Quantum Anomaly Detection with a Spin Processor in Diamond

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In the processing of quantum computation, analyzing and learning the pattern of the quantum data are essential for many tasks. Quantum machine learning algorithms cannot only deal with the quantum states generated in the preceding quantum procedures, but also the quantum registers encoding classical problems. In this work, the anomaly detection of quantum states encoding audio samples with a three-qubit quantum processor consisting of solid-state spins in diamond is experimentally demonstrated. By training the quantum machine with a few normal samples, the quantum machine can detect the anomaly samples with a minimum error rate of 15.4%. These results show the power of quantum anomaly detection in dealing with machine learning tasks and the potential to detect abnormal output of quantum devices.

1. Introduction

Quantum computers have demonstrated their ability to deal with high-dimensional data and corresponding linear algebra problems with quantum speed-up. Due to the natural essence as a linear system, a quantum register can efficiently interpret datasets stored as matrices and then perform matrix processing in the form of quantum algorithms. This includes both the data encoding classical problem and the quantum states generated by a quantum device, such as the intermediate states in quantum many-body systems and quantum computational chemistry. Since the complete classical description of a quantum register is usually hard to obtain and resource-consuming, the ability to investigate and process quantum data with a quantum computer is essential. In this process, quantum machine learning methods are promising tools to reveal the patterns of quantum data and use them in subsequent tasks, just as their counterparts running on classical computers. Many learning tasks, such as classification and feature extraction, have been demonstrated algorithmically or experimentally using quantum machine learning algorithms including principal component analysis, support vector machines, and generative adversarial network models. With the ability to learn from quantum data, these methods integrate machine learning into quantum algorithms, constituting a great extension to the conventional algorithms on quantum computers.

Among the learning tasks in data processing, many appear in the form of anomaly detection (AD), i.e., the identification of the outliers appearing inconsistent with others in the datasets. It has broad application in both classical problems such as medical diagnosis and fraud detection in finance, and quantum problems including quantum state identification and phase diagram analysis. In these problems, the normal cases are well sampled, while the anomalies are rare and under-sampled. This unbalance limits the performance of multi-class classification algorithms on these datasets, and gives rise to the research of anomaly detection algorithms. Multiple classical algorithms are proposed from different perspectives, such as density estimation method by estimating the probability density function of the normal data, k-nearest neighbor method by calculating the distance of a sample to its kth nearest neighbor, and one-class support vector machine by learning the boundary of the normal data. Recently, quantum algorithms for anomaly detection have been proposed showing the potential to detect anomalies with resources growing logarithmically with respect to the number and dimension of training samples. The quantum algorithms can efficiently provide the anomaly score of a new test sample of interest, and then one can label the new sample as normal or anomaly according to the anomaly score.

In this work, we report an experimental demonstration of quantum anomaly detection (QAD) with a hybrid spin system in diamond at ambient conditions. By encoding classical data into the quantum processor, we apply the algorithm to an audio recognition problem as a full proof-of-principle demonstration of QAD. The quantum processor can calculate the inner products of
multiple quantum samples in parallel and then use the results to identify whether a new audio sample is similar to the pattern of previously given samples. After learning the distribution of the training samples in the feature space, our quantum processor can efficiently classify the test samples with a minimum error rate of 15.4%.

2. Results and Discussion

The task of the anomaly detection algorithm is to assign each new sample an anomaly score that can describe how far away it is from the pattern of normal samples. After this, one can set a threshold and classify a sample as ANOMALY if its anomaly score exceeds the threshold. Here the training set labeled as NORMAL consists of M training samples \( \vec{z}_i \) (\( i = 1, 2, \ldots, M \)) and the new sample to be inspected is denoted by \( \vec{z}_{\text{test}} \). Each sample is represented by a vector in d-dimension feature space and all the training samples are pre-centralized, i.e., \( \sum_{i=1}^{M} \vec{z}_i = 0 \).

A simple way to define the anomaly score is to compute the Euclidean distance between the test sample and the centroid of the training data,[34]

\[
g(\vec{z}_{\text{test}}) = |\vec{z}_{\text{test}}|^2 
\]

A large Euclidean distance from the centroid predicts that the new sample is likely to be an ANOMALY case. The definition of Euclidean distance grants the same weight to the deviations in data along the direction of \( \vec{z}_i \) and \( \vec{z}_{\text{test}} \), and classifies a sample as anomaly if its anomaly score exceeds a threshold.

To overcome this, one needs to analyze the distribution of the training data in the feature space and quantify how well the inspected sample fits it. This can be done by using the anomaly score defined by proximity measure \( f(\vec{z}_{\text{test}}) \),[30] which compares the Euclidean distance \( g(\vec{z}_{\text{test}}) \) and the variance of the training data along the direction of \( \vec{z}_{\text{test}} \):

\[
f(\vec{z}_{\text{test}}) = |\vec{z}_{\text{test}}|^2 - \frac{\vec{z}_{\text{test}}^T C \vec{z}_{\text{test}}}{\sum_{i=1}^{M} |\vec{z}_i|^2}
\]

Here \( \vec{z}_{\text{test}} = \vec{z}_{\text{test}} / |\vec{z}_{\text{test}}| \) and \( C = \frac{1}{M-1} \sum_{i=1}^{M} \vec{z}_i \vec{z}_i^T \) is the covariance matrix which represents the distribution of all the training samples. The proximity measure can better reveal the pattern of training data, since it can provide a boundary line of NORMAL data that fits the distribution of the training data better.[44] To obtain the proximity measure for a test sample, classical computers require \( O(M \times d) \) resources to store and process the dataset, and costs \( O(M \times d) \) computing resources to obtain the covariance matrix and do the following calculations.

A quantum computer can process the above samples and compute \( \vec{z}_{\text{test}} C \vec{z}_{\text{test}} \) in Equation (2) using resources logarithmic in the dimension (d) and the number (M) of the training samples.[10] If the samples \( \vec{z}_i \) are pure quantum states in d-dimension Hilbert space, they can be directly loaded into the quantum register with standard \texttt{swap} gates. Here, the quantum register is composed of a log(d)-qubit data register and a log(M)-qubit index register, as shown in Figure 1. For classical data, a training-data oracle is employed to load the training samples into the quantum register. For each d-dimension vector \( \vec{z}_i \), the data loader returns a training state \( |\psi_i\rangle = 1/|\vec{z}_i| \sum_{j=1}^{d} (\vec{z}_i)_j |j\rangle \) and stores it into the data register. Here \( |j\rangle \) represents the computational basis, and \((\vec{z}_i)_j \) represents the jth element of the ith sample. The fast loading of all the M vectors can be addressed by using quantum random access memory (QRAM).[35] Starting with the superposition in the index register, i.e., \( 1/\sqrt{M} \sum_{i=1}^{M} |i\rangle \), the information of all training samples is stored as a superposition state \( |\Psi\rangle = \sum_{i=1}^{M} \sqrt{P_i} |i\rangle |\psi_i\rangle \), where \( P_i = |(\vec{z}_i)_j|^2 / \sum_{i=1}^{M} |(\vec{z}_i)_j|^2 \) represents the normalized module length \( |\vec{z}_i|^2 \) of the training data. At this stage, the reduced density matrix of the quantum state in the data register is

\[
\rho_{\text{cov}} = \sum_{i=1}^{M} P_i |\psi_i\rangle \langle \psi_i|
\]

which has a similar form with the covariance matrix \( C \) in Equation 2, i.e., \( \rho_{\text{cov}} = C/\xi \), where \( \xi = \sum_{i=1}^{M} |(\vec{z}_i)_j|^2 \) is the trace of \( C \).

Following the same method, the test sample \( \vec{z}_{\text{test}} \) is loaded into the quantum register in the form of test state \( |\psi_{\text{test}}\rangle = \sum_{j=1}^{d} (\vec{z}_{\text{test}})_j |j\rangle \). Then the proximity measure in Equation (2) reduces to

\[
f(\vec{z}_{\text{test}}) = |\vec{z}_{\text{test}}|^2 - \xi (\vec{z}_{\text{test}}^T \rho_{\text{cov}} \vec{z}_{\text{test}})
\]

By measuring the overlap between \( \rho_{\text{cov}} \) and \( |\psi_{\text{test}}\rangle \), the inner products of the test state and all the training states are calculated simultaneously, leading to a fast estimation of the proximity measure. In the experiments, one can store \( \rho_{\text{cov}} \) and \( |\psi_{\text{test}}\rangle \) into different quantum registers and then adopt overlap estimation methods such as the \texttt{swap} test.[36] In this case, the probability of the ancillary qubit at |0\rangle returns \( P_{|0\rangle} = (1 + |\langle \psi_{\text{test}} | \rho_{\text{cov}} |\psi_{\text{test}}\rangle|)/2 \), which can be utilized to estimate the overlap needed and then obtain the anomaly score in Equation (4), as shown in Figure 1.

As an application, we apply the QAD scheme to an audio recognition problem. This demonstration aims to identify whether a piece of audio segment belongs to a certain type of sound, e.g., the sound of the violin in our case. The acoustic samples we used come from the dataset for acoustic event recognition in Ref. [37]. Here we choose four types of audio samples: \{violin, acoustic guitar, crowd, and glass breaking\} as the dataset, with \{70, 30, 30, and 30\} samples of each type, respectively. The original waveforms are firstly analyzed by the method of Mel-frequency cepstral coefficients (MFCCs).[38,39] and then processed by the feature extraction method to reduce the dimension of each sample while keeping most of the information.[40,41] Details of the pre-processing are shown in Supporting Information.[42] After pre-processing, each audio segment is represented by a two-dimension feature vector and is ready to be analyzed by quantum processor. In our
length of training data, utilizing the advantage of long coherence is weighted by the normalized module length composed of single-qubit rotation ingsample. This is realized by a parameterized quantum circuit per position state in the index register, i.e., into the quantum processor, we begin with preparing the single-qubit rotation in superposition of the training states, i.e. \( |\Psi \rangle = \sum_{i=1}^{N} \sqrt{p_i} |i\rangle |\psi_i \rangle \), which denotes a single-qubit rotation \( R_y(\theta) \) conditioned on the carbon nuclear spin being at state \( |0\rangle \). Here \( R_y(\theta) = e^{-i\theta/2} \). The non-local gate \( C^\dagger X |\psi_i \rangle \), representing the encoding operation. In the experiment, the encoding of \( |z_i \rangle \) can be achieved by applying the selective microwave pulse at frequency \( MW_a \), which rotates the electron spin with the angle \( \theta = 2\arctan((z_i)_z/(z_i)_x) \) (Figure 2c). With an arbitrary wave generator compiling all the encoding microwave pulses into a single pulse, we prepare different \( |\psi_i \rangle \) in parallel and obtain the superposition of the training states, i.e. \( |\Psi \rangle = \sum_{i=1}^{N} \sqrt{p_i} |i\rangle |\psi_i \rangle \).

After discarding the index register, the next step is to load the information of each \( |z_i \rangle \) into the data register conditioned on the state \( |i\rangle \) in the index register, i.e. to perform \( \sum_{i=1}^{N} |i\rangle \otimes U_i \) (Figure 2b), where \( U_i |0\rangle = |\psi_i \rangle \), representing the encoding operation. In the experiment, the encoding of \( |z_i \rangle \) at each sample and the normalized module length of training data, utilizing the advantage of long coherence.

Starting from the thermal state, the three-qubit quantum system is initialized to state \( |000\rangle \) by a short laser pulse for dynamical nuclear polarization. To load the data of audio samples into the quantum processor, we begin with preparing the superposition state in the index register, i.e., \( \sum_{i=1}^{N} \sqrt{p_i} |i\rangle \), which is weighted by the normalized module length \( p_i \) of each training sample. This is realized by a parameterized quantum circuit composed of single-qubit rotation \( R_y(\alpha) \), \( R_y(\beta) \), and a non-local gate \( C^\dagger \text{SWAP} \).
Figure 2. a) The pre-processing of the audio samples. Waveforms of different types of audio samples are processed into feature vectors in the 2-dimension feature space. b) The schematic diagram of the quantum anomaly detection in this work. $^{13}$C and $^{14}$N nuclear spins are utilized as the index register, while the electron spin (NV) is used to encode each sample conditional on the state of the index register. After encoding the test sample with $U^\dagger_{\text{test}}$, the proximity measure is estimated by measuring the probability of the electron being on state $|0_e\rangle$. c) Pulse sequence used in the experiments. The non-local gate C$^2$ROT$^\alpha(\gamma)$ in (b) is realized by the conditional phase gate on the electron spin and two local operations, where the second radio-frequency pulse is $\pi$-phase shifted relative to the first one. The data-loading operations $|i\rangle\langle i| \otimes U_i$ are conducted in parallel by applying the microwave pulses with an arbitrary wave generator.

In the readout process, the proximity measure of a new test sample $\vec{z}_{\text{test}}$ is estimated by measuring the overlap between the state in the data register $\rho$, and the test state $|\psi_{\text{test}}\rangle$, i.e., $\langle\psi_{\text{test}}|\rho|\psi_{\text{test}}\rangle$ in Equation (4). Although the method of swap test can estimate the proximity measure of test samples, it is at the cost of more ancillary qubits. In the experiment, we use another efficient approach to introduce the information of the test sample $\vec{z}_{\text{test}}$, utilizing the inverse operation of the data loading, denoted by $U^\dagger_{\text{test}}$. The overlap $\langle\psi_{\text{test}}|\rho|\psi_{\text{test}}\rangle$ can be estimated by a single measurement of the population of the electron spin at
Figure 3. Anomaly detection by the methods of Euclidean distance $g(\vec{z}_{\text{test}})$ and proximity measure $f(\vec{z}_{\text{test}})$. Here, the music notes and stars represent normal (violin) samples and anomaly (non-violin), respectively. a) Anomaly scores provided by different methods. The samples are sorted in ascending order of $g(\vec{z}_{\text{test}})$. Error bars are not shown since they are much smaller than the size of the markers. b) The error rate of different methods. The threshold is scanned within the range of anomaly scores in (a), after the range is normalized to [0, 1].
quantum anomaly detection is 15.4%, which is 55.6% lower than the best performance that the Euclidean distance method can achieve (34.6%). These experimental results show that our quantum processor can efficiently learn the distribution of the training samples and classify different test samples accordingly.

To better understand how the spatial distribution of the training samples is learned, we can read out the proximity measure in the feature space through the covariance matrix stored in the electron spin. The experimental reconstructed density matrix reads as

\[ \rho_{\text{exp}} = \begin{pmatrix} 0.6996 & 0.2151 \\ 0.2151 & 0.3004 \end{pmatrix} \]

which matches the theoretical expectation \( \rho_{\text{cov}} \) with fidelity

\[ F(\rho_{\text{exp}}, \rho_{\text{cov}}) = \text{tr} \sqrt{\sqrt{\rho_{\text{exp}}} \rho_{\text{cov}} \sqrt{\rho_{\text{exp}}}} = 99\% . \]

For any point in the feature space \( \vec{v} = (\text{feature1, feature2}) \), its proximity measure is estimated as \( f(\vec{v}) = \sqrt{\langle \vec{v} | \rho_{\text{exp}} | \vec{v} \rangle} \). Then the value of proximity measure is shown in Figure 4b represented by different colors in the feature space, while the value of Euclidean distance is shown in Figure 4a. In the figure of proximity measure, the peanut-shaped boundary line shows that it can better learn the distribution of the normal data (blue) than using Euclidean distance. In the direction where the normal samples are widely distributed, the proximity measure \( f(\vec{x}_{\text{norm}}) \) rises slowly with the distance from the centroid. For example, while test-v is further from the centroid than test-c (Figure 4a), it has a lower proximity measure than test-c (Figure 4b). This indicates that it is less likely to be an anomaly sample, which is in accordance with its label in the dataset. In this case, the anomaly samples are distributed in all directions around the normal samples, which is beyond the applicability of one-class support vector machine.

3. Conclusion

In conclusion, we demonstrated a quantum algorithm for anomaly detection on a real quantum processor, i.e., the three-qubit hybrid spin system in diamond. Although the demonstration here is implemented in a classical dataset, the method itself can be adopted to identify quantum data, i.e., quantum states. In this work, we utilized the spin processor to demonstrate a full quantum anomaly detection process. The quantum machine was trained with audio samples which are labeled as normal, and then estimated the anomaly scores of the new samples. The experimental results show that this quantum method efficiently analyzes the distribution of the training set in the feature space, which leads to the lower error rate in detecting the anomalies. Given a larger quantum processor, our work can be naturally extended to deal with more complicated classical problems efficiently, such as credit card fraud analysis with much more samples of higher dimensions. Furthermore, a quantum processor can efficiently receive and process samples transported by quantum internet (e.g., by receiving photons containing quantum states). When errors arise from quantum devices, the quantum states will deviate from the normal states. Thus our method can work as a subroutine in distributed quantum computation, quantum communication and entanglement-enhanced quantum metrology, to detect the anomalies in the quantum circuits and improve the performance, avoiding the resource-consuming process of reading out high-dimension quantum states using quantum tomography or similar methods.

4. Experimental Section

Experimental Setup: The experiments were implemented using an NV center with a proximal \( ^{13}\text{C} \) nuclear spin and an intrinsic \( ^{14}\text{N} \) nuclear spin in a [100]-oriented diamond. In the rotating frame, the effective Hamiltonian of this spin system reads as

\[ H_{\text{NV,eff}} = |1\rangle \langle 1| \otimes (A_{\text{F}}^x \sigma_{\text{F}}^x / 2 + A_{\text{N}}^y \sigma_{\text{N}}^y / 2) \]

where \( \sigma_{\text{F,N}} \) are Pauli operators, \( A_{\text{F}}^x \approx 12.8 \text{ MHz} \) and \( A_{\text{N}}^y \approx -2.16 \text{ MHz} \) are the hyperfine coupling strengths between the electron spin and the two nuclear spins. The dephasing times of the spins were measured as \( T_2^\perp \approx 5.4 \mu s, T_2^\perp \approx 2.0 \mu s \) and \( T_2^\perp \approx 5.0 \mu s \). An external magnetic field of around 510 Gauss was applied by a permanent magnet along the symmetry axis of the NV center, so that the three-qubit system can be efficiently polarized to \( m_e = 0, m_c = 1/2, m_N = 1 \) after the polarization transfer in the excited state during laser pumping. In the experiment, a 1 \( \mu s \) 532 nm laser pulse was applied to the spin system, and the polarization of the \( ^{13}\text{C} \) and \( ^{14}\text{N} \) nuclear spins was estimated to be
The readout of the possibility of electron spin at $|0\rangle$. Here $\rho_{\text{final}}$ is the three-qubit state to be measured. $\rho_{\text{exp}}$ and $\rho_{\text{cov}}$ represent single-qubit $\pi$ pulse on carbon spin and nitrogen spin, respectively. $F_i$ ($i = 1, 2, 3, 4$) is the number of photons detected in corresponding experiment.

The average of the photon numbers

$$F_1 + F_2 + F_3 + F_4 = \frac{P_0 \times N_0 + N_1 + N_2 + N_4}{4} + \frac{P_1 \times N_4 + N_5 + N_6 + N_7}{4}$$

(9)

effectively averages the photon luminescence rates of different sublevels, and thus leads to the readout of $P_0$. Then the proximity measure of the test sample $\tilde{z}_{\text{test}}$ can be obtained after having $P_0$.

In the experiment, the fidelity of the RF pulses was estimated to be over 99%. To suppress the thermal effect on the fidelity of MW pulses, idles were added between the repetitions of the pulse sequences. The pulse sequences were repeated for $10^6$ times to suppress the photon shot noise in the readout process. The spin state readout had a duration of 400 ns, and the error bars of the readout results were 0.01.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Author Contributions

J.D., Z.L., and Y.W. supervised the experiments. Z.L. and Y.W. proposed the idea and designed the experiments. Z.C. and Y.L. performed the experiments. M.W. fabricated the structure. Z.L., Z.C., and Y.W. analyzed the data. Y.W., Z.L., and Z.C. wrote the manuscript. All authors discussed the results and commented on the manuscript.
Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

anomaly detection, machine learning, nitrogen-vacancy center, quantum algorithm, quantum computing

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