Computing expectation values of adaptive Fourier density matrices for quantum anomaly detection in NISQ devices

Diego H. Useche, Oscar A. Bustos-Brinez, Joseph A. Gallego, Fabio A. González

MindLab Research Group, Universidad Nacional de Colombia, Bogotá, Colombia
E-mail: {diusecher, oabustosb, jagallegom, fagonzalezo}@unal.edu.co

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Abstract.

This article presents a novel classical-quantum anomaly detection model based on the expected values of density matrices and a new data embedding called adaptive Fourier features. The method works by estimating a probability density function of training data and classifying new samples as anomalies if they lie below a certain probability density threshold. As a core subroutine, we present a new method to estimate the expected value of a density matrix based on its spectral decomposition on a quantum computer. The anomaly detection model is tested with pure and mixed states and both adaptive and random Fourier features on a synthetic data set for density estimation and on a widely used data set for anomaly detection; results show the superior performance of adaptive Fourier features for density estimation and anomaly detection, and of mixed states for density estimation. An important finding of this work is to show that it is possible to perform anomaly detection with high performance on noise intermediate-scale quantum computers. Code and experiments are available at https://github.com/diegour1/QuantumAnomalyDetection.

1. Introduction

A problem of interest in many areas of science and engineering is anomaly detection (AD). This problem consists in determining which samples from a given data set are “ordinary” or “normal” (being the interpretation of “normal” defined for each particular case) and which samples depart or are deviated from “normal” data (commonly known as “anomalies”). Some common applications of anomaly detection methods include fraud detection [1] and medical diagnosis [2]. Many classical algorithms have been proposed for AD [3,4]; however, recent works have shown some advantages of combining quantum computation with AD tasks [5,6,7]; for instance, these methods have shown to utilize fewer resources and to present exponential speed-ups in contrast to their classical counterparts.
A well-known approach to performing AD is density estimation (DE), which consists of estimating a probability density function (pdf) of training data to detect anomalous data. Some classical techniques include the ADDE (algorithm detection based on density estimation) [8], and the SmartSifter method, which uses a finite mixture model [9]. Some quantum anomaly detection (QAD) algorithms include the quantum ADDE which operates with amplitude estimation [5, 10], and a quantum clustering method that exploits the variations in the density function to detect anomalies [11].

In this article, we present a novel classical-quantum anomaly detection strategy that combines a density estimation algorithm called density matrix kernel density estimation (DMKDE) [12] with a new quantum representation of data called adaptive Fourier features (AFF). The method induces probability density functions from training data and classifies new samples as “normal” or “anomalies” if they lie either above or below a certain probability threshold.

One of the main results of the article is the statement of a quantum protocol to estimate the expected value of a mixed density matrix in a quantum computer, through a quantum circuit used to implement the prediction phase of the DMKDE. In contrast to methods like quantum state tomography [13, 14, 15] or the variational quantum eigensolver (VQE) [16], which estimate and codify a density matrix in terms of the Pauli matrices, our quantum algorithm uses the spectral decomposition of the density matrix to measure its expected value. In addition, we propose the adaptive Fourier features (AFF), a new trainable quantum feature mapping, based on random Fourier features (RFF) [17], and suitable for both classical and quantum computers. It represents classical data as quantum states, where the inner product in the Hilbert space approximates a Gaussian kernel in the original space. We show that the AFF in conjunction with the DMKDE quantum algorithm allows us to perform density estimation and anomaly detection with a reduced number of components in both a quantum simulator and a real quantum computer. Furthermore, we show that the proposed method is a viable quantum anomaly detection strategy for noise intermediate-scale quantum (NISQ) devices. In sum, the contribution of the article is threefold:

(i) A new classical-quantum anomaly detection strategy for NISQ computers based on density estimation and the DMKDE algorithm [12].

(ii) A novel trainable quantum feature mapping called adaptive Fourier features which leverages random Fourier features [18, 17].

(iii) A new quantum protocol to estimate the expected value of a density matrix based on its diagonal representation.

The outline of the document is as follows: in Sect. 2 we describe the related work; in Sect. 3 we present the theoretical background of the DMKDE algorithm, the RFF, the notation of the quantum circuits, and a previously proposed quantum protocol [19] to estimate the expected value of a density matrix of a pure state; in Sect. 4 we introduce our proposed quantum anomaly detection method, outline the proposed quantum circuit to estimate the expected value of a mixed state density matrix, and
show the proposed adaptive Fourier features; in Sect. 5, we illustrate the results of our proposed method for density estimation and anomaly detection; and in Sect. 6, we establish our conclusions and future outlook.

2. Related Work

Anomaly detection is an important problem in machine learning and solving it using quantum computers is an interesting challenge for the field of quantum machine learning. Recent approaches to quantum anomaly detection (QAD) include variational quantum algorithms, for instance, Herr et al. [7] use the variational method in conjunction with quantum generative adversarial networks, and in Ref. [20], they combine the variational quantum eigensolver with quantum autoencoders. In the non-variational side, some proposals perform QAD with quantum clustering [21, 11], and build density functions from data with multivariate Gaussian distributions [5, 10].

Besides VQE-based algorithms, most quantum machine learning methods are based on pure states. One QAD method based on mixed states was proposed by Liu et. al. [6], they proposed a quantum one-class support vector machine, which codifies the density matrix based on the Krauss operators. Our proposed method is also based on mixed states, by estimating the expected values of density matrices.

If we consider a density matrix as an operator, its expectation value is equivalent to a quantum state overlap between a pure state and the mixed state density matrix. The most commonly used protocol for quantum state projection is the swap test [22] which was conceived to find the state overlap between pure states, in Ref. [23], they showed that this protocol can also be used for mixed states. Other protocols to measure the state overlap were proposed in Refs. [19, 24]. In addition, the VQE method [16] can estimate the expected value of a density matrix, by writing the quantum state in terms of the Pauli matrices. Our method departs from the aforementioned techniques, by estimating the expected value of a density matrix from its spectral decomposition.

González et. al. [18] proposed the use of random Fourier features (RFF) [17] as quantum feature maps. RFF approximates shift-invariant kernels by calculating an explicit mapping to a low-dimensional feature space. Enhancing the capability of random Fourier features to approximate shift-invariant kernels is an active area of research. Two of the main approaches to the problem include refining the original RFF Monte Carlo sampling and using optimization techniques to find the optimal Fourier parameters. Regarding the RFF sampling, Kammonen et. al. [25] proposed a method to find non-Gaussian Fourier features based on Metropolis-hastings, also Ref. [26] proposed reducing the number of features by the kernel polarization method [27]. Other methods include a surrogate leverage sampling based on kernel alignment [28], compressing the dimension of the RFF by using only a subset of features which reduces the Frobenius norm error [29], and using a multilayer generative network to select the optimal sampled Fourier weights [30].

On the optimization side, there have been multiple proposals that use neural
networks to make the parameters of the random Fourier features trainable. For instance, Li et. al. [31] proposed learnable Fourier features in conjunction with dense networks for positional encoding, and Ref. [32] propose the RFFNET, a deep learning architecture that trains layers of RFF for kernel learning. Other methods for kernel learning include using LSTM to learn the parameters of the RFF [33], learning the RFF weights for multiple kernel learning [34] and employing a generative adversarial network to translate the RFF sampling from a base Gaussian distribution to more complex distributions [35]. In addition, Ref. [36] proposed a method to find the peaks in the Fourier parameters which maximize kernel alignment. Our adaptive Fourier features technique can be framed in this last category of methods, but using a siamese network to find the optimal parameters which reduce the mean squared distance between the expected kernel and its Fourier feature approximation. These optimized features are then used to construct pure and mixed quantum states for quantum anomaly detection.

3. Preliminaries

In this section, we present the DMKDE algorithm proposed by Gonzalez et al. [12], which is a non-parametric density estimation method based on density matrices and random Fourier features [17], and a special case of the quantum measurement classification algorithm (QMC) [18]. In particular, we describe two approaches to the method: pure and mixed states. Additionally, we explain the notation of the quantum circuits used through the article and present a previous work [19] to compute the expected value of a pure state density matrix in a quantum computer.

3.1. Density Matrix Kernel Density Estimation and Random Fourier Features

The machine learning algorithm density matrix kernel density estimation (DMKDE) [12] constructs a density matrix from training data and estimates the probability density of a test sample by computing the expected value of the test state with the training density matrix.

The method starts by applying a quantum feature map, based on random Fourier features [17] [18], to each sample in the train and test data set \(x_i \rightarrow |\psi_i\rangle\), where \(x_i \in \mathbb{R}^D\) and \(|\psi_i\rangle \in \mathbb{R}^d\) with \(\langle \psi_i | \psi_i \rangle = 1\). The RFF technique creates a quantum embedding whose inner product approximates a shift-invariant positive definite kernel; in this article we use the Gaussian kernel \(k(x - y) = e^{\gamma |x - y|^2}\). The parameters of the RFF are the inverse of the variance of the Gaussian kernel, denoted by \(\gamma\) (gamma), and the dimension of the quantum features \(d\).

Once the random Fourier feature map is established, the DMKDE method explores two approaches to train the density matrix; pure and mixed states. For the training states \(|\psi_i\rangle\) for \(i \in \{1, \cdots, N\}\), the pure state training density matrix is computed by,

\[
|\phi_{\text{train},1}\rangle = \frac{\sum_i |\psi_i\rangle}{\sum_i |\psi_i\rangle |}, \quad \text{and} \quad \rho_{\text{train},1} = |\phi_{\text{train},1}\rangle \langle \phi_{\text{train},1}|, \tag{1}
\]
and, the mixed state by,

\[ \rho_{\text{train},2} = \frac{1}{N} \sum_{i=1}^{N} |\psi_i\rangle \langle \psi_i|, \]

the indices 1 and 2 refer to pure and mixed approaches respectively. The probability density estimators of a testing sample \( x \rightarrow |\psi\rangle \) are computed by,

\[ \hat{p}_1(|\psi\rangle) = C_{\gamma,1} \sqrt{\langle \psi | \rho_{\text{train},1} | \psi \rangle} = C_{\gamma,1} \sqrt{|\langle \phi_{\text{train},1} | \psi \rangle|^2}, \]

\[ \hat{p}_2(|\psi\rangle) = C_{\gamma,2} \langle \psi | \rho_{\text{train},2} | \psi \rangle, \]

where \( C_{\gamma,1} \) and \( C_{\gamma,2} \) are normalization constants that depend on the parameter \( \gamma \).

The DMKDE algorithm in conjunction with RFF is an efficient approximation of the Parzen–Rosenblatt window [37, 38], a non-parametric method for density estimation. In this document, we consider the DMKDE with RFF [12] as a baseline for the proposed classical-quantum implementation of the DMKDE with adaptive Fourier features (discussed in Sect. 4.1).

3.2. Notation and DMKDE quantum circuit for pure states

We now introduce the notation of the quantum circuits used in the article, which is the same notation used in Ref. [39]. Any state of the canonical basis of an \( n \)-qubit state can be written as \( |b_0 b_1 \cdots b_{n-1}\rangle \) with \( b_i \in \{0, 1\} \), hence, we may write any state in the canonical basis as a string in its binary form. This notation can be simplified by writing such state as \( |\sum_{i=0}^{n-1} b_i 2^i\rangle_n \), namely, the bit-string is written in decimal form and the subindex indicates the number of qubits of the state. For example, the 4-qubit state \( |1010\rangle \) can be written as \( |5\rangle_4 \). We make use of the same subindex to illustrate the number of qubits upon which a unitary gate or a quantum state initialization acts.

Once established the notation of the circuits, we present a previously proposed quantum circuit by Liu et al. [19] to compute the expected value of a pure state density matrix, which is equivalent to calculating the inner product of two pure quantum states,
as indicated by Eq. 3. The circuit starts by initializing a \( n \)-qubit state with the state \( |\psi_n\rangle \in \mathbb{C}^d \), with \( 2^{n-1} < d \leq 2^n \), by means of amplitude encoding [40], and then it applies a unitary matrix \( U_n \), which satisfies that \( U_n |0\rangle_n = |\phi_{\text{train},1}\rangle_n \), see Eq. 1 and Figure 1. By measuring all the \( n \) qubits, the probability of the state \( |0\rangle_n \) is the expected value of a pure state density matrix, i.e. \( P(|0\rangle_n) = |\langle \phi_{\text{train},1}|\psi \rangle|^2 \). Other quantum techniques to measure the fidelity of quantum states can be seen in Refs. [22, 24]. In this article, we present a new quantum protocol to estimate the expected value of a mixed state density matrix based on its eigendecomposition in a qubit-based quantum computer.

4. Quantum anomaly detection method

We propose a hybrid classical-quantum model for anomaly detection based on the DMKDE algorithm [12] and the novel adaptive Fourier features technique. Fig. 2 shows the main steps of the method: (i) quantum feature map, (ii) training phase, (iii) density estimation of new samples, and (iv) threshold selection and classification. The steps (i), (ii), and (iv) are calculated in a classical computer, while the step (iii) is computed in a real quantum computer and a quantum simulator. These steps are explained in more detail below.

(i) Quantum feature map: Given a dataset to classify, split it into three partitions: train, validation, and test, in such a way that each of them is composed of both “normal” and “outlier” data. Then apply a quantum feature map \( x_i \rightarrow |\psi_i\rangle \) to all of these partitions; the selected embedding from data to quantum states can be based on the proposed adaptive Fourier features, see Sect 4.1, or on random Fourier features [17, 18].

(ii) Training phase: Use the training data to compute either the training quantum state \( |\phi_{\text{train},1}\rangle \) for the pure state or the training density matrix \( \rho_{\text{train},2} \) for the mixed state, see Equations 1 and 2. When using the mixed state approach, also calculate the spectral decomposition of the training density matrix \( \rho_{\text{train},2} = V\Lambda V^\dagger \). The
training pure and mixed quantum states encode probability distributions of the training dataset.

(iii) Density estimation of new samples: Estimate the probability density values of the validation and test partitions by computing the probability estimation of the samples with the training density matrix. The estimator of the pure state (see Eq. 3) is obtained using the quantum circuit shown in Fig. 1 [19]. To calculate the probability estimator of a mixed state (see Equation 4), use the proposed quantum circuit shown in Fig. 3. See Sect. 4.2 for the mathematical details of the mixed state quantum circuit.

(iv) Threshold selection: Once given the probability density estimations, use the validation dataset to select a threshold to separate the samples: if a sample has a density lower than the threshold, then it is considered an “outlier”. Since the validation samples include both normal data and outliers, the threshold must be somewhere between the maximum and minimum density values; the specific threshold value to choose is found using percentiles, but other metrics can be used. Finally, use this threshold to classify the samples in the test partition.

In the next sections, we present the theoretical details of the new adaptive Fourier features method, and the proposed DMKDE quantum protocol to compute the expected value of a mixed state density matrix.

4.1. Adaptive Fourier Features Quantum Feature map

To build the quantum features of the classical-quantum anomaly detection strategy, we propose the adaptive Fourier features (AFF) technique: a new trainable feature embedding based on random Fourier features [17], which maps classical data samples \( x \in \mathbb{R}^D \) to quantum state-like representations \( |\psi\rangle \in \mathbb{R}^d \), where the inner product on the quantum feature space approximates a positive definite shift-invariant kernel on the original space. In this work, we use the Gaussian kernel given by \( k(x, y) = e^{\gamma|x-y|^2} \).

In general terms, the method utilizes the training data set \( \mathcal{X} \) in the original space to train the parameters of the adaptive Fourier features, hence obtaining a quantum state-like representation of the data. The AFF method involves the following steps: (i) build a synthetic data set, composed of two random orderings of the original data set, where the labels are formed by computing the Gaussian kernel between these two subsets, (ii) construct a siamese neural network and initialize its parameters using conventional random Fourier features, (iii) train the siamese network with the synthetic data set to adjust the parameters of the adaptive Fourier features, (iv) make predictions on the original data set to obtain the AFF representations.

As mentioned before the strategy for AFF starts by creating two random shuffles \( \mathcal{X}_1 \) and \( \mathcal{X}_2 \) of the original data set \( \mathcal{X} \), with \( N \) training samples, and then computing the Gaussian kernel between these two subsets to form the synthetic set of labels \( y_i \in \mathcal{Y} \),
for \( i \in \{1, \cdots, N\} \), such that,

\[
y_i = \exp(\gamma_s |x_{i,1} - x_{i,2}|^2),
\]

with \( \gamma_s \) the shape parameter of the kernel, and \( x_{i,1} \) and \( x_{i,2} \) the \( i \)th sample vectors of \( X_1 \) and \( X_2 \) respectively.

Next, we build a siamese neural network with a trainable weight matrix \( W \in \mathbb{R}^{d \times D} \), whose weights are initialized by sampling a normal distribution \( \mathcal{N}(0,1) \), and then multiplying the weight matrix by a factor of \( \sqrt{2\gamma} \), this factor establish the Gaussian spread of the Fourier features, the inverse of the variance of the Fourier features \( \gamma \) might differ from the shape parameter \( \gamma_s \), also a trainable bias vector \( b \in \mathbb{R}^d \) is initialized by sampling from a uniform distribution \( \mathcal{U}(0, 2\pi) \). The forward pass to obtain the adaptive Fourier features resembles conventional RFF:

\[
z(x) = \sqrt{2/d} \cos\left[ (\sqrt{2\gamma}W)x + b \right], \quad |\psi\rangle = \frac{z(x)}{|z(x)|}. \tag{6}
\]

We then use the synthetic data set composed of \( X_1, X_2 \) and \( Y \) to train the siamese network. We use the Mean Squared Error (MSE) loss function to find the optimal parameters \( W \) and \( b \) of the network,

\[
\mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} (y_i - |\langle \psi_{i,1} | \psi_{i,2} \rangle|^2)^2. \tag{7}
\]

Finally, the quantum state-like representation with adaptive Fourier features is obtained by making predictions on the original data set \( X \), see Eq. 6.

### 4.2. DMKDE quantum circuit for mixed states

To implement the prediction phase of the DMKDE, see Eq. 4, we also propose a novel quantum protocol to estimate the expected value of a mixed state density matrix in a qubit-based quantum computer. This circuit extends to qubits a previous implementation of the mixed state DMKDE in a high-dimensional quantum computer [41], and to mixed states, a previous implementation of the DMKDE with pure states in a qubit-based quantum computer [42, 19].

We want to compute the expected value of a density matrix \( \rho \in \mathbb{C}^{d \times d} \) with a quantum state \( |\psi\rangle \in \mathbb{C}^d \) in a quantum computer. This calculation requires \( 2 \times n \) qubits, with \( 2^{n-1} < d \leq 2^n \). The first \( n \) qubits encode the state \( |\psi\rangle \) and the unitary matrix \( V^\dagger \) whose rows are the complex conjugate eigenvectors of \( \rho \), and the remaining \( n \) qubits encode the eigenvalues of the density matrix.

To begin with, as noted in [41], we have that,

\[
\langle \psi | \rho | \psi \rangle = \langle \psi | V \left( \sum_{i=0}^{d-1} \lambda_i |i\rangle \langle i| \right) V^\dagger | \psi \rangle = \sum_{i=0}^{d-1} \lambda_i |\langle i | V^\dagger | \psi \rangle|^2, \tag{8}
\]
where, $V \in \mathbb{C}^{d \times d}$ is the unitary matrix of eigenvectors and $\Lambda = \sum_{i=0}^{d-1} \lambda_i |i\rangle \langle i|$ is the diagonal matrix of eigenvalues.

The proposed DMKDE quantum circuit starts by initializing the first $n$ qubits with the state $|\psi\rangle_n$, see the notation in Sect. 3.2, and the remaining $n$ qubits with the state $|\lambda\rangle_n = \sum_{i=0}^{d-1} \sqrt{\lambda_i} |i\rangle_n$, state that encodes the eigenvalues of $\rho$, see Fig. 3. This operation can be performed thanks to amplitude encoding [40]. We have that,

$$|\psi\rangle_n \otimes |\lambda\rangle_n = |\psi\rangle_n \otimes \sum_{i=0}^{d-1} \sqrt{\lambda_i} |i\rangle_n.$$  (9)

Next, we construct a unitary matrix $U_n^\dagger$, see Eq. 10, whose first quadrant is composed of the unitary matrix $V^\dagger$ and its fourth quadrant with the identity matrix $I_{2^n-d}$,

$$U_n^\dagger = \begin{pmatrix} V^\dagger \\ I_{2^n-d} \end{pmatrix},$$  (10)

this unitary matrix $U_n^\dagger$ is applied to the first $n$ qubits in the form of an isometry [39]. We would have,

$$U_n^\dagger |\psi\rangle_n \otimes \sum_{i=0}^{d-1} \sqrt{\lambda_i} |i\rangle_n.$$  (11)

We can write the state of the first $n$ qubits as, $U_n^\dagger |\psi\rangle_n = \sum_{i=0}^{d-1} a_i |i\rangle_n$. Where,

$$|a_i|^2 = |\langle i_n U_n^\dagger |\psi\rangle_n|^2 = |\langle i | V^\dagger |\psi\rangle|^2,$$  (12)
DMKDE quantum circuit is, i.e., target the $i$th qubit and consider the circuit, as shown in Fig. 3. The gates can be observed by writing, \[ \sum_{d=0}^{d-1} \sum_{j=0}^{d-1} a_i \langle i | \lambda_j | j \rangle_n \]

\[ \sum_{i=0}^{d-1} a_i \sqrt{\lambda_i} | i \rangle_n \otimes | j \rangle_n + \sum_{\{(i,j):i\neq j\}} a_i \sqrt{\lambda_j} | i \rangle_n \otimes | j \rangle_n . \]

Therefore, the circuit leads, \[ U^\dagger_n | \psi \rangle_n \otimes | \lambda \rangle_n = \sum_{i=0}^{d-1} a_i | i \rangle_n \otimes \sum_{j=0}^{d-1} \sqrt{\lambda_j} | j \rangle_n \]

where, \[ | b_0 b_1 \cdots b_{n-1} \rangle \] and \[ | b_0' b_1' \cdots b_{n-1}' \rangle \] are the binary representations of \[ | i \rangle_n \] and \[ | j \rangle_n \] respectively. The $n$ CNOT gates have the same complexity as a single CNOT, as they can be parallelized in a quantum computer \[ [24] \].

We then apply a cascade of $n$ CNOT gates, between the first and the second halves of the circuit, as shown in Fig. 3. The $i^{th}$ CNOT operates with control the $(i+n)^{th}$ qubit and target the $i$th qubit, with $i \in \{0, \cdots, n-1\}$. The effect of this series of CNOT gates can be observed by writing,

\[ | i \rangle_n \otimes | j \rangle_n = | \sum_{k=0}^{n-1} b_k 2^k \rangle_n \otimes | \sum_{l=0}^{n-1} b'_l 2^l \rangle_n , \] (13)

where, \[ | b_0 b_1 \cdots b_{n-1} \rangle \] and \[ | b_0' b_1' \cdots b_{n-1}' \rangle \] are the binary representations of \[ | i \rangle_n \] and \[ | j \rangle_n \] respectively. The $n$ CNOT gates have the same complexity as a single CNOT, as they can be parallelized in a quantum computer \[ [24] \].

We represent this series of $n$ CNOT gates with the $2n$-qubit unitary operation $U^\text{Cnot}_{2n}$. The outcome of this transformation is a qubit-wise summation modulo 2 (denoted by $\oplus$) on the first half of the circuit,

\[ U^\text{Cnot}_{2n} (| i \rangle_n \otimes | j \rangle_n ) = | \sum_{k=0}^{n-1} (b_k \oplus b'_k) 2^k \rangle_n \otimes | \sum_{l=0}^{n-1} b'_l 2^l \rangle_n . \] (14)

If $i = j$, we would have that,

\[ U^\text{Cnot}_{2n} (| i \rangle_n \otimes | i \rangle_n ) = | 0 \rangle_n \otimes | \sum_{l=0}^{n-1} b'_l 2^l \rangle_n \] (15)

In contrast, if $i \neq j$, the state \[ | \sum_{k}(b_k \oplus b'_k) 2^k \rangle_n \] would be distinct to the $| 0 \rangle_n$ state. Therefore, after applying the series of $n$ CNOT gates, the resulting state of the DMKDE quantum circuit is,

\[ \sum_{i=0}^{d-1} a_i \sqrt{\lambda_i} | 0 \rangle_n \otimes | i \rangle_n + \sum_{\{(i,j):i\neq j\}} a_i \sqrt{\lambda_j} | \sum_{k}(b_k \oplus b'_k) 2^k \rangle_n \otimes | j \rangle_n . \] (16)

By measuring the first $n$ qubits the probability of state $| 0 \rangle_n$ would be,

\[ P(| 0 \rangle_n ) = \sum_{i=0}^{d-1} | a_i |^2 \lambda_i = \sum_{i=0}^{d-1} \lambda_i \langle i | V^\dagger | \psi \rangle^2 = \langle \psi | \rho | \psi \rangle , \] (17)

see Eqs. 8 and 12.
5. Results

5.1. Quantum density estimation

As mentioned in Sect. 3, the DMKDE algorithm along with the RFF embedding [12] encodes in a density matrix a probability distribution of the training data and estimates the probability density of new testing samples. Therefore, the algorithm can be used to approximate probability density functions.

To test the DMKDE algorithm with the new adaptive Fourier features and the proposed DMKDE quantum circuit for mixed states, we constructed a one-dimensional probability density function corresponding to a mixture of two Gaussians. The training data set was composed of 1000 points sampled from the pdf, and the testing data set was formed by 250 equidistant points. Two quantum feature maps based on AFF and RFF were applied to both train and test data sets, we chose features of 16 components with $\gamma = 1$, for both adaptive and random features. We found that a value of $\gamma$ with the same order of magnitude as the inverse of the variance of the training data was appropriate for density estimation. For each quantum feature embedding, we constructed pure and mixed training density matrices of dimensions 16x16, see Eqs. 1 and 2. For the prediction step, we computed the probability density estimator for both pure and mixed states, see Eqs. 3 and 4; the pure state estimator was computed with the circuit proposed by Liu et al. [19], see Fig. 1 and the mixed state estimator with our proposed DMKDE quantum circuit, see Fig. 3. In total, we report 4 experiments, one for each configuration, with the Qiskit QASM simulator of the IBM-Qiskit platform.

In Fig. 4, we show the probability density estimation for pure and mixed states with both random and adaptive Fourier features. In comparison with the pure state, the mixed state creates a better approximation of the pdf for both quantum embeddings, especially, in high-density regions. We found also better and less noisy results with AFF compared with RFF. It should be highlighted that for RFF, we chose the best performing features for density estimation, out of 20 random Fourier configurations; in contrast, for AFF, we obtained satisfactory density estimation results through multiple training iterations. To improve the estimation of the pdf and reduce the noise in low-density regions, it is required a higher number of Fourier features and henceforth bigger density matrices.

5.2. Quantum anomaly detection

Once the ability of the proposed circuits to approximate probability density functions was established, a similar experiment was performed with a previously labeled anomaly detection dataset. For this purpose, we used a modified version, from Ref. [43], of the Cardiotocography dataset from the UCI Machine Learning Repository, related to fetal heart rate. It consists of 1831 samples, where each sample contains 21 attributes, with two classes: the normal class for the inliers, and the pathologic class for the outliers. This dataset was divided into three partitions: train (60%), validation (20%), and test
(a) Density estimation with random Fourier features.

(b) Density estimation with adaptive Fourier features.

Figure 4: Density estimation with both pure and mixed states and random and adaptive Fourier features. The DMKDE experiments for density estimation were performed with the Qiskit QASM simulator applied to a 4-qubit DMKDE circuit for pure states, and an 8-qubit DMKDE circuit for mixed states. Both approaches have 16 Fourier features.

(20%), all of which contained both normal samples and outliers in the same proportion (approximately, 9.6% of all samples were labeled as outliers).

As a first step, RFF and AFF were applied to the samples of all partitions as quantum feature mappings. To evaluate the effect of the number of Fourier features on the classification, we worked with 4 and 8 dimensions (which, once normalized, corresponded to quantum states of 2 and 3 qubits, respectively). With the quantum states of the training partition samples, we calculated the density matrices for pure states $\rho_{\text{train},1}$ (see Eq. 1) and for mixed states $\rho_{\text{train},2}$ (see Eq. 2), and then we used them to build the respective quantum circuits. As usual in anomaly detection algorithms, labels were not used during the training phase.

These circuits were then run on the Qiskit QASM simulator, performing an iteration of the circuit for each sample in validation and test partitions to obtain the density estimates for all samples. After obtaining the density values, the classification of each one as “normal” or “outlier” required comparing its density value with a threshold value $t$. The search for the threshold was performed over the validation partition, by setting a percentile value $t$ such that 9.6% of the samples lay below it, thus being considered anomalies. We then used the obtained boundary $t$ to classify the testing samples.

In Ref. [12], the authors highlight the influence of the $\gamma$ parameter used in RFF mapping for the performance of a classifier. For this reason, we searched for the optimal values of $\gamma_s$ and $\gamma$ in a logarithmic scale (considering only powers of two ranging from $2^{-10}$ to $2^9$); hence, in all scenarios, we set $\gamma_s = 2^{-6}$ and $\gamma = 2^{-7}$ as the best values for AFF, and $\gamma = 2^{-7}$ for RFF. For each RFF and AFF quantum embedding, we used the
same features for the pure and mixed state approaches. We simulated each circuit ten times, randomizing the RFF embedding and the initial parameters of the AFF mapping.

Then, we report the average accuracy, AUC (area under the characteristic curve), and F1 Score of the “anomalous” class, for ten experiments for each classifier, both for 4 and 8 dimensions with RFF and AFF, with both pure and mixed state approaches. The metrics were calculated using functions provided in the scikit-learn Python library. The results are presented in Table 1. We found no significant difference in performance between pure and mixed state approaches. Differences are more noticeable when considering the dimensionality of the mapping and the type of encoding: RFF of size 8 obtained better results compared to RFF of size 4, also AFF with 4 components had a slightly better performance compared to AFF with 8 components. This indicates that an increase in the RFF components improves the performance of the algorithm, in contrast, AFF can achieve satisfactory results with a low number of features. Regarding the standard deviations, we observe more consistent results across different experiments with AFF. Therefore, it shows that RFF is more sensible to randomness than AFF in a low-dimensional setting. The random initialization of the AFF was attenuated thanks to the neural network learning.

| Size  | Method | F1 Score | Accuracy | AUC       |
|-------|--------|----------|----------|-----------|
| RFF: 4| Pure   | 0.3751 ± 0.1415 | 0.8823 ± 0.0208 | 0.7661 ± 0.1133 |
|       | Mixed  | 0.3802 ± 0.1483 | 0.8839 ± 0.0215 | 0.7696 ± 0.1144 |
| AFF: 4| Pure   | 0.6843 ± 0.0311 | 0.9409 ± 0.0044 | 0.9634 ± 0.0049 |
|       | Mixed  | 0.6967 ± 0.0212 | 0.9414 ± 0.0041 | 0.9624 ± 0.0036 |
| RFF: 8| Pure   | 0.4814 ± 0.1003 | 0.9033 ± 0.0158 | 0.8702 ± 0.0722 |
|       | Mixed  | 0.4772 ± 0.1007 | 0.9035 ± 0.0159 | 0.8731 ± 0.0703 |
| AFF: 8| Pure   | 0.6607 ± 0.0269 | 0.9343 ± 0.0048 | 0.9593 ± 0.0028 |
|       | Mixed  | 0.6487 ± 0.0384 | 0.9316 ± 0.0077 | 0.9592 ± 0.0030 |

Table 1: Obtained metrics for quantum anomaly detection experiments using RFF and AFF with QASM Simulator.

We also performed some of these experiments on real noisy quantum hardware, accessible through the IBM-Quantum platform; we aimed to determine that our algorithm is a feasible approach for near-term quantum computers [44], by studying its sensitivity to quantum noise. Given the satisfactory performance and the available quantum hardware, we restricted the experiments to RFF and AFF with four components, these quantum circuits required two qubits for the pure state scenario and four qubits for the mixed state scenario.

As before, we report the accuracy, AUC, and F1 Score of the anomalous class for each case; since our experiments required a different circuit for each sample in validation and test partitions, we performed these experiments once, thus obtaining a unique value for each metric. Results are presented in Table 2. The results follow a similar
pattern as the quantum simulator: AFF leads to higher performance in comparison to RFF. However, when comparing pure and mixed state approaches, there is a noticeable advantage of the pure state; this can be explained in terms of the complexity of the quantum circuits, for instance, the pure state approach requires half of the number of qubits of the mixed state approach, hence, it might have a lower sensitivity to noise.

| Size | Method | F1 Score | Accuracy | AUC  |
|------|--------|----------|----------|------|
| RFF: 4 | Pure  | 0.4286   | 0.8910   | 0.7945 |
|       | Mixed | 0.3768   | 0.8828   | 0.7856 |
| AFF: 4 | Pure  | 0.7246   | 0.9482   | 0.9681 |
|       | Mixed | 0.6111   | 0.9237   | 0.9418 |

Table 2: Obtained metrics for the quantum anomaly detection experiments using IBM quantum computers (IBMQ-Quito and IBMQ-Santiago) with RFF and AFF for both pure and mixed states.

6. Conclusions

In this article, we presented a classical-quantum anomaly detection model, based on the density matrix kernel density estimation algorithm proposed by Gonzalez et al. [12], and the new data embedding called adaptive Fourier features. Our proposed AD technique works by estimating a probability density function from training data and classifying test data as “normal” or “outlier” by setting a probability threshold in the pdf that acts as a boundary between these regions. Within our AD method, we proposed the DMKDE quantum protocol, which estimates the expected value of any eigen-decomposed density matrix in a quantum computer with a logarithmic number of resources; and the adaptive Fourier features a new trainable representation of data, based on RFF [18, 17], which allows for a low-dimensional representation of data.

We explored four approaches within our method to perform the estimations: pure and mixed states with both random and adaptive Fourier features. We then applied them for two different purposes, density estimation of a given pdf function and anomaly detection on a dataset; we evaluated the model with quantum features of 4 and 8 dimensions for anomaly detection, and with 16 dimensions for density estimation. In comparison to conventional RFF, AFF demonstrated superior performance on both density estimation and anomaly detection, being able to estimate probability density functions with a low number of components. In addition, the results indicated a small advantage of the mixed state approach for density estimation. However, the use of pure or mixed states for quantum anomaly detection is not conclusive: the mixed state approach might be preferred on noise-free devices, while the pure state approach would be favored on real quantum computers. The experimental results show that the proposed QAD method is a feasible approach for noise intermediate-scale quantum computers.
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Future work of the proposed classical-quantum AD technique includes comparing the performance of our method with other classical and quantum anomaly detection methods, and also increasing the number of Fourier features, hence augmenting the size of the quantum circuits (given the near-term limitations in quantum hardware). Besides, we aim to apply adaptive Fourier features as mapping functions to other kernel methods and to study its theoretical implications and performance. An interesting future endeavor involves integrating the proposed DMKDE quantum circuit with variational quantum algorithms to learn mixed quantum states in a quantum computer.

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