Periodic Unitary Encoding for Quantum Anomaly Detection of Temporal Series

Daniele Lizzio Bosco^{1,2}¹, Riccardo Romanello³¹, and Giuseppe Serra¹

¹Department of Mathematics, Computer Science and Physics, University of Udine, Udine, Italy ²Department of Biology, University of Naples Federico II, Naples, Italy

³Department of Environmental Sciences, Informatics and Statistics, Ca' Foscari University of Venice, Venice, Italy

Keywords: Quantum Kernel, Anomaly Detection, Quantum Machine Learning, One-Class SVM.

Abstract: Anomaly detection in temporal series is a compelling area of research with applications in fields such as finance, healthcare, and predictive maintenance. Recently, Quantum Machine Learning (QML) has emerged as a promising approach to tackle such problems, leveraging the unique properties of quantum systems. Among QML techniques, kernel-based methods have gained significant attention due to their ability to effectively handle both supervised and unsupervised tasks. In the context of anomaly detection, unsupervised approaches are particularly valuable as labeled data is often scarce. Nevertheless, temporal series data frequently exhibit known seasonality, even in unsupervised settings. We propose a novel quantum kernel designed to incorporate seasonality information into anomaly detection tasks. Our approach constructs a Hamiltonian matrix that induces a unitary operator which period corresponds to the seasonality of the task under consideration. This unitary operator is then used to encode the data into the quantum kernel, ensuring that values sampled at instants equivalent under the period are treated consistently by the kernel. We evaluate the proposed method on an anomaly detection task for temporal series, demonstrating that embedding seasonality directly into the quantum kernel generation improves the overall performance of quantum kernel-based support vector machines.

SCIENCE AND TECHNOLOGY PUBLICATIONS

1 INTRODUCTION

In recent times, there has been a notable increase in research activity surrounding Quantum Machine Learning (QML) (Mishra et al., 2021; Peral-García et al., 2024; Wang and Liu, 2024), which has emerged as a prominent topic within the field of Machine Learning (ML). The continuous increasing in the capabilities of quantum computing, which has continued to expand in terms of computational power and scalability (Kim et al., 2023), has also contributed to the rising interest in this area.

A significant portion of ML and Deep Learning approaches relies on the computation of loss functions, which are then used to guide the optimization process with algorithms such as gradient descent (Ruder, 2017). This reliance has also extended to much of QML algorithms, such as Quantum Neural Networks (Jeswal and Chakraverty, 2018; Crooks, 2019), and, more in general, to variational quantum algorithms (Cerezo et al., 2021a).

However, the initial enthusiasm surrounding QML has been tempered by a series of studies demonstrating that computing loss functions on quantum computer is, in most cases, unfeasible, due to the phenomenon known as *barren plateaus* (Uvarov and Biamonte, 2021; Wang et al., 2021; Holmes et al., 2022; Cerezo et al., 2021b).

Recently, a paradigm shift has been proposed towards models within the $CSIM_{QE}$ class (Cerezo et al., 2024), which require quantum hardware only in the initial phase. This class of models represents a promising direction for addressing some of the scalability and hardware limitations of earlier approaches.

A significant category of models within the CSIM_{QE} framework is that of quantum kernels (Schuld and Killoran, 2019; Schnabel and Roth, 2024). Since the initial demonstration of a *quantum advantage* on a synthetic problem (Liu et al., 2021), quantum kernels have been successfully applied to

Periodic Unitary Encoding for Quantum Anomaly Detection of Temporal Series

DOI: 10.5220/0013537800004525 In Proceedings of the 1st International Conference on Quantum Software (IQSOFT 2025), pages 27-36 ISBN: 978-989-758-761-0

^a https://orcid.org/0009-0002-7372-6518

^b https://orcid.org/0000-0002-2855-1221

^c https://orcid.org/0000-0002-4269-4501

Lizzio Bosco, D., Romanello, R. and Serra, G.

Copyright © 2025 by Paper published under CC license (CC BY-NC-ND 4.0)

a range of tasks, including classification (Havlíček et al., 2019) and anomaly detection (Belis et al., 2024; Incudini et al., 2024). The model proposed in this study is a quantum kernel designed for anomaly detection in temporal series.

Other quantum models have also been developed for temporal series analysis. One of the most popular has been proposed in (Baker et al., 2024), in which the authors provide a kernel-based quantum model to address the task of classification of temporal series. In this work, we address a similar task. However, the solution we propose differs from prior work in three critical ways.

First, our model is designed to operate effectively in unsupervised settings, making it suitable for tasks where labeled data is scarce.

Second, like many quantum kernel approaches, our proposed model operates within the $CSIM_{QE}$ class. In contrast, (Baker et al., 2024) requires gradient computation, which is potentially challenging to implement efficiently on real quantum hardware.

Finally, the model allows for the integration of prior knowledge about the periodicity of the task, which is a critical factor in time-series analysis (Yousif et al., 2024). This periodic information, often available even in unsupervised tasks, enhances the model's ability to capture essential temporal patterns in the data.

The paper is structured as follows. In Section 2, we introduce the theoretical background. Section 3 focuses on the proposed method for addressing the anomaly detection task. We also outline the mathematical foundations behind our approach.

Next, in Section 4, we describe the experimental setup used to evaluate our proposal. The results of our experiments are presented and discussed in Section 5. Finally, in Section 6, we conclude the paper and suggest potential directions for future work. The source code used for the experiments is available at this link¹.

2 BACKGROUND

We provide the necessary background on kernel methods, Support Vector Machines (SVMs), quantum computing, and quantum kernels. For an in-depth discussion of kernel methods and SVMs, we refer to (Shawe-Taylor and Sun, 2014). A comprehensive introduction to quantum computing can be found in (Nielsen and Chuang, 2010). For further details on quantum kernels, we refer to (Schnabel and Roth, 2024).

2.1 Kernel Methods and Support Vector Machines

A kernel $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, defined over an input domain \mathcal{X} , is a function that can be written as

$$\kappa(x, x') = \langle \phi(x), \phi(x') \rangle.$$

where ϕ is a *mapping function* that projects points from the input space X into a higher-dimensional feature space equipped with an inner product $\langle \cdot, \cdot \rangle$.

Kernels induce a notion of similarity between data points, as they can extract meaningful patterns in high-dimensional spaces. Typical examples of kernel functions are the *linear kernel*, the *sigmoid kernel*, and the *RBF Gaussian kernel*.

A function κ is a valid kernel if and only if it satisfies Mercer's conditions (Minh et al., 2006), which state that the kernel must be symmetric and positive semi-definite. These properties ensure that the kernel corresponds to an inner product in some feature space, making it suitable for a wide range of machine learning algorithms.

Among machine learning algorithms based on kernels, Support Vector Machines (SVMs) are one of the most popular. In their simplest application, given a labeled dataset $\mathcal{D} = \{(x_i, y_i)\}$, where $x_i \in \mathbb{R}^n$ are feature vectors and $y_i \in \{-1, 1\}$ are class labels, SVMs aim to find a hyperplane that maximizes the margin between the two classes in the feature space. The hyperplane is defined as the set of points satisfying $w^T x + b = 0$, where *w* is the weight vector and *b* is the bias term.

One-Class SVMs, first introduced in (Amer et al., 2013), have been developed as a modification of SVMs to address novelty detection tasks. In contrast to standard SVMs, they can be used both for unsupervised settings with low availability of labeled data and for semi-supervised tasks to model the decision boundary around normal data. For more information on One-Class SVMs, we refer to (Alam et al., 2020).

2.2 Quantum Computing

The state of a quantum system is represented as a unit vector in the space \mathbb{C}^{2^n} , where *n* corresponds to the number of qubits of the system.

A general quantum state is expressed as:

$$\left|\psi\right\rangle = \sum_{h} c_{h} \left|v_{h}\right\rangle$$

where $\{|v_h\rangle\}$ is a basis, typically assumed to be the *canonical basis*.

¹https://github.com/Dan-LB/Periodic-Unitary-Encodin g

In a quantum system, computations are carried out by evolving the state with unitary operators, often called *unitaries*. Unitaries can be represented as matrices in $\mathbb{C}^{2^n \times 2^n}$ that satisfy the property

$$UU^{\dagger} = U^{\dagger}U = I, \qquad (1)$$

where \dagger represents the complex conjugate and *I* corresponds to the identity matrix.

The action of a unitary operator U on a quantum state $|\psi\rangle$ is expressed as:

$$\left| \mathbf{\psi}' \right\rangle = U \left| \mathbf{\psi} \right\rangle,$$

indicating that the state $|\psi\rangle$ transitions to $|\psi'\rangle$ after applying U. When a unitary operator depends on a parameter t, we denote it as U(t).

Hermitian operators are defined as matrices in $\mathbf{C}^{2^n \times 2^n}$ that satisfy the property

$$H = H^{\dagger}.$$
 (2)

When H is hermitian, the operator defined as

$$U(t) \coloneqq \exp(-iHt),\tag{3}$$

where $t \in \mathbf{R}$ and $\exp(\cdot)$ is the matrix exponential, is a unitary matrix, and is denoted as the unitary generated (or induced) by *H*.

2.3 Quantum Kernels

Quantum kernels leverage the principles of quantum computing to define similarity measures between data points.

By encoding classical data into the Hilbert space of a quantum system, quantum kernels can capture complex patterns that may be difficult to model using classical approaches (Liu et al., 2021).

The foundation of quantum kernels lies in the concept of embedding classical data into quantum states through a quantum feature map. For a classical input $x \in X$, the quantum feature map is represented by a unitary operation U_{ϕ} such that:

$$\left|\phi(x)\right\rangle = U_{\phi}(x)\left|0\right\rangle^{\otimes n},$$

where $|0\rangle^{\otimes n}$ is the initial state of the quantum system. The corresponding kernel function can be defined as the overlap between quantum states corresponding to two data points *x* and *x'*

$$\boldsymbol{\varsigma}(\boldsymbol{x},\boldsymbol{x}') = |\langle \boldsymbol{\phi}(\boldsymbol{x}) | \boldsymbol{\phi}(\boldsymbol{x}') \rangle|^2. \tag{4}$$

In practice, the quantity defined by Eq 4 can be computed by the (Buhrman et al., 2001).

Once the quantum kernel has been computed, the same properties as classical kernel methods hold, which allows to design a classical-quantum hybrid SVM, where the model weights are computed classically.

In the following, we refer to this kind of models as *quantum SVMs*, as defined in (Rebentrost et al., 2014).

3 METHOD

In this section, we describe the proposed model for collective anomaly detection in time series. The model requires a minimal amount of quantum resources to remain within the $CSIM_{QE}$ class and is particularly well-suited for addressing unsupervised tasks.

The core of the model is a quantum kernel designed to measure similarity between time series. To achieve this, we first construct a class of "small" kernels, which measure similarity between the features of a series at a given time step (or *instant*) *t*. Hereafter, we refer to these kernels as *instantaneous kernels*, denoted by k_t . These kernels are designed to incorporate both temporal dependency and, when applicable, seasonality. The instantaneous kernels are then combined to form the final kernel *K*, defined as:

$$K = \sum_{t=1}^{L} \alpha_t k_t, \tag{5}$$

where the weights α_t can be selected heuristically, or in a Multiple Kernel Learning (MKL) fashion (Gönen and Alpaydin, 2011).

In the following, we detail the components of our proposed approach:

- Construction of instantaneous kernels that incorporate temporal and seasonal dependencies;
- Generation of periodic unitaries to account for seasonality;
- Composition of the final kernel *K* and its key properties.

3.1 Time-Related Properties

Before describing the three aforementioned components, we provide an intuition for the concepts of temporal dependency and seasonality that are integral to our model.

3.1.1 Temporal Dependency

Temporal dependency refers to the ability of a kernel to distinguish between values occurring at different time steps within a time series. To illustrate, consider instantaneous kernels k_t that are independent of time, where $k_t(x_t, y_t)$ depends solely on the values at time step *t*. If we construct a uniform combination of such kernels as:

$$K = \frac{1}{L} \sum_{t=1}^{L} k_t, \tag{6}$$

then the kernel becomes invariant to any permutation σ_L of the time steps $\{1, \ldots, L\}$. Formally:

$$K(\mathbf{x}, \mathbf{y}) = K(\sigma_L(\mathbf{x}), \sigma_L(\mathbf{y})).$$
(7)

This invariance indicates that the kernel does not capture temporal relationships between features, effectively losing the temporal component of the data.

In contrast, when k_t explicitly incorporates t (e.g., through a time-dependent mapping), the temporal structure is preserved. For example, if $t \neq t'$, then $k_t(x,y) \neq k_{t'}(x,y)$. Consequently, the kernel treats values at different time steps differently, retaining the temporal dependency of the series.

However, if the weights α_t in $K = \sum_{t=1}^{L} \alpha_t k_t$ are non-uniform, the kernel loses invariance to permutations of time steps, as certain steps are weighted more heavily than others. In this case, the kernel remains non-temporal unless temporal dependency is explicitly encoded in the instantaneous kernels.

3.1.2 Seasonality and Periodicity

While temporal dependency is crucial, there are scenarios where certain time steps should be treated similarly. This arises in time series with seasonal patterns. For instance, consider a series sampled hourly over several days. A kernel with injective temporal dependency would treat values at the same hour on different days as entirely distinct. However, for tasks where seasonality is significant, such as detecting daily patterns, it is desirable for the kernel to evaluate these values similarly.

We refer to this capability as *considering the periodicity* of the data. Specifically, periodicity allows the kernel to recognize and account for recurring patterns in the series, such as daily or weekly cycles. This ensures that elements in the same part of a period are evaluated equivalently, maintaining the seasonal context of the data.

3.2 Instantaneous Kernels

The first step in our proposal involves constructing a quantum kernel that incorporates temporal dependency and can accommodate periodic (or "seasonal") information. We consider a set of time series X, where each element $\mathbf{x} \in X$ is a sequence of vectors $x_1, \ldots, x_L \in \mathbb{R}^F$, where $F \ge 1$ corresponds to the number of features measured at each instant.

We assume that each time series **x** consist of the same number of observations, *L*, and that observations from different series with the same index *t* are measured at the same time. For simplicity, the time axis is scaled such that the first sample x_1 corresponds to t = 0, while the final sample x_L corresponds to t = 1.

To construct the quantum kernel, classical data must first be encoded into quantum states. Given that each element \mathbf{x} in X has the same length L, we encode

each x_t independently using a fixed static feature map $U : \mathbb{R}^F \to \mathcal{H}_{2^n}$. This map embeds the feature space into the Hilbert space of a system of *n* qubits. To introduce temporal dependency, we augment the encoding by applying a time-dependent transformation, represented as $t \mapsto \exp(-iHt)$, where *H* is a Hamiltonian matrix, similarly to the approach proposed in (Baker et al., 2024).

The resulting mapping for the encoded data, incorporating both feature information and temporal dependency, is defined as:

$$\phi(x_t, t) := U(x_t) \exp(-iHt) |0\rangle^{\otimes n}.$$
(8)

This mapping allows the kernel to capture timedependent structures in the data while leveraging the quantum state representation of the features.

In general, the feature map and the Hamiltonian H can be chosen in various ways, depending on the specific problem and computational requirements.

3.2.1 Feature Map Selection

Feature maps can often be selected heuristically or by exploiting symmetries inherent to the problem (Ragone et al., 2023). For instance, many quantum kernel applications employ heuristically constructed kernels to model domain-specific patterns (Belis et al., 2024). In other scenarios, such as Quantum Neural Networks, feature maps (frequently referred to as *encodings*) are chosen according to desired properties such as minimal circuit depth or noise resilience. Examples of common encoding strategies include parameterized rotations, basis encoding, and amplitude encoding (Rath and Date, 2024).

3.2.2 Hamiltonian Design and Learning

The Hamiltonian H can either be explicitly designed based on problem properties or learned as a parameterized model. In the latter case, $H(\theta)$ is constructed as a parametric Hamiltonian with a parameter vector θ , as demonstrated in (Baker et al., 2024). This approach enables gradient-based optimization of H obtained via *parameter-shift-rule* (Wierichs et al., 2022). However, this method has two notable limitations:

- 1. **Trainability Issues:** The computation of gradients may be infeasible in the presence of hardware noise or limited measurement shots, potentially leading to barren plateaus or vanishing gradients.
- Supervised Setting Requirement: Learning the Hamiltonian typically relies on a supervised setting, which may not always be available in realworld applications. For instance, anomaly detec-

tion tasks often lack labeled data, making this approach less applicable.

Seasonality plays a crucial role in analyzing time series, even in unsupervised approaches. It refers to recurring patterns within the data, such as daily cycles influenced by night and day, weekly fluctuations associated with operational schedules, or longer-term trends driven by periodic events (Yousif et al., 2024). These recurring patterns are essential for effectively modeling temporal data and identifying anomalies within their broader temporal context (Darban et al., 2024).

In the following, we outline our proposed method for incorporating seasonality into the instantaneous kernel. By embedding seasonal information, the kernel is better equipped to capture periodic structures and evaluate similarities in time series data that exhibit recurring behaviors.

3.3 Periodic Unitary Construction

To incorporate seasonality into the model, we construct Hamiltonians that induce periodic unitaries through the mapping $U(t) = \exp(-iHt)$. Consider a time series of length *L* with a pattern repeated every *S* time steps. We define *P* as the number of repetition patterns within the time series, given by P = L/S (i.e. the period of the time series).

For a given diagonal Hamiltonian matrix H, the unitary operator U(t) is expressed as:

$$U(t) = \operatorname{diag}\left(e^{-it\lambda_1}, \dots, e^{-it\lambda_N}\right),\tag{9}$$

where $(\lambda_1, \ldots, \lambda_N)$ are the eigenvalues of H. For $t \in \mathbb{R}$, each component $e^{-it\lambda}$ can be rewritten as $\cos(t\lambda) + i\sin(t\lambda)$, which has a period of $1/(2\pi\lambda)$. Thus, U(t) is periodic if and only if there exists a real number $\overline{\lambda}$ such that all eigenvalues $\lambda_1, \ldots, \lambda_N$ multiplied by $\overline{\lambda}$ are rational or, equivalently, integers. When the eigenvalues are coprime integers (not necessarily pairwise co-prime), the period of U(t) is exactly 2π .

Conveniently, the same property holds even when the generating hamiltonian *H* is not diagonal. In particular, this can be proved by observing the characterization of period matrices as matrices with eigenvalues satisfying $\lambda^k = \lambda$ for a certain *k* (Benitez and Thome, 2006), and the fact that if λ is an eigenvalue of a matrix *A*, then e^{λ} is eigenvalue of $\exp(A)$.

To construct a generic Hamiltonian *H* that induces periodic unitaries, we represent *H* as MDM^{-1} , where *M* is a unitary matrix and *D* is the diagonal matrix of eigenvalues. The eigenvalues $(\lambda_1, \ldots, \lambda_N)$ are selected as coprime integers. The periodic unitary is then given by:

$$U(t) \coloneqq \exp(-2\pi i HPt). \tag{10}$$

This construction ensures that the periodicity of U(t) aligns with the seasonality of the dataset. An example of the behavior of a periodic unitary constructed in this way is given in Figure 1.



Figure 1: Plot of the trace distance between U(t) and I, where U is generated respectively by a random hamiltonian (in orange), a hamiltonian with period 1 (in green), and a hamiltonian with period 3 (in blue), for 2 (up) and 4 (down) qubits. Periodic hamiltonians are generated starting from integer eigenvalues uniformly sampled in $\{-15, ..., 15\}$.

3.3.1 Optimization and Practical Considerations

While the eigenvalues and unitary M can theoretically be optimized, this process requires efficient gradient computation and typically a supervised setting. Such optimization may be impractical for anomaly detection tasks, which are often unsupervised or semisupervised. Moreover, prior work (Baker et al., 2024) has shown that random parameter selection in similar kernels often performs comparably to optimized parameters, suggesting that optimization might not justify the additional complexity.

Randomly selected weights are commonly used in other QML approaches, such as Quanvolutional Neural Networks (Henderson et al., 2019). Additionally, as discussed in (Mattern et al., 2021), evaluations with trained and random parameters yield similar results, indicating that parameter optimization may not always provide significant benefits for QML models.

3.4 Resulting Kernel K

The final step involves selecting the coefficients of the kernel *K*. This step determines how the instantaneous kernels are combined to form the final kernel defined in Equation 5. Two approaches can be employed to select the coefficients α_i : heuristic selection and optimization using Multiple Kernel Learning (MKL).

3.4.1 Heuristic Selection

The simplest approach involves selecting the coefficients randomly or based on predefined properties. For instance, using uniform weights $\alpha_i = 1/L$ yields an average kernel, which has been shown to perform well in many contexts (Xu et al., 2013).

To incorporate periodicity, weights can be chosen such that $\alpha_i = \alpha_{i+P}$, where *P* represents the periodicity of the series. This ensures that values sampled at intervals of *P* are evaluated equivalently. Formally, for a translation of *P* steps, denoted as δ_P , the kernel satisfies:

$$K(\mathbf{x}, \mathbf{y}) = K(\delta_P(\mathbf{x}), \delta_P(\mathbf{y})).$$
(11)

This invariance under translations is particularly useful for tasks where the starting time step of the series is irrelevant. For example, in a time series with weekly periodicity, the series may start on different days of the week without affecting the analysis.

3.4.2 Optimization via Multiple Kernel Learning

The second approach involves using MKL techniques to optimize the coefficients α_i based on a target property or function. A prominent example is the EasyMKL algorithm (Aiolli and Donini, 2015), which maximizes a specified metric between data points. Specifically, it maximizes the distance between positive and negative examples with a unitary norm vector holding the coefficients of the Kernel's combination.

A key advantage of this approach is that the optimization process is entirely classical, requiring no access to quantum resources once the kernels are computed. As a result, the proposed kernel remains within the CSIM_{QE} class. However, it is important to note that MKL techniques typically rely on supervised settings, which may not be suitable for many anomaly detection tasks.

4 EXPERIMENTAL DESIGN

To evaluate our proposed model, we addressed an anomaly detection task for a time series with a given periodicity. In particular, we considered the wellknown Taxi Request dataset². This dataset contains the number of taxi requests recorded by the NYC and Limousine Commission from July 2014 to January 2015, and provides the aggregated count of passenger at each 30 minutes interval. It presents 5 "documented anomalies", corresponding to significant events during the tested period: the NYC Marathon (November 2, 2014), Thanksgiving (November 27, 2014), Christmas (December 25, 2014), New Year's Day (January 1, 2015), and a severe New England blizzard (January 27, 2015). For this reason, it provides a good ground truth for evaluating anomaly detection algorithms.

We preprocessed the dataset with the following steps:

- First, we divided the series in windows of size corresponding to 7 days;
- For each window, we label it as "anomalous" if it contains one of the five anomalous days.

4.1 Tested Models

We compare our proposed model with periodic unitary encoding with other One-Class SVMs using several classical kernels, As a first classical baseline, we compare our model with periodic unitary encoding to One-Class SVMs using several classical kernels that do not take into account temporal properties. In particular, we evaluated classical SVMs built on linear, polynomial, and Radial Basis Function kernels.

In addition, we evaluate a One-Class SVM model based on the Dynamic Time Warping (DTW) (Berndt and Clifford, 1994), a widely used distance for sequential pattern matching. The model implemented uses as the kernel matrix the similarity values obtained by inverting the distances, similarly to what is done in (Shimodaira et al., 2001; Bahlmann et al., 2002). However, is important to note that DTW is not a Positive Definite Symmetric function, and thus does not induce a proper kernel function (Lei and Sun, 2007).

As quantum models, we considered

- Quantum temporal kernel with Random Hamiltonian;
- Quantum temporal kernel with periodical unitary of period 1 (1-P hamiltonian);

²Accessible at https://www.kaggle.com/datasets/julien jta/nyc-taxi-traffic.

• Quantum temporal kernel with periodical unitary of period 7 (7-P hamiltonian), corresponding to a period equal to one day.

The Random Hamiltonian model is used as baseline to evaluate the 7-P model. The 1-P model is used to determine if variations in the performances depend on the periodicity component, or just on the differences in the generation of the kernel.

4.2 Implementation Details

Each model is trained only on non-anomalous data (corresponding to weeks with no anomalous days). After the training, the remaining data is split in a small validation set, used to select hypeparameters, and on test set, used for the final evaluation. In details, for each experiment, we first split the non-anomalous data with a 0.7, 0.3 ratio to obtain the train set. Validation and test sets are obtained with a split of 0.3, 0.7on the remaining samples, and contains both anomalous and non-anomalous samples. Hyperparameters selection (corresponding to the v value and the threshold value of the SVM) is performed by maximizing the balanced accuracy of the model on the validation set. This step does not require to recompute the kernels, and can be done efficiently without using quantum resources.

Quantum kernels are obtained with 2-qubits circuits, simulated in a noiseless environment with the Qiskit library (Javadi-Abhari et al., 2024). Periodic Hamiltonians are constructed starting from random eigenvalues uniformly sampled in $\{-15, ..., 15\}$. The data encoding, corresponding to $U(x_t)$ in the Equation 8, is the angle encoding $R_X(x\pi)$. Each experiment is repeated 30 times.

5 RESULTS

5.1 Performance Metrics

We evaluate the models using well-known metrics such as Precision, Recall, F1-Score, and Balanced Accuracy. Average results with standard deviation are given in Table 1, and plotted in Figure 2.

5.1.1 Quantum Models

Among the quantum models, the 7-period Hamiltonian demonstrates the best performance, achieving a balanced accuracy of 81.56% and an F1-Score of 73.33%. This indicates its superior ability to differentiate between normal and anomalous data. In comparison, the 1-period Hamiltonian and the random Hamiltonian models exhibit similar performances, with balanced accuracies of 75.6% and 76.1%, respectively, and slightly lower F1-Scores around 61% and 63%. The 7-period Hamiltonian obtained also the highest Precision and Recall compared to other quantum models.

5.1.2 Classical Models

Classical methods such as the linear kernel, polynomial kernel, and radial basis function (RBF) kernel treat time series as simple vectors with L elements, disregarding temporal dependencies. Among these, the RBF kernel achieves the highest precision (94.1%) and balanced accuracy (86.9%), indicating its ability to make reliable predictions with fewer false positives. The polynomial kernel follows with a balanced accuracy of 73% and an F1-Score of 60.4%, showing moderate performance. The linear kernel achieves a balanced accuracy of 71.6%, which is lower than the RBF but still competitive.

On the other hand, Dynamic Time Warping, a method specifically designed to account for temporal dynamics, achieves a balanced accuracy of 85% and an F1-Score of 80.2%. Despite obtaining the highest Recall between tested models (equal to 80%), other metrics are lower then RBF.

5.2 Discussion

The results demonstrate the importance of incorporating temporal information into model design. In particular, the 7-period Hamiltonian model consistently outperformed both the random Hamiltonian, and the 1-period models, highlighting the value of leveraging periodic structures in time series data. Is it interesting to note that, even if the generation of the hamiltonian between the Random Hamiltonian and the 1-P model is different, they perform in a similar manner, showing that the increased performance on the 7-P model depends on selecting the correct period.

The 7-P model obtains Precision and Balanced Accuracy competitive to the ones obtained by the DTW model, which is, in general, expensive to compute (Wang et al., 2010). However, RBF has a better overall performance, suggesting that this particular task do not require necessarily temporal understanding.

6 CONCLUSION

In this work, we tackled the problem of anomaly detection for temporal series with some form of season-

Model	Precision	Recall	F1 Score	Balanced Accuracy
Linear Kernel	0.855 ± 0.275	0.478 ± 0.243	0.581 ± 0.218	0.716 ± 0.110
Polynomial Kernel	0.871 ± 0.268	0.500 ± 0.244	0.604 ± 0.222	0.730 ± 0.109
Dynamic Time Warping	0.882 ± 0.156	$\textbf{0.800} \pm \textbf{0.241}$	0.802 ± 0.155	0.850 ± 0.111
Radial Basis Function	$\textbf{0.941} \pm \textbf{0.122}$	0.778 ± 0.295	$\textbf{0.814} \pm \textbf{0.222}$	$\textbf{0.869} \pm \textbf{0.153}$
Random Hamiltonian	0.764 ± 0.376	0.589 ± 0.358	0.630 ± 0.329	0.761 ± 0.170
1-P Hamiltonian	0.721 ± 0.396	0.578 ± 0.381	0.610 ± 0.356	0.756 ± 0.185
7-P Hamiltonian	$\textbf{0.860} \pm \textbf{0.272}$	$\textbf{0.678} \pm \textbf{0.297}$	$\textbf{0.733} \pm \textbf{0.263}$	$\textbf{0.816} \pm \textbf{0.148}$

Table 1: Performance metrics of classical and quantum models on anomaly detection tasks. The table reports mean values and standard deviations for Precision, Recall, F1 Score, and Balanced Accuracy.



Figure 2: Barplot of average Precision, Recall, F1-Score, and Balanced Accuracy of the considered models.

ality. We proposed a Periodic Unitary Encoding for a quantum kernel model that leverages the seasonality of temporal series to provide a better classical data representation. This unitary transformation is induced by a Hamiltonian constructed from a set of coprime eigenvalues.

Testing our method against an anomaly detection task showed that, by leveraging the correct period of the data, the quantum model obtained better results. Nevertheless, a comparison of our results with those obtained using RBF indicates that the latter achieves superior performance. Given that RBF does not utilize temporal correlation, we can suppose that the task we addressed is not strongly dependent on timerelated information. Therefore it would be worth investigating if our approach outperforms other quantum models also when addressing tasks that have a deeper connection to time-related properties.

To conclude, it is interesting to note that the proposed periodic unitary encoding has potential applications beyond anomaly detection, offering a flexible approach for tasks where the quantum representation of classical data must satisfy specific properties, such as equivariance under translations (Bronstein et al., 2017). By introducing this method, we provide a step forward in exploring how domain-specific knowledge can inform quantum data encoding, contributing to the advancement of Quantum Machine Learning in practical and meaningful ways.

REFERENCES

- Aiolli, F. and Donini, M. (2015). Easymkl: a scalable multiple kernel learning algorithm. *Neurocomputing*, 169:215–224. Learning for Visual Semantic Understanding in Big Data ESANN 2014 Industrial Data Processing and Analysis.
- Alam, S., Sonbhadra, S. K., Agarwal, S., and Nagabhushan, P. (2020). One-class support vector classifiers: A survey. *Knowledge-Based Systems*, 196:105754.
- Amer, M., Goldstein, M., and Abdennadher, S. (2013). Enhancing one-class support vector machines for unsupervised anomaly detection. pages 8–15.
- Bahlmann, C., Haasdonk, B., and Burkhardt, H. (2002). Online handwriting recognition with support vector machines - a kernel approach. In *Proceedings Eighth International Workshop on Frontiers in Handwriting Recognition*, pages 49–54.
- Baker, J., Park, G., Yu, K., Ghukasyan, A., Goktas, O., and

Kumar, S. (2024). Parallel hybrid quantum-classical machine learning for kernelized time-series classification. *Quantum Machine Intelligence*, 6.

- Belis, V., Woźniak, K., Puljak, E., Barkoutsos, P., Dissertori, G., Grossi, M., Pierini, M., Reiter, F., Tavernelli, I., and Vallecorsa, S. (2024). Quantum anomaly detection in the latent space of proton collision events at the lhc. *Communications Physics*, 7.
- Benitez, J. and Thome, N. (2006). k -group periodic matrices. SIAM Journal on Matrix Analysis and Applications, 28:9–25.
- Berndt, D. and Clifford, J. (1994). Using dynamic time warping to find patterns in time series. In *KDD workshop*, volume 10, pages 359–370.
- Bronstein, M., Bruna, J., LeCun, Y., Szlam, A., and Vandergheynst, P. (2017). Geometric deep learning: going beyond euclidean data. *IEEE Signal Processing Magazine*, 34(4):18–42.
- Buhrman, H., Cleve, R., Watrous, J., and de Wolf, R. (2001). Quantum fingerprinting. *Phys. Rev. Lett.*, 87:167902.
- Cerezo, M., Arrasmith, A., Babbush, R., Benjamin, S., Endo, S., Fujii, K., McClean, J., Mitarai, K., Yuan, X., Cincio, L., and Coles, P. (2021a). Variational quantum algorithms. *Nature Reviews Physics*, 3(9):625–644.
- Cerezo, M., Larocca, M., García-Martín, D., Diaz, N., Braccia, P., Fontana, E., Rudolph, M., Bermejo, P., Ijaz, A., Thanasilp, S., Anschuetz, E., and Holmes, Z. (2024). Does provable absence of barren plateaus imply classical simulability? or, why we need to rethink variational quantum computing.
- Cerezo, M., Sone, A., Volkoff, T., Cincio, L., and Coles, P. (2021b). Cost function dependent barren plateaus in shallow parametrized quantum circuits. *Nature Communications*, 12.
- Crooks, G. (2019). Gradients of parameterized quantum gates using the parameter-shift rule and gate decomposition.
- Darban, Z., Webb, G., Pan, S., Aggarwal, C., and Salehi, M. (2024). Deep learning for time series anomaly detection: A survey. ACM Comput. Surv., 57(1).
- Gönen, M. and Alpaydin, E. (2011). Multiple kernel learning algorithms. Journal of Machine Learning Research, 12(64):2211–2268.
- Havlíček, V., Córcoles, A., Temme, K., Harrow, A., Kandala, A., Chow, J., and Gambetta, J. (2019). Supervised learning with quantum-enhanced feature spaces. *Nature*, 567(7747):209–212.
- Henderson, M., Shakya, S., Pradhan, S., and Cook, T. (2019). Quanvolutional neural networks: Powering image recognition with quantum circuits.
- Holmes, Z., Sharma, K., Cerezo, M., and Coles, P. (2022). Connecting ansatz expressibility to gradient magnitudes and barren plateaus. *PRX Quantum*, 3:010313.
- Incudini, M., Lizzio Bosco, D., Martini, F., Grossi, M., Serra, G., and Di Pierro, A. (2024). Automatic and effective discovery of quantum kernels. *IEEE Transactions on Emerging Topics in Computational Intelligence*, PP:1–10.

- Javadi-Abhari, A., Treinish, M., Krsulich, K., Wood, C., Lishman, J., Gacon, J., Martiel, S., Nation, P., Bishop, L., Cross, A., Johnson, B., and Gambetta, J. (2024). Quantum computing with Qiskit.
- Jeswal, S. and Chakraverty, S. (2018). Recent developments and applications in quantum neural network: A review. Archives of Computational Methods in Engineering, 26:793 – 807.
- Kim, Y., Eddins, A., Anand, S., Wei, K., Berg, E., Rosenblatt, S., Nayfeh, H., Wu, Y., Zaletel, M., Temme, K., and Kandala, A. (2023). Evidence for the utility of quantum computing before fault tolerance. *Nature*, 618:500–505.
- Lei, H. and Sun, B. (2007). A study on the dynamic time warping in kernel machines. In 2007 Third International IEEE Conference on Signal-Image Technologies and Internet-Based System, pages 839–845.
- Liu, Y., Arunachalam, S., and Temme, K. (2021). A rigorous and robust quantum speed-up in supervised machine learning. *Nature Physics*, 17:1–5.
- Mattern, D., Martyniuk, D., Willems, H., Bergmann, F., and Paschke, A. (2021). Variational Quanvolutional Neural Networks with enhanced image encoding.
- Minh, H. Q., Niyogi, P., and Yao, Y. (2006). Mercer's theorem, feature maps, and smoothing. In Lugosi, G. and Simon, H. U., editors, *Learning Theory*, pages 154– 168, Berlin, Heidelberg. Springer Berlin Heidelberg.
- Mishra, N., Kapil, M., Rakesh, H., Anand, A., Mishra, N., Warke, A., Sarkar, S., Dutta, S., Gupta, S., Prasad Dash, A., Gharat, R., Chatterjee, Y., Roy, S., Raj, S., Kumar Jain, V., Bagaria, S., Chaudhary, S., Singh, V., Maji, R., Dalei, P., Behera, B. K., Mukhopadhyay, S., and Panigrahi, P. K. (2021). Quantum machine learning: A review and current status. In Sharma, N., Chakrabarti, A., Balas, V. E., and Martinovic, J., editors, *Data Management, Analytics and Innovation*, pages 101–145. Springer Singapore.
- Nielsen, M. A. and Chuang, I. L. (2010). *Quantum Computation and Quantum Information: 10th Anniversary Edition.* Cambridge University Press.
- Peral-García, D., Cruz-Benito, J., and García-Peñalvo, F. (2024). Systematic literature review: Quantum machine learning and its applications. *Computer Science Review*, 51:100619.
- Ragone, M., Braccia, P., Nguyen, Q., Schatzki, L., Coles, P., Sauvage, F., Larocca, M., and Cerezo, M. (2023). Representation theory for geometric quantum machine learning.
- Rath, M. and Date, H. (2024). Quantum data encoding: a comparative analysis of classical-to-quantum mapping techniques and their impact on machine learning accuracy. *EPJ Quantum Technology*, 11.
- Rebentrost, P., Mohseni, M., and Lloyd, S. (2014). Quantum support vector machine for big data classification. *Physical Review Letters*, 113(13).
- Ruder, S. (2017). An overview of gradient descent optimization algorithms.
- Schnabel, J. and Roth, M. (2024). Quantum kernel methods under scrutiny: A benchmarking study.

- Schuld, M. and Killoran, N. (2019). Quantum machine learning in feature hilbert spaces. *Physical Review Letters*, 122(4).
- Shawe-Taylor, J. and Sun, S. (2014). Kernel Methods and Support Vector Machines, volume 1, pages 857–881.
- Shimodaira, H., Noma, K., Nakai, M., and Sagayama, S. (2001). Dynamic time-alignment kernel in support vector machine. In Dietterich, T., Becker, S., and Ghahramani, Z., editors, Advances in Neural Information Processing Systems, volume 14. MIT Press.
- Uvarov, A. and Biamonte, J. (2021). On barren plateaus and cost function locality in variational quantum algorithms. *Journal of Physics A: Mathematical and Theoretical*, 54(24):245301.
- Wang, S., Fontana, E., Cerezo, M., Sharma, K., Sone, A., Cincio, L., and Coles, P. (2021). Noise-induced barren plateaus in variational quantum algorithms. *Nature Communications*, 12.
- Wang, X., Ding, H., Trajcevski, G., Scheuermann, P., and Keogh, E. (2010). Experimental comparison of representation methods and distance measures for time series data.
- Wang, Y. and Liu, J. (2024). A comprehensive review of quantum machine learning: from nisq to fault tolerance. *Reports on Progress in Physics*, 87(11).
- Wierichs, D., Izaac, J., Wang, C., and Lin, C. (2022). General parameter-shift rules for quantum gradients. *Quantum*, 6.
- Xu, X., Tsang, I., and Xu, D. (2013). Soft margin multiple kernel learning. 24(5):749 – 761.
- Yousif, M., Mohammed, M., Celik, M., Hamdoon, A., Jassim, R., and Abdullah, N. (2024). Periodicity analysis of most time series methods: A review. In 2024 8th International Symposium on Multidisciplinary Studies and Innovative Technologies (ISMSIT), pages 1–7.