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Fidelity and Accuracy trade-off in quantum kernels

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Abstract

Quantum computing is an influential technological outcome 21st century which blend principles of quantum physics with information theory for leap and bound enhancement of computational powers. Various quantum errors such as noise, decoherence, imperfect hardware operations etc. are impediments in harnessing the full potential of this promising technology. Recently Quantum Support Vector Machine (QSVM) is found to have immense applications in quantum error correction for fault-tolerant quantum computing in NISQ era. Due to statistical insinuation, selection of an idyllic quantum kernel is a herculean task. To overcome this issue an optimal trade-off is required between fidelity and accuracy of quantum kernel which are averse to each other. This research paper evaluated nine quantum kernels for effective trade-off between fidelity and accuracy the outcome of study is much useful in quantum kernel selection of Quantum Error Correction (QEC) applications.

Keywords: SVM, QSVM and quantum kernel, quantum computing, quantum error correction

Introduction

and classical information theory. The reliance on the principles of quantum mechanics offers some computational advantages which are absent in classical computing ^[1]. The key difference among classical and quantum computing are due to advent of quantum bits (qubits) which differs from binary bits in classical systems. In particular, while bits can only store values of either 0 or 1 but a qubit can hold information as $|0\rangle, |1\rangle$ or a state of superposition *i.e.* they are in both states at the same time. The other anomaly in qubits is a due to phenomenon of entanglement which signify the correlated qubits. The quantum circuits can be realized by preparing quantum circuits consisted of quantum gates and registers to perform specific quantum computations ^[2]. These quantum components are suffered by curse of quantum errors which are inherently different from their classical counterpart and can't be mitigated easily. This technical barrier hinders the conversion of quantum promises in to effective quantum advantages. Some quantum error correction (QEC) schemas, known as quantum error correction codes (QECC) have been designed for correction of some specific types of quantum errors which encode redundancy of qubit to protect it from noise due to environmental interaction ^[3, 4].

Recently, artificial intelligence (AI) and machine learning (ML) approaches found immense application in design and development of scalable and robust QECC. Support vector machine (SVM) is a supervised learning algorithm commonly used for classification and regression of structured data ^[5]. SVM has bizarre ability to effectively handle the complex tasks of error classification, syndrome decoding, hardware error analysis and fault-optimization etc. Quantum support vector machine (QSVM) leverage the principles of quantum mechanics to SVM to offer various advantages such as high dimensional feature mapping, scalability, enhanced pattern recognition in noise models, simulations of error channels, adaptability and reduce computational costs ^[6]. The QSVM can be implemented either by variational quantum circuit or through a gate-based approach which deploy quantum kernels to emancipate machine learning. Since the quantum operations are governed under the principles of statistical mechanics which can yield only deterministic outputs. Owing to inherent probabilistic nature. Various researches reveal that gate-based deployment of quantum kernels is easy to implement and more accurate than quantum variational circuit approaches but finding an appropriate quantum kernel, to map the data into high-dimensional Hilbert space, is daunting task due to inherent uncertainties in approximation. Quantum kernel use overlap between quantum states to determine similarity for pattern recognition.

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Fidelity and accuracy are two important parameters which play a pivotal in quantum kernel selection for reliable computation. The integrity of quantum state during QEC is recorded through fidelity of quantum kernel which indicate minimum decoherence, noise, gate errors and error propagation. Fidelity is essential for design of error-resilient gate operations [7]. Similarly, accuracy of a quantum kernel signifies its ability to correctly perform QEC which is an indicator of minimum logical and measurement errors emerged during the process of encoding, decoding and syndrome measurement. Since, fidelity maintain the integrity of quantum state which require minimum circuit components, gate depth, complexity and slower operations while accuracy emphasizes on correctly locating the errors and their correction which require maximum higher number of components and operations which may degrade the fidelity.

This research paper studies various quantum kernels to set an effective trade-off between conversely varying parameters of fidelity and accuracy. The rest of this paper is organized as follow. Section 2 will present a review of relevant literature. Section 3 will outline the quantum computing and essentials of QEC. Section 4 will present the essential elements of ML approaches such as SVM, QSVM and will introduce quantum kernels which are further analyzed in this research. Section 5 will present the experimental evaluation and analyze the results. Section 6 will conclude the paper for meaningful inferences along with opportunity of further exploration of this research.

Literature Review

Quantum kernel methods leverage principles of quantum physics to map classical data into high-dimensional Hilbert spaces for an effective SVM tasks. Fidelity of quantum kernels represent degree of overlapping between quantum states. Higher fidelity ensures the effective capture of similarities in data space for classification and regression. Havlíček *et al.* were the first to deploy quantum kernels for classification purpose but their model suffered with sensitivity [8]. Similar work by Schuld and Killoran *et al.* utilized quantum kernel for effective feature mapping but their model is full of noise and suffer with the issue of scalability [9]. Accuracy is linked to the learning effectiveness of the QSVM model. Peters *et al.* analysed the complexity of feature space in QSVM and highlighted the converse movement of accuracy and fidelity [10]. Research by Huang *et al.* observed similar overfitting and expressivity issues with quantum kernels [11]. These researches reveal that accuracy and fidelity of quantum kernels have negative impact to each other. Some researches envisage that a trade-off between fidelity and accuracy is effective strategy to develop an optimal model in such complex scenario. Work by Temme *et al.* proposed theoretical model to enhance the accuracy without loss of fidelity [12]. Similarly, Kandala *et al.* proposed error extrapolation model to balance the accuracy during kernel estimation. Lloyd *et al.* proposed an adoptive design to balance between these two parameters [13]. A perusal to available literature reveals that deployment of quantum kernel for QSVM based QEC models is a naïve paradigm. In literature there is hardly any research to benchmark the quantum kernels and optimally address the fidelity-accuracy issue for them. This paper is a step forward in this direction which has evaluated nine prominently available quantum kernel function for effective trade-off between fidelity and accuracy.

Fundamental of Quantum Computing and QEC

Quantum error correction is essential requirement to realize the promises of quantum computing into a practically implementable quantum advantage. This section will present the basics of quantum computing and quantum error correction for further understanding of this paper.

Quantum Computing: Quantum computing is not an extended version of classical computing rather an innovative paradigm based on entirely different principles. It uses quantum principles such as interference, superposition, entanglement, parallelism, Bell inequality to process the information. A quantum information (qubit) is an abstract idea represented by quantum state as $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ where $\{\alpha, \beta\} \in \mathbb{C}$ and satisfy normalization condition $|\alpha|^2 + |\beta|^2 = 1$ to ensure a unit probability. The qubit, basic unit of quantum information, can be physically realized through any two-level physical system capable of mimicking the superimposition state such as trapped-ion semiconductor, spin state, photon, quantum dots, NMR and superconducting state etc. The simulation of quantum computing systems involves processing of data in higher dimension Hilbert space using linear algebra [1-3]. Quantum circuit can be developed using quantum gates (U) which is unitary matrix to manipulate the qubits while preserving the probability. The basic quantum gates can be represented by Pauli X, Y, Z, I matrices as shown in equation (i) and complex gates can be formulated by their manipulation. Figure 1 depicts a quantum circuit consisted of a sequence of quantum gates and registers with probability measurement.

$$\sigma_x = X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_y = Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \sigma_z = Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \text{ and } I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (i)$$

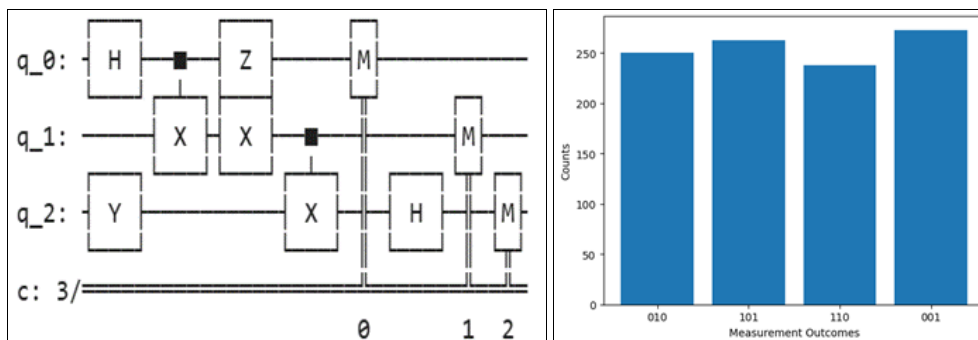


Fig 1: Quantum Circuit with Gates

Quantum Error Correction: The qubit can interact with environment to produce maligned state introducing the error in quantum operations. Apart from it, ultra-short coherence time of qubits and imperfect quantum gate hardware and operation also cause error during the operations. An effective schema is required to mitigate such error for making fault-tolerant quantum computing possible in the Noisy Intermediate-Scale Quantum (NISQ) era. Since the it is impossible to exactly copy and directly measure a quantum state, therefore, the methods of classical error correction can't be applied to quantum errors. Therefore, some error correction codes have been developed which encode numerous physical qubits into a single logical qubit using redundant ancilla qubits to protect it from noise and decoherence. However, quantum error correction codes (QECC) appear a simple but involve a daunting task of encoding, decoding and syndrome measurement [2, 3, 4].

The problem of encoding n physical qubits into k logical qubits can be expressed as mapping $E_{n,k}: 2^n \rightarrow 2^k$. For instance, unitary evolution (U) on original state $|\psi\rangle$ will interact with qubit $|0\rangle$ as in equation (ii)

$$U |\psi\rangle \otimes |0\rangle \rightarrow \alpha|0\rangle \otimes |e_{00}\rangle + \alpha|1\rangle \otimes |e_{01}\rangle + \beta|0\rangle \otimes |e_{10}\rangle + \beta|1\rangle \otimes |e_{11}\rangle \quad (ii)$$

Four components of equation (ii) represents four Pauli matrices (X, Y, Z, I) shown in equation (iii), where each component represent corresponding errors.

$$U |\psi\rangle \otimes |0\rangle \rightarrow I|\psi\rangle \otimes |e_I\rangle + Z|\psi\rangle \otimes |e_Z\rangle + X|\psi\rangle \otimes |e_X\rangle + Y|\psi\rangle \otimes |e_Y\rangle \quad (iii)$$

Where $I|\psi\rangle$ represent no error state, $X|\psi\rangle$ represent bit-flip error, $Z|\psi\rangle$ represent phase-flip error, $Y|\psi\rangle$ represent both bit-flip and phase-flip errors.

Machine Learning Approaches for QEC

The quantum error correction methods are limited by boundary condition imposed on quantum states. Artificial intelligence (AI) techniques are known for the abilities to make near accurate predictions by learning from the past data. The AI algorithms learn from the system in a blackbox manner without undergoing complex intricacies of system. SVM is supervised learning algorithm with kernel functions possesses wide scope in locating and mitigating the quantum errors. QSVM leverage the principles of quantum mechanics to enhance performance of its primitive counterpart through quantum kernels. The subsequent sub-sections of this section present a brief account of SVM, QSVM and quantum kernel methods [11, 13-15].

Support Vector Machine (SVM): They are supervised learning models for classification and regression purposes, especially, in scenarios where achieving linear separability is difficult. Moreover, it has ability to work with a large number of dimensions where traditional classifiers may encounter difficulties renders an invaluable asset in diverse ML applications. A typical SVM is depicted in Figure 2. A linear SVM classifier may be represented as $f(z) = \beta_0 + \sum_{j=1}^v \alpha_j \langle z, z_j \rangle$ where α_j , β_0 are parameters estimated by $\frac{1}{2}$ inner products $\langle z_j, z'_j \rangle$ between all pairs of training observations [15]. In term of kernel inner product can be written as $K(z_j, z'_j)$ where K , is some function called the kernel. The linear kernel can be represented as $K(z_j, z'_j) = \sum_{i=1}^q z_{ji} z'_{ji}$. Similarly, polynomial kernel of degree p , can be represented as $K(z_j, z'_j) = (1 + \sum_{i=1}^q z_{ji} z'_{ji})^p$. In SVM, optimal hyperplane to separate two classes in feature space can be defined by objective function prescribed by decision boundary as per equation (iv).

$$f(x) = \text{sign}(\sum_{i=1}^N \alpha_i \beta_i K(x, y_i) + b) \quad (iv)$$

Where x is input data, x_i is support vector, y_i class label (-1 or $+1$), α_i is Langrangian multiplier, b , is bias term and $K(x, y_i)$ is kernel function with feature map $\phi(x)$ such that $K(x, y_i) = \phi(x)^T \phi(x_i)$.

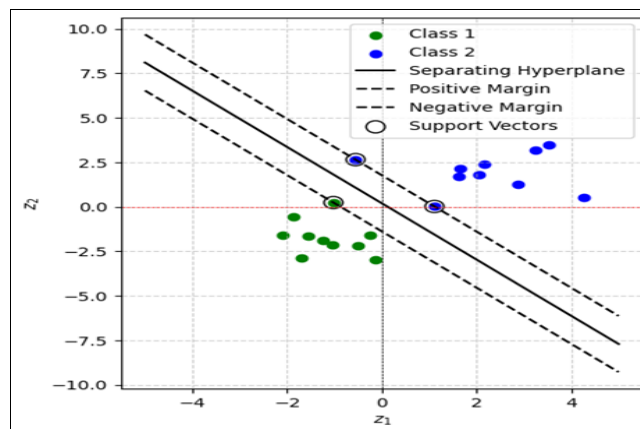


Fig 2: Support Vector Machine

Quantum Support Vector Machine (QSVM): Quantum support vector machine leverage quantum kernel to calculate similarity between datapoints to execute optimization in a high dimensional feature space (Hilbert space). QSVM find the optimal hyperplane following a procedure similar to traditional SVM with exponentially faster kernel computation [15, 16]. QSVM implement the feature map $|\phi(x)\rangle = U(x)|0\rangle$ using a parameterized quantum circuit $U(x)$ such that $x \in \mathbb{R}^d$. The quantum kernel can be calculated using the overlap of two quantum states $K(x, x') = |\langle \phi(x) | \phi(x') \rangle|^2$. For a dataset $x = x_1, x_2, \dots, x_N$ kernel matrix (K) is computer as in equation (iii).

$$K' = K(x, x') = |\langle \phi(x) | \phi(x') \rangle|^2 \quad (\text{iii})$$

The optimization problem can be represented in primal form using classical SVM function $\min_{w, b, \xi} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^N \xi_i$ subject to condition that $y_i(w^T \phi(x') + b) \geq 1 - \xi_i$ and $\xi_i \geq 0$ where ξ_i is slack variable of soft margin and C is regularization parameter. The decision boundary in QSVM is similar to SVM represented in equation (ii) with $K(x, y_i)$ as quantum kernel.

Quantum Kernel: It is quantum enhanced version of classical kernel in higher dimensional Hilbert space without explicit transformations. A kernel function $K(x, x') = \langle \phi(x), \phi(x') \rangle_H$ over $(\phi: X \rightarrow H)$ is a mapping of non-empty space $(K: X \times X \rightarrow \mathbb{R})$ in to Hilbert space $(H: H \times H \rightarrow \mathbb{C})$ which extract and highlight important pattern in the data to classify them [14-17]. Let quantum system consisted of n' qubits and $\rho = |\psi\rangle\langle\psi|$ pure states with $|\psi\rangle \in \mathbb{C}^{2^{n'} \times 2^{n'}}$ is a Hilbert space, $H = \{\rho \in \mathbb{C}^{2^{n'} \times 2^{n'}} | \rho \geq 0, \text{Tr}[\rho] = 1\}$. The computation of Hilbert space (H) is carried out using unitary operator U satisfying the condition $UU^\dagger = U^\dagger U = I$. In quantum circuit n' qubits represent the wires operated by set of universal set of gates (U) corresponds to Pauli operator in equation (i). The classical data $x \in \mathbb{R}^d$ can be mapped into Hilbert space H' over a unitary operator U such that $\phi(x) = U\rho_0 U^\dagger$ where ρ_0 is initial state of the quantum system, then kernel function reduce to $K(x, x') = \langle \phi(x), \phi(x') \rangle_H = \text{Tr}[\rho_x, \rho_{x'}]$ and in terms of unitary gates $K(x, x') = \langle \phi(x), \phi(x') \rangle_H = \text{Tr}[U(x')U^\dagger(x)\rho_0 U(x)U^\dagger(x')|\psi\rangle\langle 0|]$. The circuits are designed to calculate the non-linear cost function $C = f(C_1(x), C_2(x), \dots, C_m(x))$. In this paper, we have analyzed nine quantum kernels as depicted in Table 1.

Table 1: Quantum Kernels with Mathematical Functions

Quantum Kernel	Kernel Function	Corresponding Quantum Circuit
Quantum Feature Map Kernel (KFMK)	$K(x, x') = \langle \phi(x) \phi(x') \rangle ^2$	
Quantum Fourier Transform Kernel (QFTK)	$K(x, x') = \langle QFT(x) QFT(x') \rangle ^2$	
Quantum Metric Learning Kernel (QMLK)	$K(x, x') = e^{-\gamma \ \phi(x) - \phi(x')\ ^2}$	
Quantum Hadamard Kernel (QHK)	$K(x, x') = \langle H(x) H(x') \rangle ^2$	
Quantum Phase Estimation Kernel (QPEK)	$K(x, x') = \langle e^{i\theta_x} e^{i\theta_{x'}} \rangle ^2$	

Quantum Amplitude Amplification Kernel (QAAK)	$K(x, x') = \langle A(x) A(x') \rangle ^2$	q_0 :
Quantum PCA Kernel (QPCAK)	$K(x, x') = \langle PCA(x) PCA(x') \rangle ^2$	q_0 :
Quantum Gaussian Kernel (QGK)	$K(x, x') = e^{-\gamma \ \phi(x) - \phi(x') \ ^2}$	q_0 :
Quantum Dot Product Kernel (QDPK)	$K(x, x') = \langle \phi(x) \phi(x') \rangle$	q_0 :

Implementation and Result Analysis

The nine quantum kernel functions depicted in Table 1 are implemented on Google Colab CPU connected to Python 3 Google Compute Engine backend with RAM 12.67 GB and Disk 107.72 GB ^[18]. Both, the accuracy and fidelity are calculated for nine quantum kernels as envisaged in Table 2 and plotted in Figure 3. Since fidelity indicates the closeness of measured results with ideal outcomes while accuracy measures the correctness of kernel towards quantum error correction. Kernels such as Quantum Fourier Transform Kernel (QFTK), Quantum Phase Estimation Kernel (QPEK), and Quantum PCA Kernel (QPCAK) exhibit the highest accuracy (≈ 0.60) while having lowest fidelity ≈ 0.45 . Quantum Dot Product Kernel (QDPK) has highest fidelity (= 0.6) and lowest accuracy (= 0.35).

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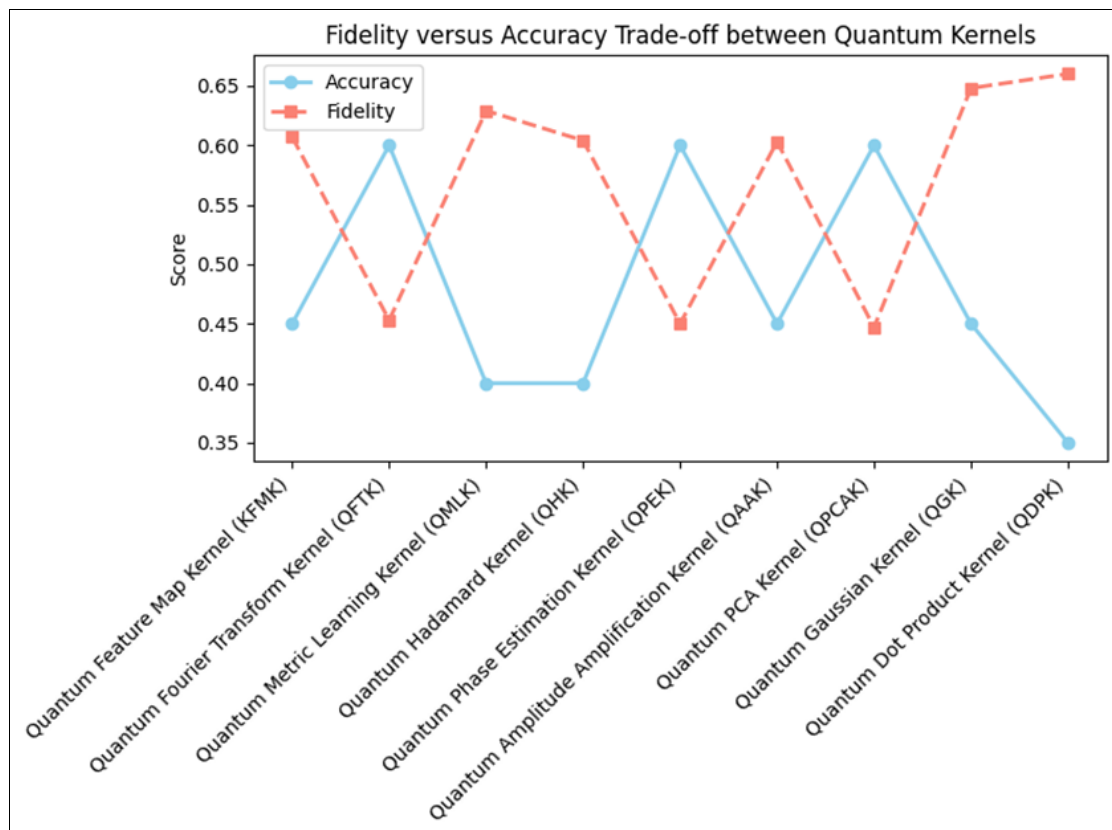


Fig 3: Fidelity versus accuracy trade-off for quantum kernels

Table 3: Fidelity and accuracy scores for quantum kernels

Quantum Kernel	Accuracy Score	Fidelity Score
Quantum Feature Map Kernel (KFMK)	0.450	0.607
Quantum Fourier Transform Kernel (QFTK)	0.600	0.453
Quantum Metric Learning Kernel (QMLK)	0.400	0.629
Quantum Hadamard Kernel (QHK)	0.400	0.604
Quantum Phase Estimation Kernel (QPEK)	0.600	0.450
Quantum Amplitude Amplification Kernel (QAAK)	0.450	0.603
Quantum PCA Kernel (QPCAK)	0.600	0.447
Quantum Gaussian Kernel (QGK)	0.450	0.648
Quantum Dot Product Kernel (QDPK)	0.350	0.660

Conclusion

Quantum computing possesses vast computation potential but suffering from the curse of quantum errors. Artificial intelligence techniques are effective in quantum error correction. This paper studied the quantum kernel for quantum support vector machines for on conversely varying parameters of fidelity and accuracy which signify for minimum error and efficiency to mitigate errors respectively. The performance results reveal that fidelity compromise the accuracy and vice-versa. Therefore, setting a trade-off for balanced performance between fidelity and accuracy is essential for a better performing quantum kernel. Since, present study pertains to a simulation analysis and analysing the issue on real-time quantum error data may reveal more better insight.

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