Quantum K-nearest neighbor classification algorithm based on Hamming distance

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K-nearest neighbor classification algorithm is one of the most basic algorithms in machine learning, which determines the sample's category by the similarity between samples. In this paper, we propose a quantum K-nearest neighbor classification algorithm with Hamming distance. In this algorithm, quantum computation is firstly utilized to obtain Hamming distance in parallel. Then, a core sub-algorithm for searching the minimum of unordered integer sequence is presented to find out the minimum distance. Based on these two sub-algorithms, the whole quantum frame of K-nearest neighbor classification algorithm is presented. At last, it is shown that the proposed algorithm can achieve a quadratical speedup by analyzing its time complexity briefly.

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I. INTRODUCTION

Recently, with the development of quantum mechanics and information science, quantum information, the product of the combination of these two disciplines, has gradually attracted people's attention. One of the most popular issues is quantum machine learning (QML) [1]. Since the proposal of quantum linear system algorithm by Harrow et al. [2], a series of quantum algorithms have been presented to solve various machine learning tasks, such as quantum dimensionality reduction algorithm [3–5], quantum regression algorithm [6, 7], quantum association rules mining [8], quantum decision tree classifier [9], quantum support vector machine [10–12], quantum nearest neighbor classification algorithm [13–18], and so on. They combine classical algorithms with quantum computation, and are shown to achieve significant speedup over their classical counterparts.

As one of the most common algorithms in machine learning, classification has been widely applied in image recognition [17] and text categorization [19]. Typically, K-nearest neighbor (KNN) classification algorithm determines the testing sample's category based on the metric of distance with excellent performance, and has been combined with quantum computation as well, arousing widespread interest of scholars. In 2011, Lloyd et al. presented a quantum method to calculate Euclidean distance [14] with the help of swap test [20]. Based on that, Wiebe et al. proposed a quantum version of nearest-centroid classification algorithm [15] where Grover's search algorithm [21], in the form of the Dürr Høyer minimization algorithm [22] was utilized to find the closest cluster. However, for non-numerical data, it doesn't make sense to compute the Euclidean distance, while Hamming distance is significative and can be obtained easily. In terms of that, Ruan et al. proposed a quantum KNN algorithm based on Hamming distance [16]. However, in their algorithm, besides K, a new parameter t is added, which is used to find out the training samples from whom the distance to the test sample is less than t, so that there are two parameters to set and optimize, increasing the amount of computation. Moreover, a key step of KNN algorithm, searching the K nearest neighbors, is ignored.

Further studying on these problems, we propose a whole quantum KNN classification algorithm based on Hamming distance, which is shown to be quadratically faster than its classical counterpart when the sample vectors lie in a low-dimensional feature space. In the proposed algorithm, a core sub-algorithm is put forward to search the minimum distance which is more efficient and more applicable to integer data than Dürr Høyer minimization algorithm [22] which is utilized commonly in quantum machine learning algorithms [15, 17]. Moreover, we present the whole quantum frame of KNN classification algorithm where the testing sample's category can be obtained clearly.

The rest of this paper is organized as follows. In Sec. II, we review the classical KNN classifier. Sec. III presents two quantum sub-algorithms, calculating Hamming distance and searching the minimum of unordered integer sequence. Sec. IV gives the whole quantum frame of KNN classification algorithm. Conclusions are given in the last section.

II. PRELIMINARIES

In this section, we briefly review the basic idea and main processes of the classical KNN classification algorithm [19].

KNN is one of the most common classification algorithms of supervised learning, where the testing sample is classified according to the similarity between it and training samples. For example, as shown in Fig. 1, there are two classes, blue square and red triangle. The task is to
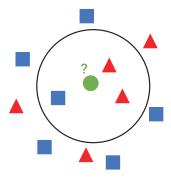
FIG. 1: The illustration of KNN algorithm.

determine what the green circle whose class is unknown belongs to. At first, the distance metric is utilized to calculate similarities between the green circle and other samples. It's easy to see that the K nearest neighbors include two red triangles and one blue square when $K = 3$. Finally, based on "majority voting" principle, the green circle is classified to the category of red triangle.

The general processes of classical KNN classifier can be summarized as follows.

(1) Compute the similarity between the testing sample (unclassified sample) and each training sample.

(2) Find out K nearest neighbors of the testing sample.

(3) Count categories of K nearest neighbors, then assign the most frequent category to the testing sample.

Obviously, the runtime of KNN classification algorithm is dominated by the computation of distance which should be implemented M times. Thus, its time complexity is $O(M)$.

There are many ways to calculate similarity. One of the most common metrics is Hamming distance. It can be applied to KNN classification algorithm to classify non-numerical data points efficiently, which is concerned in this paper. Given the testing sample vector $\overrightarrow{x} = (x_1, x_2, \cdots, x_N)^T$ $(x_j \in \{0,1\};\ j = 1, 2, \cdots, N)$, whose class is unknown, and training sample vectors $\overrightarrow{v_i} = (v_{i1}, v_{i2}, \cdots, v_{iN})^T$ $(v_{ij} \in \{0,1\};\ j = 1, 2, \cdots, N)$ with class c_i, where $i = 1, 2, \cdots, M;\ c_i \in \{0, 1, \cdots, L\}$. Hamming distance between $\overrightarrow{x}$ and $\overrightarrow{v_i}$ is given by

$$d_i = |\overrightarrow{x} - \overrightarrow{v_i}| = \sum_{j=1}^{N} (x_j \oplus v_{ij}), \qquad (1)$$

which shows the difference of two bit vectors. For example, the Hamming distance between 01101 and 11001 is 2.

Ruan et al. presented a quantum KNN classification algorithm for implementing this algorithm based on the metric of Hamming distance [16]. In their algorithm, a new parameter t is introduced to help finding out the K nearest neighbors. Specifically, if the Hamming distance between a training sample and the test sample is less than t, it is considered to be one of the K nearest

neighbors. Obviously, the value of t is difficult to determine because there is no direct correlation between t and K. In addition, generally speaking, the value of K is much less than the number of training samples M. Then if the K nearest neighbors are obtained by performing a projection measurement on the quantum register directly (mentioned in Sec. 3.2 of Ref. [16]), the success probability $\frac{K}{M}$ may be very small. Therefore, this problem should also be considered in the practical implementation of the algorithm presented in Ref. [16]. In the next section, we will give possible solutions to these problems.

III. TWO QUANTUM SUB-ALGORITHMS

From the classical frame of KNN classification algorithm, it is evident that there are two key steps, i.e. steps (1) and (2). So, before presenting the whole quantum frame of KNN classifier, two corresponding quantum sub-algorithms are put forward in this section. The first quantum sub-algorithm is computing Hamming distance, which is described in Sec. III A. The second sub-algorithm in Sec. III B is a quantum method for searching the minimum of unordered integer sequence. In Sec. III C, we perform runtime analysis on the two sub-algorithms respectively.

A. Quantum method for computing Hamming distance

Computing similarity is an important subprogram in classification algorithms. For the classification of non-numerical data, Hamming distance is one of the popular ways to calculate similarity. Here, we describe a quantum method to calculate Hamming distance between $\overrightarrow{x}$ and $\overrightarrow{v_i}$ in parallel.

A1: Prepare the superposition state

$$|\phi_1\rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |\boldsymbol{v_i}\rangle |\boldsymbol{x}\rangle. \qquad (2)$$

where $|\boldsymbol{x}\rangle = |x_1 x_2 \cdots x_N\rangle = |x_1\rangle|x_2\rangle \cdots |x_N\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_N\rangle$ and $|\boldsymbol{v_i}\rangle = |v_{i1} v_{i2} \cdots v_{iN}\rangle$ respectively.

Considering a binary training data set $\overrightarrow{v_i}$, we can use a decimal value $\boldsymbol{v_i}$ to represent the vector, where $\boldsymbol{v_i} = v_{i1} 2^{N-1} + \cdots + v_{iN} 2^0$. Thus, the dataset can be taken as a new vector $\overrightarrow{V} = (\boldsymbol{v_1}, \boldsymbol{v_2}, \cdots, \boldsymbol{v_M})$. We assume we have a quantum access to the vector in a quantum random access memory (QRAM) [23–26], and the classical elements $\boldsymbol{v_i}$ $(i \in [M])$ store in M memory cells. Possible physical realizations and architectures for the QRAM are discussed in detail in Ref. [23] and Ref. [25]. Then there exists an oracle O_V

$$O_V : |i\rangle |0\rangle \mapsto |i\rangle |\boldsymbol{v_i}\rangle, \qquad (3)$$

which can efficiently access $\boldsymbol{v_i}$ in time $O(\log_2 M)$.

Before performing O_V, one important step is preparing the state $\frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle$. Ref. [17] gives an efficient approach to generating this state by performing a product of Hadamard gates, $H = \frac{1}{\sqrt{2}} ((|0\rangle + |1\rangle) \langle 0| + (|0\rangle - |1\rangle) \langle 1|)$, and the quantum comparator that can be applied to compare the size of two numbers [27]. At first, prepare $m = \lceil \log_2 (M + 1) \rceil$ qubits in $|0\rangle$, and perform Hadamard gates to obtain $\frac{1}{\sqrt{2^m}} \sum_{i=0}^{2^m-1} |i\rangle$. Next, we append two flag qubits. If $i = 0$, flip the first qubit, and if $i > M$, flip the second qubit. The first operation can be implement by CNOT gate, and the second operation can be achieved with the help of the quantum comparator. Then measure the flag qubits, and we can obtain the state $\frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle$. The measure probability is $M/2^m$, thus, the running time is $O(2^m/M) = O(1)$. Next, performing oracle O_V, we can obtain the state $\frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |\boldsymbol{v_i}\rangle$.

For the testing vector $\overrightarrow{x}$, we need prepare N qubits. If $x_j = 0$, the jth qubit is in the state $|0\rangle$. Otherwise, it is in the state $|1\rangle$. In this way, we have $|\boldsymbol{x}\rangle$. As a result, we can generate the state $|\phi_1\rangle$ in $O(\log_2 M)$.

A2: Implement the CNOT gate to see whether the state in the same place is equal. The CNOT gate is one of the most common controlled operations in quantum computing, with two input qubits, known as the target qubit and control qubit, respectively. The action of the $CNOT_{ct}$ gate is given by $|x\rangle_c |y\rangle_t \to |x\rangle_c |x \oplus y\rangle_t$, where $x, y \in \{0, 1\}$, c and t represent the control qubit and the target qubit respectively; that is, if $x = y$, then the target qubit t is in the state $|0\rangle$, otherwise t is in the state $|1\rangle$. By implementing CNOT gates on the qubits in the same place of $|\boldsymbol{x}\rangle$ and $|\boldsymbol{v_i}\rangle$, and labeling the result state of the target qubit $|x_i\rangle$ with $|r_{ij}\rangle$, we have

$$|\phi_2\rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} \bigotimes_{j=1}^{N} CNOT_{c_{ij}t_j} |i\rangle |\boldsymbol{v_i}\rangle_{c_{i1}\cdots c_{iN}} |\boldsymbol{x}\rangle_{t_1\cdots t_N}$$
$$= \frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |v_{i1} \cdots v_{iN}\rangle_{c_{i1}\cdots c_{iN}} |r_{i1} \cdots r_{iN}\rangle_{t_1\cdots t_N},$$
$$(4)$$

A3: Add a register in the state $|0\rangle$ with $n = \lceil \log_2 (N + 1) \rceil$ qubits to store Hamming distance d_i. After calculating $\sum_{j=1}^{N} r_{ij}$, the state becomes

$$|\phi_3\rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |v_{i1} \cdots v_{iN}\rangle |r_{i1} \cdots r_{iN}\rangle |d_i\rangle. \quad (5)$$

This step can be achieved by using $d_i + r_{ij}$ quantum circuit proposed by Kaye[28] as shown in Fig. 2(a). In Fig. 2(a), d_i is described as $d_{i1}d_{i2} \cdots d_{in}$ in binary representation, and the controlled circuit consists of a series of controlled NOT operations and a Pauli operation $X = |0\rangle \langle 1| + |1\rangle \langle 0|$, where controlled NOT operation requires more than one control qubits. It's easy to verify
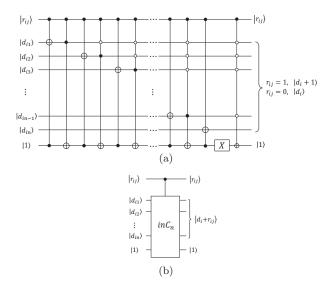

FIG. 2: The $d_i + r_{ij}$ quantum circuit. The hollow circle on the control qubit indicates that the operation is applied to the target qubit conditioned on the control qubit equalling 0. While, the solid circle is in opposite condition.

that this circuit can obtain the result of $d_i + r_{ij}$. Moreover, this circuit can be taken as a controlled operation inC_n, as shown in Fig. 2(b).

Fig. 3 shows the processes of the calculation of Hamming distance. After preparing the state $|\phi_1\rangle$, implement CNOT gates and we can obtain $|\phi_2\rangle$. Then, perform inC_n to obtain Hamming distance d_i stored in R_D. An example is given for illustrating this circuit more clearly. Given two vectors, $\overrightarrow{v_i} = (01101)^T$ and $\overrightarrow{x} = (11001)^T$, their corresponding quantum states are $|v_{i1} \cdots v_{i5}\rangle_{R_V} = |01101\rangle$ and $|x_1 \cdots x_5\rangle_{R_X} = |11001\rangle$. Perform CONT gates, and the state of register R_X becomes $|r_{i1} \cdots r_{i5}\rangle_{R_X} = |10100\rangle$. Then, implement the operation inC_3 to obtain Hamming distance, $\sum_{j=1}^{5} r_{ij}$. Here, inC_3 needs to be performed 5 times. For the first, the first qubit of the register R_X is the control qubit, and after performing the operation inC_3, the state of the register R_D becomes $|0 + r_{i1}\rangle = |1\rangle$. For the second, perform the operation inC_3 controlled by the second qubit of the register R_X, and the state of the register R_D becomes $|1 + r_{i2}\rangle = |1\rangle$. The last three operations are similar to the first two. As a result, we have the Hamming distance between $\overrightarrow{v_i}$ and $\overrightarrow{x}$, $|d_i\rangle = |2\rangle$.

B. Quantum method for searching the minimum of unordered integer sequence

The second step of KNN classification algorithm is finding out K nearest neighbors, that is, searching the K minimum Hamming distances between the testing sample and training samples. In other words, this task can be depicted as a problem: searching the K minimum elements of the set $D = \{d_1, d_2, \cdots, d_M\}$, where
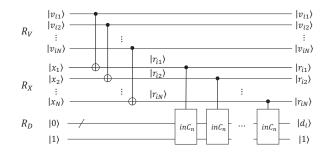
FIG. 3: The circuit for computing Hamming distance d_i. The last qubit in the state $|1\rangle$ is used for the implementation of inC_n operation.

$d_i \in \{1, 2, \cdots, N\}$. Here, because the case where the distance is equal to 0 is trivial and easy to solve, we don't take it into account in this section, and the solution of that is presented in Sec. IV. To solve this problem, we propose a quantum algorithm for searching the minimum value of unordered integer sequence with runtime $O\left(\sqrt{M} \log_2 M\right)$. Compared with the classical algorithm, our algorithm can achieve quadratical speedup.

To find out the minimum element of D, we introduce a parameter $key_j \in \{1, 2, \cdots, N\}$ with its binary representation $key_{j1} key_{j2} \cdots key_{jn}$, where $n = \lceil \log_2 (N + 1) \rceil$. The binary representation of d_i is $d_{i1} d_{i2} \cdots d_{in}$. Add a bit in 0 before d_i and key_j, i.e., $d_i = 0d_{i1}d_{i2} \cdots d_{in}$ and $key_j = 0key_{j1}key_{j2} \cdots key_{jn}$. Then we have $d_i \ominus key_j = d_i - key \mod 2^{n+1}$. Suppose the result is b_i with the binary representation $b_{i0} b_{i1} \cdots b_{in}$. If $d_i < key$, we can obtain $b_{i0} = 1$, and $b_{i1} \cdots b_{in}$ is the binary representation of $d_i - key_j \mod 2^n$. That is, if $d_i < key_j$, the bit b_{i0} will be flipped to 1, otherwise $b_{i0} = 0$. This idea inspires us that the elements less than key_j can be reserved by measuring an ancillary qubit with outcome 1, if d_i and key_j are encoded to quantum represents $|d_i\rangle$ and $|key_j\rangle$. What's more, thanks to quantum parallelism, $|d_i - key\rangle$ can be computed in parallel, which makes the process more efficiently. Based on these analysis, a quantum algorithm for searching the minimum value of unordered integer sequence is given as follows.

B1: Prepare the quantum state

$$|\alpha_1\rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |d_i\rangle_{R_D}, \qquad (6)$$

For easy of depiction, R_D is used to denote the register storing d_i which has n qubits.

To prepare $|\alpha_1\rangle$, assume we are provided the quantum oracle

$$O_D : |i\rangle |0\rangle \mapsto |i\rangle |d_i\rangle, \qquad (7)$$

which can efficiently access the entries of D in $O(\log_2 M)$ time. This holds when the entries of D are efficiently computable or are stored in QRAM [23–26]. We start with performing the oracle O_D on the state

$\frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |0\rangle$ to have $\frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |d_i\rangle$. Here, the preparation of the state $\frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle$ is shown clearly in step A1 of Sec. III A.

B2: Add the second ancillary qubit a_2 in the state $|0\rangle$ before R_D, and we have

$$|\alpha_2\rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |0\rangle_{a_2} |d_i\rangle_{R_D}. \qquad (8)$$

B3: Append a register storing key denoted by R_k. At first, suppose $max_0 = N$, $min_0 = 1$, then $key_0 = \left\lfloor \frac{max_0 + min_0}{2} \right\rfloor$ with the binary representation $key_0 = key_{01} key_{02} \cdots key_{0n}$. Generate state $|key_0\rangle = |0key_{01}key_{02} \cdots key_{0n}\rangle$ stored in R_K, and obtain

$$|\alpha_3\rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |0\rangle_{a_2} |d_i\rangle_{R_D} |key_0\rangle_{R_K}. \qquad (9)$$

B4: Reserve the elements less than key_0.
Calculate $|d_i - key_0\rangle$ in parallel, and the state becomes

$$|\alpha_4\rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |d_i \ominus key_0\rangle_{a_2, R_D} |key_0\rangle_{R_K}, \qquad (10)$$

where, $a \ominus b$ represents $a - b \mod 2^{n+1}$.

If there exist elements less than key_0 in sequence D, labeled with d_{i_p}, then $a_2 : |0\rangle \rightarrow |1\rangle$. We have

$$|\alpha_4\rangle = \frac{1}{\sqrt{M}} \left(\sum_{p=1}^{l} |i_p\rangle |1\rangle_{a_2} |d_{i_p} - key_0\rangle_{R_D} |key_0\rangle_{R_K} + \sum_{q=1}^{M-l} |i_q\rangle |0\rangle_{a_2} |d_{i_q} - key_0\rangle_{R_D} |key_0\rangle_{R_K} \right), \qquad (11)$$

where, l is the number of the elements less than key_0; and d_{i_q} is the element bigger than or equal to key_0.
Otherwise,

$$|\alpha_4\rangle = \frac{1}{\sqrt{M}} \sum_{q=1}^{M} |i_q\rangle |0\rangle_{a_2} |d_{i_q} - key_0\rangle_{R_D} |key_0\rangle_{R_K}. \qquad (12)$$

At this time, if measure a_2 to see the outcome 1, after successful measurement, we retain the elements less than key_0. According to Eq. (11), the probability of obtaining measurement outcome 1 is $Prob_2(1) = l/M$. The state after measurement is

$$|\alpha_5\rangle = \frac{1}{\sqrt{l}} \sum_{p=1}^{l} |i_p\rangle |1\rangle_{a_2} |d_{i_p} - key_0\rangle_{R_D} |key_0\rangle_{R_K}. \qquad (13)$$

Here, we need $O(M)$ measurements. By utilizing amplitude amplification [29], the runtime can be speed up to $O\left(\sqrt{M}\right)$. If all the measurement outcomes are 0, then the conclusion is that no element is less than key_0.

Next, restore R_D to d_i. Perform quantum addition operation, and we obtain

$$|\alpha_6\rangle = \frac{1}{\sqrt{l}} \sum_{p=1}^{l} |i_p\rangle |0\rangle_{a_2} |d_{i_p}\rangle_{R_D} |key_0\rangle_{R_K}, \qquad (14)$$

or,

$$|\alpha_6\rangle = \frac{1}{\sqrt{M}} \sum_{q=1}^{M} |i_q\rangle |0\rangle_{a_2} |d_{i_q}\rangle_{R_D} |key_0\rangle_{R_K}. \qquad (15)$$

After implementing step B4, we obtain the elements less than key_0 if they exist.

B5: Update the value of key based on the idea of binary searching. If the outcome of measuring a_2 is 1, then $max_j = key_{j-1} - 1$, $min_j = min_{j-1}$. Otherwise, $min_j = key_{j-1} + 1$, $max_j = max_{j-1}$. We have $key_j = \left\lfloor \frac{max_j + min_j}{2} \right\rfloor$. For example, we assume that the minimum value of set D, $d_{min} = \frac{5N}{16}$, and N is a multiple of 16, as shown in Fig. 4. Then, the initial $max_0 = N$, $min_0 = 1$, and $key_0 = \left\lfloor \frac{N+1}{2} \right\rfloor = \frac{N}{2}$. In the next three iteration, we have $key_1 = \frac{N}{4}$, $key_2 = \frac{3N}{8}$, $key_3 = \frac{5N}{16}$, respectively. Obviously, through three iterations, key is close to d_{min}.
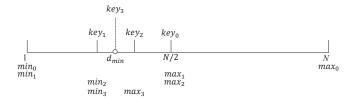

FIG. 4: The process of updating the value of key, where d_{min} denotes the minimum value of set D, and min_j, max_j, key_j is the value of min, max, key in jth iteration respectively.

Then, update R_K to store $|key_j\rangle$. Repeat step B4 until $max_j = min_j$. After measuring a_2, the state will be in two cases:

$$|\alpha_7\rangle = \frac{1}{\sqrt{E}} \sum_{e=1}^{E} |i_e\rangle |1\rangle_{a_2} |d_{i_e} - key_j\rangle_{R_D} |key_j\rangle_{R_K}, \quad (16)$$

$$|\alpha_7\rangle = \frac{1}{\sqrt{E}} \sum_{e=1}^{E} |i_e\rangle |0\rangle_{a_2} |d_{i_e} - key_j\rangle_{R_D} |key_j\rangle_{R_K}, \quad (17)$$

where, E is the number of the elements whose value are the minimum; $d_{i_1} = d_{i_2} = \cdots = d_{i_E} = d_{min}$, d_{min} is the value of the minimum of set D. Eq. (16) can be obtained when the measure outcome is 1, where $d_{min} < key_j$, and Eq. (17) can be obtained when the measure outcome is 0, where $d_{min} = key_j$. Then performing addition operation on register R_D and R_K, the final state is

$$|\alpha_{min}\rangle = \frac{1}{\sqrt{E}} \sum_{e=1}^{E} |i_e\rangle |0\rangle_{a_2} |d_{i_e}\rangle_{R_D} |key_j\rangle_{R_K}. \quad (18)$$

Measuring the index register and R_D in computational basis, we obtain the value of the minimum elements of D, d_{min} and its index.

C. Runtime analysis

One of the clear advantages of quantum algorithm is that it is faster than classical algorithm. Hence, in this section, the runtime of the above two quantum sub-algorithms are discussed respectively. Similarly to the representative quantum algorithm, we analyze the number of quantum operations in each step of the two sub-algorithms and obtain the time complexity of them. It is shown that the presented sub-algorithms achieve significant speedup over their classical counterparts.

The sub-algorithm A presents a quantum method for calculating Hamming distance. Obviously, in step A1, the runtime of state preparation is $O(\log_2 M)$. Then, N CNOT gates are utilized to obtain $|r_{i1} \cdots r_{iN}\rangle$ in step A2, so the time complexity of this step is $O(N)$. Finally, to compute the sum of r_{ij}, N inC_n operations are used in step A3. According to Ref. [28], the depth of inC_n is

$$\begin{cases} 1 & n = 1 \\ 10 & n = 2 \\ 2n^2 + n - 5 & n \geq 3 \end{cases} \qquad (19)$$

Thus, each inC_n operation has $O(n^2)$ elementary gates, which means that step A3 takes runtime $O(Nn^2)$. Based on the runtime of each step of sub-algorithm A shown in Table I, we can obtain the overall runtime of this sub-algorithm is $O(\log_2 M + N + Nn^2)$. Considering a low-dimensional feature space, i.e., $N \ll M$, we can ignore the effect of N on the overall algorithm. In this case, the time complexity of the quantum sub-algorithm A is $O(\log_2 M)$. As compared to the classical counterpart, the runtime of which is $O(M)$, the proposed quantum sub-algorithm greatly reduces the time complexity.

TABLE I: The runtime of the sub-algorithm A.

Step	Runtime
A1	$O(\log_2 M)$
A2	$O(N)$
A3	$O(Nn^2)$
Overall time complexity	$O(\log_2 M + N + Nn^2)$

The sub-algorithm B is a quantum sub-algorithm for searching the minimum of unordered integer sequence which can be used to find out the K nearest neighbors in KNN classification algorithm. In step B1, QRAM [23–26] is utilized to state preparation with the runtime $O(\log_2 M)$. Then, in step B2 and step B3, the particle a_2 in state $|0\rangle$ and the register R_K in state $|key_0\rangle$ are appended respectively, so the runtime of the two steps is $O(1)$. After that, in Step B4, $|d_i - key\rangle$ is calculated in parallel, and a_2 is measured to reserve the elements

less than key. The probability of obtaining measurement outcome 1 of a_2 is l/M where l is unkonwn, so it need $O\left(\sqrt{M}\right)$ repetitions by utilizing amplitude amplification [29]. Finally, key is updated $O\left(\log_2 N\right)$ times to obtain the minimum value in step B5. Based on Table II, the overall time complexity of the sub-algorithm B is $O\left(\log_2 N\sqrt{M}\log_2 M\right)$. Here, the case where the sample vectors lie in a low-dimensional feature space is also taken into account, i.e., $N \ll M$, the time complexity is $O\left(\sqrt{M}\log_2 M\right)$. Compared with the classical searching algorithm with runtime $O\left(M\right)$, obviously, our algorithm achieves the speedup.

TABLE II: The runtime of sub-algorithm B.

Step	Runtime
B1	$O\left(\log_2 M\right)$
B2	$O\left(1\right)$
B3	$O\left(1\right)$
B4	$O\left(\sqrt{M}\right)$
B5	$O\left(\log_2 N\right)$
Overall time complexity	$O\left(\log_2 N\sqrt{M}\log_2 M\right)$

Involving the problem of searching the minimum value, Christoph Dürr and Peter Høyer proposed a quantum algorithm for finding the minimum value based on Grover's search algorithm [21] with running time $O\left(\sqrt{M}\right)$ (M is the sample scale) in 1996 [22]. Given a set containing M elements, their algorithm utilizes an oracle to compare the value of elements with one of them and mark the smaller. The element can be in a arbitrary numeric set. Different with their algorithm, the data set in our algorithm is required to be a set of integers in a known range. We search the minimum based on the properties of elements and we don't rely on the oracle to mark the index register. The elements less than key are reserved by measuring a flag qubit, which can be implemented via the present quantum technique, such as QRAM [23–26], quantum addition operation [28] and amplitude amplification [29]. In practical term, there exist lots of application scenarios where the element requires to be a integer and its scope has made requirement as well, such as finding the minimum students' test score in student management system, finding the minimum age in Demographic and Health Surveys and finding the minimum Hamming distance which we concern in this paper.

IV. WHOLE QUANTUM FRAME FOR KNN CLASSIFIER

Based on the above two sub-algorithms, in this section, we present the whole quantum frame for KNN classifier based on Hamming distance in detail in Sec. IV A. Its runtime analysis is in Sec. IV B.

A. Quantum algorithm

Given testing sample vector $\overrightarrow{x}$, and training sample vectors $\{\overrightarrow{v_i}, c_i\}_{i=1}^{M}$, the detail of the algorithm is as follows.

Step W1: Prepare the initial quantum state.

In this step, the initial quantum state

$$|\psi_0\rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |v_{i1}\cdots v_{iN}\rangle_{R_V} |c_i\rangle_{R_C} |x_1\cdots x_N\rangle_{R_X} \tag{20}$$

is generated.

We assume training samples are stored in QRAM [23–26], and oracle O_{VC} is provided, where

$$O_{VC} : |i\rangle |0\rangle |0\rangle \mapsto |i\rangle |\boldsymbol{v_i}\rangle |c_i\rangle \tag{21}$$

Then, the state $\frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |\boldsymbol{v_i}\rangle |c_i\rangle$ can be obtained in $O\left(\log_2 M\right)$. To generate $|\boldsymbol{x}\rangle = |x_1 x_2 \cdots x_N\rangle$, prepare the state $|0\cdots 0\rangle$ with N qubits at first. If $x_j = 1$, then the jth qubit is flipped to $|1\rangle$. Otherwise, it is still in $|0\rangle$. Thus, we can obtain $|\boldsymbol{x}\rangle$ stored in R_X. As a result, $|\psi_0\rangle$ is generated in $O\left(\log_2 M\right)$.

Step W2: Calculate Hamming distance.

In this step, the first sub-algorithm is utilized to compute Hamming distances between the testing sample and training samples. Based on the quantum circuit as shown in Fig. 3 to calculate Hamming distance described in Sec. III A. firstly, perform CNOT gates on R_V and R_X to see whether the state in the same place is equal. Then, N controlled operation inC_n are performed to obtain $|d_i\rangle$. The state becomes

$$|\psi_1\rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |v_{i1}\cdots v_{iN}\rangle_{R_V} |c_i\rangle_{R_C} |r_{i1}\cdots r_{iN}\rangle_{R_X} |d_i\rangle_{R_D}$$

$$= \frac{1}{\sqrt{M}} \sum_{i=1}^{M} |i\rangle |\boldsymbol{v_i}\rangle_{R_V} |c_i\rangle_{R_C} |\boldsymbol{r_i}\rangle_{R_X} |d_i\rangle_{R_D}. \tag{22}$$

Step W3: Search K nearest neighbors.

Considering the case where $d_i \neq 0$, d_i is an integer between 1 and N. We can use the second sub-algorithm proposed in Sec. III B. to search K nearest neighbors of $\overrightarrow{x}$ directly. When the case where $d_i = 0$ is taken into account, the distance d_i plus 1 can be calculated in advance so that the scope becomes $\{1, 2, \cdots, N+1\}$, and the second sub-algorithm is also applicable in this case. Here, we present the process in the case where $d_i \neq 0$. At this time, by implementing the second sub-algorithm, we obtain the index i_{min} and category $c_{i_{min}}$ of the nearest neighbor. Next, the steps are described in brief.

Step W3.1: As shown in steps B2 and B3, append the second ancillary qubit a_2 as a flag particle in the state $|0\rangle$, and a register R_K to store the state $|key_0\rangle$, where $key_0 = \lfloor \frac{max_0 + min_0}{2} \rfloor$ with the binary representation $key_0 = key_{01}key_{02}\cdots key_{0n}$ and initial $max_0 = N$, $min_0 = 1$.

Step W3.2: Perform step B4 to reserve the elements less than key_0. Calculate $|d_i - key_0\rangle$ at first, then measure a_2. If the outcome is 1, the elements less than key will be reserved. The probability of the outcome 1 will be l/M, so to perform measurements, we need to make $O\left(\sqrt{M}\right)$ measurements. One case is that all the measurement outcomes are equal to 0, which shows all elements are not less than key_0. Restore R_D to d_i, we obtain the state

$$|\psi_2\rangle = \frac{1}{\sqrt{l}} \sum_{p=1}^{l} |i_p\rangle \left|\boldsymbol{v_{i_p}}\right\rangle_{R_V} \left|c_{i_p}\right\rangle_{R_C} \left|\boldsymbol{r_{i_p}}\right\rangle_{R_X} |0\rangle_{a_2}$$
$$\left|d_{i_p}\right\rangle_{R_D} |key_0\rangle_{R_K}, \tag{23}$$

or

$$|\psi_3\rangle = \frac{1}{\sqrt{M}} \sum_{q=1}^{M} |i_q\rangle \left|\boldsymbol{v_{i_q}}\right\rangle_{R_V} \left|c_{i_q}\right\rangle_{R_C} \left|\boldsymbol{r_{i_q}}\right\rangle_{R_X} |0\rangle_{a_2}$$
$$\left|d_{i_q}\right\rangle_{R_D} |key_0\rangle_{R_K}. \tag{24}$$

Step W3.3: Update the value of key as step B5 shows, and repeat step W3.2 until $max_j = min_j$. Finally, after measuring the index register and register R_C, i_{min} and $c_{i_{min}}$ can be obtained.

Step W3.4: Take $\overrightarrow{v_{i_{min}}}$ out of the training sets, and repeat the second sub-algorithm, then we can obtain the second nearest neighbor. Therefore, repeating the second sub-algorithm K times, we can obtain the K nearest neighbors with their index k_i ($i \in \{1, \cdots, K\}$) and category c_{k_i}.

Step W4: Determine the testing sample's category.

The task of this step is to find out the category whose frequency is the highest of the K nearest neighbors. Here, the quantum measurement is utilized to avoid quantum-classical interaction, so that the whole algorithm is more efficient. Firstly, based on the result we obtain in step W3, we prepare the state,

$$|\theta\rangle = \frac{1}{\sqrt{K}} \sum_{i=1}^{K} |i\rangle |c_{k_i}\rangle, \tag{25}$$

where, c_{k_i} is category of the k_ith nearest neighbor. Suppose c_{k_i} is stored in QRAM [23–26], and the oracle O_{C_k}

$$O_{C_k} : |i\rangle |0\rangle \mapsto |i\rangle |c_{k_i}\rangle \tag{26}$$

is provided. After generating $\frac{1}{\sqrt{K}} \sum_{i=1}^{K} |i\rangle |0\rangle$, we can implement the oracle O_{C_k} and obtain the state $|\theta\rangle$ in time $O(\log_2 K)$.

Assume the number of category j in K nearest neighbors is ρ_j, $j \in \{0, 1, \cdots, L\}$. Measuring the second register R_C in computational basis, the probability of outcome j is

$$Prob(j) = \langle\theta| (I \otimes |j\rangle \langle j|) |\theta\rangle = \frac{\rho_j}{K}. \tag{27}$$

It's easy to see that the higher the frequency of category is, the bigger measurement probability is. Besides, $O(K)$ repetitions are enough to obtain the category whose frequency is highest in K nearest neighbors. At the end, assign the most frequent category to the testing sample.

B. Runtime analysis

In this section, the time complexity of the proposed quantum KNN classification algorithm is analyzed briefly. Based on the results of Sec. III C, we analyze the runtime of each step and obtain the overall time complexity of the whole algorithm is $O\left(\sqrt{M} \log_2 M\right)$. As shown in Table III, a detailed analysis of each step of the whole quantum algorithm is depicted as follows.

At first, in step W1, the state $|\psi_0\rangle$ is generated in time $O(\log_2 M)$ with the help of QRAM [23–26]. Then, in step W2, the Hamming distance between testing sample and training samples are calculated in parallel by utilizing the sub-algorithm A, where N CNOT gates and N inC_n operations are implemented. Thus, the runtime of step W2 is $O(N + Nn^2)$. Next, sub-algorithm B is utilized to search K nearest neighbors in step W3, which is the most time consuming. The substeps of step W3 have the corresponding steps of sub-algorithm B, where step W3.1 corresponds step B2 and B3; step W3.2 and step W3.3 correspond step B4 and step B5 respectively. According to the runtime analysis of sub-algorithm B in Sec. III C, steps B2 to B5 cost $O\left(\log_2 N\sqrt{M}\right)$ in total. Besides, the sub-algorithm B is required to perform K times to search the K minimum distances, so the runtime on step W3 is $O\left(K \log_2 N\sqrt{M}\right)$. Finally, the testing sample's category is determined in step W4. As generating the state $|\theta\rangle$ costs $O(\log_2 M)$ and $O(K)$ measurements are taken, the runtime on step W4 is $O(K \log_2 K)$.

To sum up, the overall time complexity of the presented quantum KNN classification algorithm is $O\left(K^2 \log_2 K \log_2 N\sqrt{M} \left(\log_2 M + N + Nn^2\right)\right)$. Generally speaking, the vector dimension N and the number of categories K are always far less than the sample scale M, so they have a trivial impact on the overall runtime. It means that the overall time complexity of the quantum KNN classification algorithm is $O\left(\sqrt{M} \log_2 M\right)$. Compared with the classical KNN classification algorithm whose time complexity is $O(M)$, our algorithm achieves quadratical speedup when the sample size is large.

V. CONCLUSIONS

To sum up, in this paper, we consider quantum algorithm for KNN classifier based on Hamming distance, which is one of the most basic algorithms in machine

TABLE III: The runtime of the quantum KNN classification algorithm.

Step	Runtime
W1	$O\left(\log_2 M\right)$
W2	$O\left(N + Nn^2\right)$
W3	$O\left(K \log_2 N \sqrt{M}\right)$
W4	$O\left(K \log_2 K\right)$
In total: $O\left(K^2 \log_2 K \log_2 N \sqrt{M} \left(\log_2 M + N + Nn^2\right)\right)$	

learning and can be a significant subprocess in lots of classification algorithms [18, 19] as well. To achieve this task, two core sub-algorithms are proposed firstly. One is quantum method to calculate Hamming distances between testing sample and training samples, where the addition circuit presented by Kaye [28] is utilized. Another is the sub-algorithm for searching the minimum of unorder integer sequence aiming at finding out the nearest neighbor, which also can be efficiently applied to solve some statistical problems. Based on the above methods, we put forward the whole quantum frame of KNN classification algorithm.

Through a brief analysis, the presented algorithm can classify the testing sample with the time complexity $O\left(\sqrt{M} \log_2 M\right)$ when the sample vectors lie in a low-dimensional feature space. Thanks to the characteristics of quantum computation, the algorithm achieves quadratical speedup over the classical algorithm. However, when the dimension of sample vectors is large, it is hard to obtain the quadratical acceleration, which is a new issue we will study in the future. Moreover, how to efficiently select K in quantum KNN classification algorithm also deserves further investigation.

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