proposed method 2. Fig.4 shows the numerical example the comparison between method 1 and proposed method 2 for \( N = 1024, m = 1, l = 512 \).

C. The application to Grover search algorithm of the proposed methods

In this section, let us apply the proposed method 2 obtained in the section B to Grover search algorithm shown in Fig.1. Fig.6 shows the proposed method 3 (in digital time) corresponding to the proposed method 2. Let us compute the
1. Initial state $|\psi\rangle$
2. Repeat $T_1$ times
3. $|\psi\rangle = I_p|\psi\rangle$
4. $|\psi\rangle = G|\psi\rangle$
5. Repeat $T_2$ times
6. $|\psi\rangle = I_p|\psi\rangle$
7. $|\psi\rangle = G|\psi\rangle$
8. Observe the system

Fig. 6 The algorithm of the proposed method 3

As $T_1 = 2$, $I_p$ and $G$ to the Eq.53 are iterated one more time. As a result, the following state is obtained:

$|\psi\rangle = \frac{1}{4}(-1,-1,-1,-1,-1,-1,1,-1,1,-1,1,1)$ (54)

Further, iterating the steps 5 to 8 of the proposed method 3 to the Eq.54, the desired data is obtained with the probability 0.96.

Next, supposing that the stored data are $|0\rangle, |2\rangle, |3\rangle, |6\rangle, |7\rangle, |10\rangle, |11\rangle, |12\rangle$ as follows:

$|\psi\rangle = \frac{1}{2\sqrt{2}}(1,0,1,1,0,0,1,1,1,0,0,0)^t$ (55)

When the steps 2 to 4 of the proposed method 3 are iterated for the Eq.55, the following state is obtained:

$|\psi\rangle = -\frac{1}{2\sqrt{2}}(1,0,1,1,0,0,1,1,1,0,0,0)^t$ (56)

Then, the desired data is obtained with the probability 0.5 after applying the steps 5 to 8. It shows that the proposed method 3 does not always give a good result.

As shown in Fig.7, we can not always get the maximum result, because the maximum value of $T_1$ is real number in analog model. Therefore, in order to improve the result we can introduce the phase rotation[8]. These are represented as the following unitary matrixes:

$W = I - (1-e^{-i\alpha}) \sum_{\lambda=1}^{l} |\rho_{\lambda}\rangle \langle \rho_{\lambda}|$ (57)

$V = (1-e^{i\beta})|s\rangle\langle s| + e^{i\beta}I$ (58)

1. Initial state $|\psi\rangle$
2. Repeat $T_2$ times
3. $|\psi\rangle = W|\psi\rangle$
4. $|\psi\rangle = V|\psi\rangle$
5. Repeat $T_2$ times
6. $|\psi\rangle = I_p|\psi\rangle$
7. $|\psi\rangle = G|\psi\rangle$
8. Observe the system

Fig. 8 The algorithm for the proposed method 4

The method is called the proposed method 4 The Fig.8 shows the algorithm for the proposed method 4. Matrixes $I_p$ and $G$ used before are the special case for $\alpha = \beta = \pi$ of $W$ and $V$, respectively. Let us compute the time $T_2$. Let us consider the case of $T_2 = 2$. Then, as the imaginary parts of $\psi_a(2)$ and $\psi_b(2)$ are agree, we will find the condition that the real parts of $\psi_a(2)$ and $\psi_b(2)$ are agree. The following relation is satisfied with the condition:

$\alpha = \arccos\left(-\frac{N - 2l}{2l}\right)$ (59)

where $l \geq (1/4)N$

Fig.7 shows the results of Grover and two proposed algorithms.

Example 3:

Let $n = 4$ and $N = 16$. Let the initial state be defined as the Eq. 55. In the proposed method 4, $\alpha$ is set to $\pi/2$. 

Fig. 7. The comparison among the proposed algorithms of numerical simulation for $N = 256$.

Example 2:

Let $n = 4$ and $N = 16$. Let $|2\rangle, |6\rangle, |11\rangle, |12\rangle$ be stored data.

$|\psi\rangle = \frac{1}{2}(0,0,1,0,0,0,0,0,1,0,0,0,1,0,0,0)^t$ (52)

The suffix $t$ means the transpose of the vector. The following result is obtained by applying $I_p$ and $G$ to the initial state of the Eq.52.

$|\psi\rangle = \frac{1}{4}(-1,-1,-1,-1,-1,-1,-1,-1,1,-1,1,-1,1,1,-1,1)^t$ (53)
TABLE I

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As $T_2 = 2$, the steps 3 to 4 of the proposed method 4 are iterated two times. Then, the following state is obtained:

$$|\psi\rangle = \frac{1}{4\sqrt{2}} \left( -1+i, -1+i, -1+i, -1+i, -1+i, -1+i, -1+i, -1+i \right) t$$  \hspace{1cm} \text{(60)}$$

Grover algorithm shows good performance only in the case of $N = l$. The proposed method 3 shows better performance compared with Grover algorithm, but does not always show good performance in the case of $N \neq l$.

The proposed algorithm 4 shows best performance of three algorithms in digital model.

V. CONCLUSIONS AND FUTURE WORK

The result in this paper is summarized in Table I. The method 1 and the proposed method 2 are obtained by solving the Schrodinger equation. The method 1 and the proposed method 2 in analog time lead to Grover algorithm and the proposed method 3 in digital time. The proposed method 2 in analog time gives the optimum solution, but the proposed method 3 in digital method 3 does not give the optimum solution, because the optimum time is real number. Therefore, we propose the method 4 and show that it gives the optimum solution. As the future work, we will consider the relation between the proposed method 2 and 4.

REFERENCES