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## Entanglement-enabled quantum kernels for enhanced feature mapping

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# Entanglement-enabled quantum kernels for enhanced feature mapping

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## ABSTRACT

Classical machine learning, extensively utilized across diverse domains, faces limitations in speed, efficiency, parallelism, and processing of complex datasets. In contrast, quantum machine learning algorithms offer significant advantages, including exponentially faster computations, enhanced data handling capabilities, inherent parallelism, and improved optimization for complex problems. In this study, we used the entanglement enhanced quantum kernel in a quantum support vector machine to train complex respiratory datasets. Compared to classical algorithms, our findings reveal that quantum support vector machine (QSVM) performs better with higher accuracy (45%) for complex respiratory datasets while maintaining comparable performance with linear datasets in contrast to their classical counterparts executed on a 2-qubit system. Through our study, we investigate the efficacy of the QSVM-Kernel algorithm in harnessing the enhanced dimensionality of the quantum Hilbert space for effectively training complex datasets.

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## I. INTRODUCTION

In the ever-evolving landscape of machine learning (ML) in various sectors, from accelerating industrial automation to revealing the fundamental aspects of nature. ML algorithms have demonstrated remarkable efficacy in processing and analyzing data across multiple dimensions.<sup>1–3</sup> However, the performance of the ML algorithms is very dependent on the input datasets, which have limitations in training random datasets and intricate optimizations. Classical algorithms, such as classical support vector machines (SVMs), are extensively utilized in solving various problems in diverse domains; their strength lies in their ability to effectively solve classification problems, particularly through the use of kernel functions. Their capability to handle non-linear relationships between features makes them suitable for a wide range of applications, including bioactivity modeling, protein classification, and image enhancement.<sup>4,5</sup> As the feature space becomes large and the kernel functions become computationally expensive to estimate, SVM faces challenges in successfully solving such problems. The choice of kernel function and regularization parameter are key

parameters to effectively training the datasets.<sup>6</sup> In addition, the computational complexity of increasing the non-linearity of kernels can lead to higher power consumption, posing practical challenges in real-world applications.<sup>7,8</sup>

In contrast, quantum machine learning algorithms, including quantum support vector machines, have been performing better in speed, efficiency, and parallel processing of complex datasets.<sup>9–12</sup> Different quantum machine algorithms have been utilized for various tasks, including drug discovery,<sup>13</sup> classification of particles produced by the large hadron collider (LHC),<sup>14</sup> detection of quantum anomalies,<sup>15</sup> calculation of electronic structure,<sup>16</sup> and monitoring of healthcare.<sup>17</sup> Quantum SVM (QSVM) offers a significant speed-up gain in overall run-time complexity.<sup>18</sup> The inherent volatility of random data, their high-dimensional feature spaces, and the absence of clear patterns result in compromised accuracy and computational efficiency. Despite concerted efforts to enhance the performance of classical SVMs in such datasets through custom kernel functions and dimensionality reduction techniques, the problem persists. The ZZ feature map of QSVM plays a crucial role in transforming random data into a higher-dimensional space, thereby enhancing the

training of QSVM in comparison to classical SVM. It is a non-linear mapping that extracts local properties of the input data, allowing for a more effective representation of the data in a higher-dimensional space.<sup>19</sup> This transformation is significant, as it changes the relative position between data points, making the dataset easier to classify in the feature space.<sup>9,10</sup> In addition, the QSVM kernel method utilizes the large dimensionality of the quantum Hilbert space to replace the classical feature space, further enhancing the discriminative power of the QSVM.<sup>20</sup>

In this work, we used QSVM to classify the random dataset of different breathings acquired by the piezoelectric sensor (see [supplementary material](#), Sec. I for a detailed description of the sensor fabrication and data acquisition). By merging the principles of quantum computing with the established SVM framework, our approach harnesses the intrinsic parallelism of the quantum realm and the ability to handle superpositions and entanglements. Using quantum-enhanced kernel functions (KQ-SVM) seeks to navigate the intricacies of random data distributions and offers a viable solution to classical SVM limitations. Through empirical analyses spanning random-infused datasets, our research validates the superior performance of KQ-SVM, with 45% higher precision than its classical counterparts. Therefore, our study makes a pivotal advancement in quantum machine learning, setting a precedent for future explorations into the integration of quantum computing into the realm of data analysis.

## II. METHODS

Kernel methods and quantum computing represent two intriguing yet distinct approaches for deciphering complex data. While both have their merits, quantum algorithms, particularly Quantum Support Vector Machines (QSVMs), demonstrate superiority, especially when dealing with random datasets. Kernel methods rely on the application of kernel functions to project data into a higher-dimensional feature space, unraveling intricate relationships within the data. This method, while effective, operates within the constraints of classical computation. However, quantum computing leverages the principles of quantum mechanics, utilizing qubits that exhibit superposition and entanglement to manipulate information in ways beyond classical capabilities.<sup>21,22</sup> Quantum SVMs, specifically designed for quantum computers, provide a unique advantage by harnessing the power of quantum parallelism to process information more efficiently than classical SVMs. One notable distinction lies in the data representation paradigms employed by these approaches. Kernel methods visualize data as points that reside within the feature space, a representation limited by the classical computational framework.<sup>23,24</sup> Quantum computers, on the contrary, utilize qubits existing in a vast Hilbert space, allowing for a more nuanced and flexible representation of the data. This fundamental difference underscores the diverse avenues through which information can be captured and manipulated, giving quantum algorithms an edge in handling complex, unpredictable datasets.

Although kernel methods have excelled in various ML tasks, boasting a well-established theoretical framework and diverse algorithms, they may face challenges when dealing with highly random datasets where the underlying patterns are elusive and non-linear. Quantum SVMs, on the other hand, offer a promising solution

to this issue. The inherent quantum parallelism allows these algorithms to explore multiple solutions simultaneously, providing a more robust approach to capture intricate patterns in seemingly chaotic data. These are computationally demanding problems where classical SVMs and kernel methods may struggle due to their inherent limitations. The quantum advantage lies in its ability to process large amounts of information in parallel, offering a potential breakthrough for solving problems that were once deemed impractical for classical computation.

The captivating journey into the heart of a QSVM is a meticulous exploration of the intricate dance of quantum states, feature transformations, and learning algorithms that orchestrate this powerful ML tool. It begins with the preparation of qubits, the fundamental building blocks of quantum computation, in a specific configuration, which lays the foundation for subsequent transformations.<sup>24</sup> The dynamical map then takes center stage, orchestrating the evolution of the quantum state under the combined influence of the input data and the chosen kernel function.<sup>21,25</sup> This map acts as a translator, encoding the complex relationship between raw data and the feature space where classification ultimately occurs.<sup>9</sup> As the qubits evolve through this map, their state transforms into the evolved density matrix, reflecting the inherent uncertainty that defines the quantum realm. The measured feature vector then collapses the quantum wavefunction, transforming the probabilistic quantum state into a concrete classical vector suitable for classification algorithms. This vector serves as the bridge between the quantum realm and the classical world, carrying the distilled essence of the data within the feature space.

The feature map plays a pivotal role in this transformation, acting as a portal that transports the data from its original input space to a higher-dimensional realm known as the feature space. Within this expanded canvas, complex relationships between data points that were previously hidden can become readily apparent, potentially leading to superior classification accuracy in challenging datasets. The training function plays a crucial role in guiding the behavior of the dynamical map and the resulting feature map, ultimately enabling the QSVM to navigate the vast feature space and distinguish between classes effectively. By meticulously optimizing this function through a training process, the QSVM gradually refines its ability to separate the data in the feature space, ultimately leading to more accurate classifications (Fig. 1).<sup>11,26</sup> Classical SVM seeks to find a hyperplane that maximizes the margin between the two classes. The decision function  $f(\mathbf{x})$  for SVM is

$$f(\mathbf{x}) = \mathbf{w} \cdot \phi(\mathbf{x}) + b, \quad (1)$$

where  $\phi: \mathbb{R}^d \rightarrow \mathbb{F}$  is the feature map that transforms the input data into a higher-dimensional feature space  $\mathbb{F}$ . The optimization problem is

$$\min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^{2n} \max(0, 1 - y_i(\mathbf{w} \cdot \phi(\mathbf{x}_i) + b)), \quad (2)$$

where  $\mathbf{w}$  is the weight vector,  $b$  is the bias term,  $\|\mathbf{w}\|^2$  is the squared norm of  $\mathbf{w}$ ,  $C$  is the regularization parameter,  $\phi(\mathbf{x}_i)$  is the feature mapping of input  $\mathbf{x}_i$ ,  $y_i$  is the label, and  $\max[0, 1 - y_i(\mathbf{w} \cdot \phi(\mathbf{x}_i) + b)]$  is the hinge loss, which measures the penalty for misclassified points and the degree of correctness for correctly classified points that lie

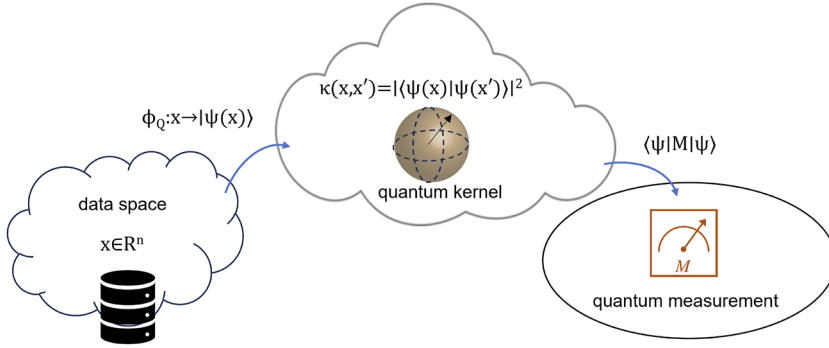


FIG. 1. Visual representation illustrating the conceptual flow of the quantum support vector machine (QSVM).

within the margin. Classical SVM uses a feature map  $\phi: \mathbb{R}^n \rightarrow H$  to map input data  $x \in \mathbb{R}^n$  to a higher-dimensional feature space  $H$  as  $\phi(x)$  with the kernel function,

$$K(x_i, x_j) = \phi(x_i) \cdot \phi(x_j). \quad (3)$$

This leads to the following decision function of SVM:

$$f(\mathbf{x}) = \sum_{i=1}^N \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}) + b, \quad (4)$$

where  $\alpha_i$  are the Lagrange multipliers,  $y_i \in \{-1, 1\}$  are the labels, and  $b$  is the bias term.

While quantum feature maps input  $x$  to a quantum state  $|\phi_q(x)\rangle$  in Hilbert space  $H_q$ ,

$$|\phi_q(\mathbf{x})\rangle = U(\mathbf{x})|0\rangle. \quad (5)$$

Entangling gates such as the CNOT gate create correlations between qubits,

$$\text{CNOT}(|0\rangle \otimes |+\rangle) = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \quad (6)$$

where  $U(x)$  is a quantum circuit parameterized by  $x$ , which leads to generating the quantum kernel as an inner product between quantum states,

$$K_q(\mathbf{x}_i, \mathbf{x}_j) = |\langle \phi_q(\mathbf{x}_i) | \phi_q(\mathbf{x}_j) \rangle|^2. \quad (7)$$

Quantum feature maps embed data into an exponentially larger space, enabling better separation of complex data distributions,

$$\mathcal{H} = \text{span}\{|0\rangle, |1\rangle, \dots, |2^n - 1\rangle\}. \quad (8)$$

Entangled states represent dependencies between features more effectively than classical methods,

$$|\phi(\mathbf{x})\rangle = \sum_{k=0}^{2^n-1} c_k(\mathbf{x})|k\rangle. \quad (9)$$

The quantum kernel naturally incorporates non-linear boundaries, making it ideal for datasets with complex structures. The quantum kernel is defined as

$$K_{\text{quantum}}(\mathbf{x}_i, \mathbf{x}_j) = \left| \sum_{k=0}^{2^n-1} c_k^*(\mathbf{x}_i) c_k(\mathbf{x}_j) \right|^2, \quad (10)$$

where  $\mathbf{x}_i$  and  $\mathbf{x}_j$  are the input feature vectors, and  $c_k(\mathbf{x})$  represents the coefficients of the quantum state corresponding to the input  $\mathbf{x}$ . Further entanglement maps to an entangled quantum state  $|\phi_{q,e}(x)\rangle$ ,

$$|\phi_{q,e}(\mathbf{x})\rangle = U_e(\mathbf{x})|\text{entangled state}\rangle, \quad (11)$$

where  $U_e(\mathbf{x})$  is an entanglement operation based on the input  $\mathbf{x}$ . This leads to the entanglement-enhanced quantum kernel. The entanglement introduced by the ZZ feature map allows the kernel to naturally incorporate non-linear boundaries, making it ideal for datasets with complex structures such as respiratory data. The entangled state representation is

$$|\phi_{\text{ent}}(\mathbf{x})\rangle = \exp(i\mathbf{x}_1\mathbf{x}_2Z \otimes Z) \left( \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \right), \quad (12)$$

where  $\mathbf{x}_1$  and  $\mathbf{x}_2$  are components of the input feature vector  $\mathbf{x}$ , and  $Z \otimes Z$  represents the tensor product of Pauli-Z operators acting on the qubits. The enhanced quantum kernel with entanglement is

$$K_{q,e}(\mathbf{x}_i, \mathbf{x}_j) = |\langle \phi_{q,e}(\mathbf{x}_i) | \phi_{q,e}(\mathbf{x}_j) \rangle|^2, \quad (13)$$

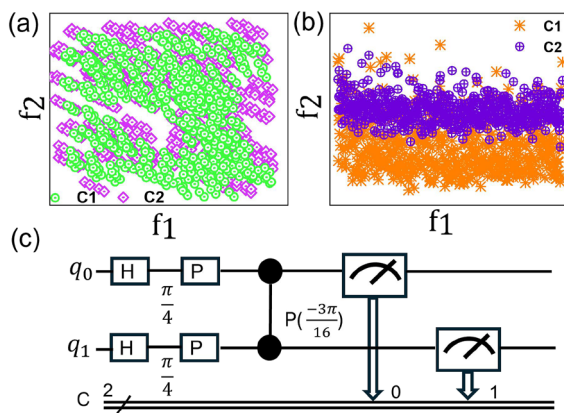
$$f(\mathbf{x}) = \sum_{i=1}^N \alpha_i y_i K_{q,e}(\mathbf{x}_i, \mathbf{x}) + b. \quad (14)$$

The higher accuracy of the quantum SVM is attributed to the entangled quantum states effectively mapping data to a much higher-dimensional space compared to classical or nonentangled quantum mappings, capturing intricate correlations between features, representing complex patterns more effectively, and the decision function now leverages the enhanced kernel.

### III. LITERATURE REVIEW

Quantum support vector machines (QSVMs) have emerged as a promising approach in quantum machine learning, leveraging quantum computational advantages for classification tasks. Rebstroff *et al.*<sup>9</sup> proposed a quantum implementation of support vector machines (SVMs) with logarithmic complexity in the size of feature vectors and training sets, highlighting their exponential speedup compared to classical counterparts. This work utilized quantum matrix inversion techniques and principal component analysis (PCA) to efficiently compute inner products in

high-dimensional feature spaces, demonstrating their applicability in big data scenarios where classical algorithms face significant computational challenges. Expanding on this foundation, Li *et al.*<sup>27</sup> experimentally realized a QSVM algorithm on a four-qubit nuclear magnetic resonance (NMR) system, showcasing its ability to classify handwritten digits with minimal features. The study emphasized the potential of QSVMs to address resource-intensive machine learning tasks by transforming training data into quantum feature spaces and optimizing hyperplanes through quantum parallelism. Their work demonstrated the feasibility of implementing quantum machine learning algorithms on current quantum devices. Building on the integration of kernel methods and quantum computing, Blank *et al.*<sup>21</sup> introduced a quantum classifier based on quantum state fidelity. This approach allows for tailored quantum kernels, enabling the design of weighted power sums of quantum state fidelities and showcasing the flexibility of quantum circuits for kernel customization. The classifier's performance was validated through experiments on IBM's quantum cloud platform, highlighting the practical benefits of leveraging quantum Hilbert spaces for machine learning tasks. Applications of QSVMs in large-scale problems were explored by Wu *et al.*<sup>14</sup> in high-energy physics analyses at the Large Hadron Collider (LHC). This study applied a quantum kernel estimator to classify collision events associated with Higgs boson production, demonstrating comparable performance to classical algorithms while utilizing the high dimensionality of quantum state spaces. The research underscored the potential for quantum machine learning to address computational bottlenecks in processing vast datasets, as encountered in physics experiments. From a theoretical perspective, Oppen and Urbanczik<sup>7</sup> analyzed the generalization performance of SVMs using statistical physics. Their work revealed the universal asymptotics of learning curves, showing that SVMs with infinite kernel complexity can achieve optimal generalization error, even in noisy data scenarios. This insight provides a theoretical basis for employing high-dimensional feature spaces, such as those enabled by quantum kernels, in machine learning tasks.



**FIG. 2.** (a) Respiratory complex dataset. (b) Breast cancer dataset. (c) 2-qubit equivalent quantum circuit. Where  $f_1$  and  $f_2$  represent two distinct features, and  $C_1$  and  $C_2$  represent the two classes.

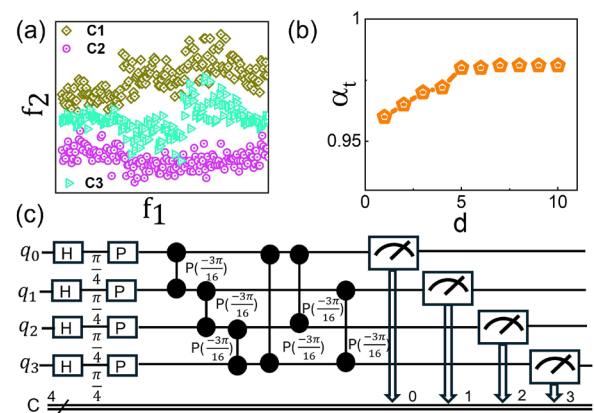
#### IV. RESULTS AND DISCUSSION

In our investigation of unfolding the power of kernel-enhanced quantum machine learning (QML) models, such as the Kernel-Enhanced Quantum Support Vector Machine (KQ-SVM), on random datasets compared to classical SVMs, the following equations have been considered: 1. Classical SVM Optimization Problem: The classical SVM solves the following optimization problem to find the optimal hyperplane. In order to test the strength of the KQ-SVM in comparison to the classical SVM, various datasets have been selected, such as the breast cancer dataset, the Iris dataset, and the randomly generated respiratory datasets. Figure 2(a) provides a visual representation of the respiratory dataset in a two-dimensional feature space, where  $f_1$  on the  $x$  axis and  $f_2$  on the  $y$  axis represent the two features.

The breast cancer dataset has been taken as a linear dataset, where the two classes are distinguishable [Fig. 2(b)]. A quantum circuit of 2 qubits comprising the two Hadamard gates to create the entanglement and two CNOT gates has been utilized to perform the quantum measurement of both datasets [Fig. 2(c)]. The QSVM enhanced with the kernel has been found to perform more accurately with 45% higher accuracy for the randomly acquired respiratory dataset. While providing almost comparable performance for the separate classes of the breast cancer dataset, for a comprehensive discussion on the machine learning and quantum machine learning algorithms, see [supplementary material](#), Sec. II.

This approach holds promise for more accurate classifications by addressing complex relationships within the data.<sup>28</sup> It depicts the learning journey of a quantum circuit, showing that as the depth of the circuit increases, its training precision increases, indicating its ability to grasp more refined patterns in the data. This suggests that the model effectively uses quantum computing to learn complex relationships and improve its diagnostic capabilities.

Understanding the specific operations and interactions within this circuit is crucial for interpreting its predictions and ensuring its transparency and reliability in medical applications.<sup>29,30</sup> The



**FIG. 3.** (a) Iris dataset for different classes. (b) Training accuracy vs depth plot. (c) Equivalent quantum circuit for classification of the Iris dataset. Where  $f_1$  and  $f_2$  are the features,  $C_1$ ,  $C_2$ , and  $C_3$  are the three different classes,  $\alpha_t$ , and  $d$  are the training accuracy and depth, respectively.



potential of combining kernel methods and quantum computing for breast cancer diagnosis is further supported by the literature. To extend our investigation to more than binary classes, we have utilized the Iris dataset, which has three classes. Figure 3(a) presents a scatter plot that depicts instances of a dataset with features related to classification. However, the lack of clear labeling obscures the specific attributes used for classification, making precise interpretations difficult to find. The quantum circuit learning journey shows an increase in the training accuracy as the depth of the circuit increases, indicating its ability to grasp more refined patterns in the data [Fig. 3(b)]. Quantum circuit, emphasizing the importance of understanding its functionality, specific gates, and connections to interpret the results and discern the potential advantages of this approach.

The 4-qubit quantum circuit consists of a 4-Hadamard gate to create the entanglement [Fig. 3(c)]. The ability of quantum circuits to uniformly address the Hilbert space has been linked to classification accuracy, emphasizing the relevance of quantum computing in machine learning tasks.<sup>27,31</sup> The experiment depicted in the image explores the impact of different kernel types and learning rates on the performance of a machine learning model [Fig. 4(a)]. The study involved the use of a linear kernel, a polynomial kernel, a radial basis function (RBF) kernel, and a sigmoid kernel, with variations in the learning rate for each kernel. Performance evaluation was performed on both training and test data. The findings revealed that the choice of kernel and learning rate significantly influences model performance. For example, the RBF kernel with a learning rate of 0.01 exhibited the highest accuracy of 50% on the training data but the lowest accuracy of 40% on the testing data, indicating potential overfitting. In contrast, the linear kernel with a learning rate of 0.5 achieved the best performance on the test data with an accuracy of 60%, suggesting a better generalization to unseen data. However, it showed a lower accuracy of 57% in the training data, indicating potential underfitting. The other kernels yielded mixed results, with the polynomial kernel achieving 53% precision on the training data and 50% on the testing data, and the sigmoid kernel achieving 48%

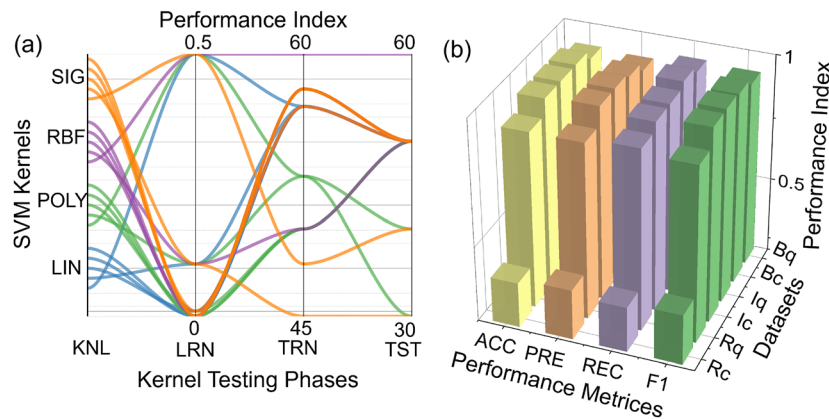
accuracy on the training data and 40% on the testing data. These results underscore the critical importance of carefully selecting the kernel and learning rate for machine learning models. The evaluation metrics for training the classical and quantum algorithms have indicated that there is not much deviation in accuracy when training the linear data, while for the random datasets [a detailed classification report has been provided in the [supplementary material](#), Sec. III], quantum machine learning performs better with higher accuracy, 45% [Fig. 4(b)]. It indicates the different evaluation metrics, such as precision, recall, and F1 score, to compare the performance among different databases, where *i* indicates the iris dataset, *r* indicates the randomly generated respiratory dataset, and *b* represents the breast cancer dataset. The optimal choice depends on the specific problem and the dataset, emphasizing the need for experimentation to identify the best combination for a given task.<sup>32–35</sup>

## V. CONCLUSION

Classical SVMs often struggle with complex and randomly distributed datasets, compromising their accuracy and efficiency. Our proposed KQ-SVM leverages quantum-enhanced kernel functions and quantum parallelism to address these challenges. Empirical analysis across diverse datasets shows KQ-SVM significantly outperforms classical SVMs, achieving over 45% higher accuracy on complex datasets while maintaining comparable performance on linear datasets. This research demonstrates the transformative potential of quantum computing in machine learning, paving the way for enhanced performance and accuracy in real-world applications.

## SUPPLEMENTARY MATERIAL

The [supplementary material](#) provides detailed information on the experimental procedures, including the fabrication and characterization of the piezoelectric sensor (Fig. S1) and the acquisition



**FIG. 4.** (a) Comparison of different support vector machine (SVM) kernel functions (SIG: sigmoid, RBF: radial basis function, POLY: polynomial, and LIN: linear) across four key phases of SVM testing: KNL (kernel selection), LRN (learning), TRN (training), and TST (testing). The Y axis represents the normalized kernel outputs generated during these phases. Each curve corresponds to a specific kernel function, showing its behavior throughout the SVM workflow. (b) Performance comparison of classical SVM and quantum SVM for three datasets: R (respiratory), I (Iris), and B (breast cancer). The performance metrics on the X axis include ACC (accuracy), PRE (precision), REC (recall), and F1 (F1 score). The bars are color-coded to distinguish classical SVM (subscript "c") and quantum SVM (subscript "q"), with the Y axis representing the normalized performance indices (PI) ranging from 0 to 1.

of respiratory data (Fig. S2). It also includes the development and implementation of quantum and classical machine learning algorithms, with performance evaluations presented through confusion matrices for various datasets (Figs. S3 and S4). A classification report comparing quantum and classical models (Table S1) and an overview of quantum gate operations are provided at the end. See the [supplementary material](#) for a detailed discussion on sensor fabrication, respiratory data acquisition, machine learning and quantum machine learning model development, and the classification reports of different algorithms.

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## AUTHOR DECLARATIONS

### Conflict of Interest

The authors have no conflicts to disclose.

### Author Contributions

**Anand Babu:** Conceptualization (lead); Data curation (lead); Formal analysis (lead); Methodology (equal); Validation (lead); Writing – original draft (lead); Writing – review & editing (lead). **Saurabh G. Ghatnekar:** Data curation (equal); Investigation (equal); Methodology (equal); Validation (equal). **Amit Saxena:** Methodology (equal); Supervision (equal); Writing – review & editing (equal). **Dipankar Mandal:** Conceptualization (equal); Investigation (equal); Project administration (equal); Supervision (equal); Writing – original draft (equal); Writing – review & editing (equal).

## DATA AVAILABILITY

The codes implemented in this study are available on the GitHub repository at the following link: <https://github.com/ABnano/QKernelML>.

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