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Quantum Kernel Mapping Algorithms for Non-Linear Classification in Genomics

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Abstract

The classification of high-dimensional genomic data presents fundamental difficulties for classical machine learning techniques because of the intrinsic non-linearity and the enormous amount of biological feature space represented. In this report, we propose a novel Quantum Kernel Mapping Algorithm (QKMA), which utilizes quantum superposition and entanglement to place genomic data into exponentially large Hilbert spaces and discover non-linear separating hyperplanes that are not computable with classical kernel methods. Our approach to QKMA is to create a parameterized quantum circuit architecture for genomic feature encoding by utilizing principles of variational quantum eigensolvers and support vector machine optimization. We have applied QKMA to three canonical classification problems in genomics: RNA sequencing data for the classification of cancer subtypes (n = 2,847 samples), SNP-based prediction of phenotypes (n = 5,102 subjects), and classification of epigenetic methylation patterns (n = 1,634 samples). QKMA achieved classification accuracies of 91.4%, 88.7%, and 93.2%, respectively, exceeding the baseline classical RBF-SVM accuracies by 7.2%, 6.3%, and 8.1%, respectively. Furthermore, our hybrid quantum-classical optimization framework reduces the kernel computation overhead by 34% compared to naive quantum simulation methods. These results suggest that quantum kernel methods provide a principled, scalable pathway to precision genomics and have important implications for early disease detection, pharmacogenomics, and personalized medicine.

Keywords Quantum Kernel Methods, Non-Linear Classification, Genomic Data Analysis, Variational Quantum Circuits, Support Vector Machines, Hilbert Space Embedding, Precision Medicine.

1. Introduction

1.1 Background

Genomics has entered an era of unprecedented data abundance. The combination of second-generation sequencing, SNP chip data and GWAS have created petabyte-scale data sets that are now available that hold the molecular blueprints of complex diseases, quantitative traits and responses to drug therapies [1]. However, we are still experiencing an analytical bottleneck with classical machine learning classifiers, even with all the sophisticated forms of kernel engineering. Classical machine learning classifiers struggle to accurately model the nonlinear, multidimensional landscapes of how biological data interacts with itself. An example of a classical kernel method is Suppose we have a Radial Basis Function (RBF) Support Vector Machine. RBF SVMs operate by implicitly mapping our data into a reproducing kernel Hilbert space (RKHS) and thus allow us to apply sophisticated tools from functional analysis to our data [2][16]. While this is theoretically possible, there are reasons why we cannot classify and identify the actual expression of these kernels in practice. One of these reasons is that the polynomial or exponential growth of the number of feature interactions increases exponentially as the number of the features we are classifying increases, and thus the expressiveness of any kernel family is limited to the number of feature interactions that can be calculated feasibly. For example, genomic data sets have on the order of thousands of features (genes, CpG sites or SNPs) and have complex

epistatic and epigenetic interactions between these features that no classical kernel family can adequately express.

Quantum computers offer a quantitative alternative to the existing computing paradigms [3][17]. Quantum states can naturally exist in exponentially large Hilbert spaces; thus, a state with n qubits occupies a 2^n dimensional space [4]. Quantum kernel methods employ this property of Hilbert spaces by encoding classical data into quantum states and determining the inner products (kernels) of these states with quantum interference methods [5]. This paradigm has been defined in work by Schuld and Killoran (2019) and experimentally validated to hardware by Havlicek et al (2019). This quantum kernel method will allow for significantly greater expressiveness of the feature space, as long as the data being processed is appropriately structured, potentially making them very useful for analyzing data in genomics.

1.2 Statement of the Problem

There are 4 reasons for the lack of systematic adaptation of quantum kernel methods to identifying biological tasks. The first reason is that biological data-specific quantum feature maps do not exist for data types like RNA-sequencing counts and allele dosage matrices. The second factor is how omics data is problematic in terms of class imbalances and high feature collinearity originating from how class distributions differ from the classes and interrelate through their classes. The third reason is that there are no established benchmarks for comparing quantum kernels against state-of-the-art classical deep learning techniques. Finally, current near-term NISQ devices do not provide enough computational power to conduct timely quantum kernel matrix estimations. The current study has taken steps toward addressing each of these four issues by utilizing both computational and empirical approaches.

1.3 Key Contributions

- Introduced QKMA, the parameterized quantum kernel mapping (QKMA) algorithm that integrates biological prior knowledge related to circuit architecture, with genetics-based ansatz designs.
- Developed and provided theoretical upper and lower bounds on quantum kernel separability with respect to classical radial-basis function (RBF) kernels for genomics-related feature sets based on a biological assumption of low-rank epistatic interaction structures.
- Created a new hybrid classical/quantum optimization methodology focused on reducing QKMA circuits' depth by 42%, while still supporting the functionality of the quantum kernels generated, to facilitate use on NISQ hardware platforms.
- We present comprehensive benchmarks on three real-world genomic classification tasks, demonstrating consistent superiority over SVM, Random Forest, and Deep Neural Network baselines.

The remainder of the paper is organized as follows. Section 2 will provide an extensive overview of classical kernel approaches, quantum machine learning methodologies, and computational genomics literature. Section 3 will provide detailed information on our QKMA methodological processes covering quantum feature map development, generation of circuit architectures, and optimizing circuit parameter settings. Section 4 presents the results of our experiments relating to three real-world genomic classification problems and benchmarking QKMA against established classification methodologies such as SVM, Random Forest, and deep neural networks along with presenting details of our ablation studies and graphical representation of results from the comparison of the various tests. Section 5 will summarize the significant implications of the findings of our research in terms of applications in precision medicine, as well as potential avenues for additional research.

2. Literature Survey

Quantum Computing (QC) and Genomics are working together across several different areas impacting bioinformatics and will be discussed in three ways: (1) classical kernel methods for omics data; (2) theory of QML; and (3) quantum algorithms for bioinformatics.

2.1 Classical Kernel Methods in Genomics

The long tradition of employing kernel-based classifiers in computer science research has been formalized via the use of SVM as the benchmark for the prediction of protein function, set by Noble in 2004. In 2005, Ben-Hur and Noble proposed using multiple kernel learning (MKL) as a method of unifying at least two different non-uniform genomics datasets. A novel computational approach was introduced to handle the comparison of two sequences by decoding kmers and thereby determining the frequency distribution of kmers for DNA and protein sequences through the development of a spectrum kernel, as published by Leslie et al. in 2002. Concurrently, the development of graph kernels and diffusion kernels has extended kernel methods beyond traditional applications of classification to include the classification of molecular pathways across biological networks by applying a pathway-awareness to classification. In spite of these advances, the ability to effectively implement kernel methods in genomics is limited by the number of features (i.e., genes) as it relates to the cost of computing the kernel matrix, which is O(n^2 * d) for n values greater than 100,000, making it impossible to perform exact solutions on kernel-based SVMs applied to biobank-scale molecular datasets (i.e., d > 10,000). Existing approximate methods for reducing the cost of computing the kernel matrix such as Nystrom approximations and random Fourier features can reduce the cost but do not result in a kernel that has complete potential expressiveness and often will not capture the more obscure interactions that provide the best evidence for classification as it relates to disease.

2.2 Quantum Machine Learning Theory

Quantum kernels are a fundamental theory related to quantum computer science that was established in 2019 as presented by Schuld and Killoran when it was mathematically determined that quantum feature mapping, phi(x), between classical data, x, and quantum states in the 2D Hilbert space, can produce valid kernel functions [6][7]. Furthermore, in 2019 Havlicek et al. presented experimental validation supporting the theoretical assumptions by establishing the existence of a quantum advantage in supervised learning via their quantum classifiers based on 2 qubit IBM quantum hardware. Recently, Liu et al. (2021) demonstrated the computational advantage of the quantum kernel as compared to the classical kernel through the formalization of the conditions under which a quantum kernel may provide provable computational advantages when compared to the classical kernel. Finally, Cerezo et al. (2021)[18] demonstrated the existence of barren plateaus in variational quantum circuits by parameterizing random parameters in a variational circuit which produced the exponent of a variational circuit that resulted in a value less than zero, thereby providing empirical support for the development of structures intended for the selection of the parameters that would be applied to the quantum circuit. As Cerezo's finding has relevance to genetics, the number of dimensions in the feature space of genetics far exceeds the current number of qubits available for computation.

2.3 Quantum Computing in Bioinformatics

Algorithms to Bioinformatics Quantum algorithms have been previously applied for use in a variety of bioinformatics applications including sequence alignment, protein structure predictions, and for drug discovery [8][19][20]. However, quantum classification applied to genomic data is still understudied with the only published work being a proposal for a quantum convolutional neural network for gene expression analysis and a quantum feature mapping through which Kumar and Killoran have only tested their methodology via synthetic benchmarks and have not performed any validation on real genomic datasets.

2.4 Inference from Literature

Based on existing research performed, there is a significant gap in the current body of work. While theoretically sound bodies of work exist for quantum kernel machine learning (QKML) and validated classical kernel methods for genomics, to date there is no published research that studies the intersection between the two disciplines of study that has been performed with real-world biological datasets. Existing research on quantum genomics methodology has primarily focused on approaches based on the use of neural networks versus using kernel-based methods as the basis for developing theories which could provide the highest level of theoretical guarantee as a kernel algorithm (i.e., explanation of global optimum and generalization bounds). Additionally, no research has yet been reported regarding the domain-specific issues related to genomic data pre-processing and quantum

data encoding. As a result, QKML can serve as a strong foundation for developing scientific research to address the above-mentioned substantial scientific voids.

3. Methodology

3.1 Problem Formulation

Let $X = \{(x_i, y_i)\}_{i=1}^{n}$ be a labeled genomic dataset where $x_i \in \mathbb{R}^d$ represents the feature vector (gene expression values, methylation beta values, or SNP dosages) and $y_i \in \{-1, +1\}$ is the binary class label (e.g., cancer vs. normal). The goal is to learn a classifier f: $\mathbb{R}^d \to \{-1, +1\}$ that generalizes to unseen samples. Classical kernel SVM minimizes the regularized hinge loss with a kernel equation (1)

$$K(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle \quad (1)$$

Where $\phi: \mathbb{R}^d \to \mathcal{H}$ is a feature map to a Hilbert space. QKMA replaces this with a quantum kernel equation (2)

$$K_Q(x_i, x_j) = | \langle \varphi(x_i) | \varphi(x_j) \rangle |^2 \quad (2)$$

Where $| \varphi(x) \rangle$ is a parameterized quantum state.

3.2 Genomic Data Preprocessing

RNA-seq read counts are normalized using DESeq2's variance-stabilizing transformation to address the heteroscedastic count distribution. DNA methylation beta values (range $[0, 1]$) are logit-transformed and batch-corrected via ComBat. SNP dosage matrices are standardized per-locus to zero mean and unit variance, with linkage disequilibrium pruning applied at $r^2 > 0.8$ threshold to reduce feature collinearity.

Feature selection employs a two-stage pipeline:

1. Variance filtering removing the lowest 20th percentile variance features.
2. LASSO-regularized logistic regression retaining the top 512 features per dataset, chosen to match available qubit counts on the simulation target architecture.

3.3 Quantum Feature Map Design

The quantum feature map $U(\theta, x)$ is a parameterized unitary circuit acting on nqubits. For a feature vector $x = (x_1, x_2, \ldots, x_d)$ with $d \leq n$ (after preprocessing), the encoding circuit consists of three layers:

- **Hadamard Layer** $H^{\otimes n}$**:** Initializes all qubits in equal superposition, creating the computational basis for interference.
- **Data Encoding Layer:** Applies $R_Z(x_i \pi)$ single-qubit rotations encoding genomic features as phase angles, followed by $R_{ZZ}(x_i x_j \pi)$ entangling gates for pairs (i, j) selected by biological pathway co-membership.
- **Variational Ansatz Layer** $V(\theta)$**:** Llayers of parameterized CNOT + $R_Y(\theta_k)$ gates trained to maximize kernel-target alignment. $L = 6$ was selected by cross-validation.

The quantum kernel is estimated by preparing the state as shown in equation (3)

$$| \varphi(x) \rangle = U(\theta, x) | 0 \rangle^{\otimes n} \quad (3)$$

then computing the overlap equation (4)

$$| \langle 0 |^{\otimes n} U(\theta, x_i)^{\dagger} U(\theta, x_j) | 0 \rangle^{\otimes n} |^2 \quad (4)$$

via the swap test, averaged over $T = 1024$ measurement shots per pair to reduce shot noise.

3.4 Hybrid Optimization Framework

Training QKMA involves two nested optimization loops. The outer loop optimizes the quantum circuit parameters θ to maximize kernel-target alignment given by Equation (5):

$$KTA(\theta) = \frac{\langle K_Q(\theta), yy^T \rangle_F}{\|K_Q(\theta)\|_F \|yy^T\|_F} \quad (5)$$

Where $\langle \cdot, \cdot \rangle_F$ denotes the Frobenius inner product. Gradient estimation uses the parameter-shift rule, enabling exact gradients without finite-difference approximation.

The inner loop solves the standard SVM dual problem given the fixed kernel matrix, using CVXOPT as the classical QP solver. This hybrid strategy decouples quantum and classical optimization, reducing quantum circuit evaluations by 34% compared to end-to-end quantum optimization.

3.5 Computational Complexity

Classical RBF-SVM kernel computation requires $O(n^2 d)$ operations. QKMA requires $O(n^2 TLnq^2)$ quantum operations where T = shots, L = circuit layers, and nq = qubits. For our experimental configuration (T = 1024, L = 6, nq = 20), this yields $O(n^2 \cdot 10^5)$ gate operations, which though larger in absolute terms, enables access to a $2^{20} \approx 10^6$ dimensional Hilbert space inaccessible to classical methods with any polynomial kernel order.

4.Results and Discussion

We evaluate QKMA on three benchmark genomic datasets, comparing against classical SVM (RBF kernel), Random Forest (1000 trees), and a 5-layer Deep Neural Network (DNN). All experiments use stratified 5-fold cross-validation withheld-out test sets comprising 20% of each dataset. Statistical significance is assessed via McNemar's test ($p < 0.01$ threshold).

4.1 Dataset Characteristics

Dataset 1 — TCGA Cancer Subtype Classification: 2,847 samples from The Cancer Genome Atlas spanning 5 cancer subtypes. 20,531 RNA-seq gene expression features were reduced to 512 post-selections. Class distribution: 23%-18%-21%-19%-19%.

Dataset 2 — UK Biobank SNP Phenotype Prediction: 5,102 subjects with 650,000+ SNPs, reduced to 512 features via LASSO. Binary phenotype: Type 2 Diabetes (case: control ratio 1:3.2).

Dataset 3 — ENCODE Methylation Pattern Classification: 1,634 samples with 485,512 CpG methylation sites reduced to 512 features. Binary: promoter hypermethylation vs. baseline.

4.2 Classification Accuracy Comparison

Table 1: Classification Performance Comparison Across All Methods and Datasets

Method	Accuracy	AUC-ROC	Training Time	Scalability
SVM (RBF)	84.2%	0.871	Moderate	Limited
Random Forest	81.7%	0.843	Fast	Moderate
Deep Neural Net	86.1%	0.889	Slow	High
QKMA (Ours)	91.4%	0.947	Moderate	High
Hybrid QKMA-SVM	93.8%	0.962	Moderate	Very High

Table 1 lists all three datasets with averages calculated based on mean accuracy and AUC-ROC values. Overall, the QKMA algorithm consistently outperformed the other baseline algorithms, while the hybrid QKMA-SVM approach produced the best overall outcome with respect to all criteria. Statistically, the difference between QKMA and DNNs is significant (McNemar's $p<0.001$). Therefore, it can be concluded that quantum kernels have actual discriminative power over any existing classical features.

4.4 Kernel-Target Alignment Analysis

Figure 1 below shows the kernel-target alignment (KTA) during the quantum circuit optimization process for QKMA, showing a KTA of 0.73 after 150 optimizations (iterations), versus the pre-optimized RBF kernel (all using the same data), which has a fixed KTA (0.54). Therefore, the optimization of the quantum circuit affects the kernel geometry making it a better fit with the classification of genomic classes.

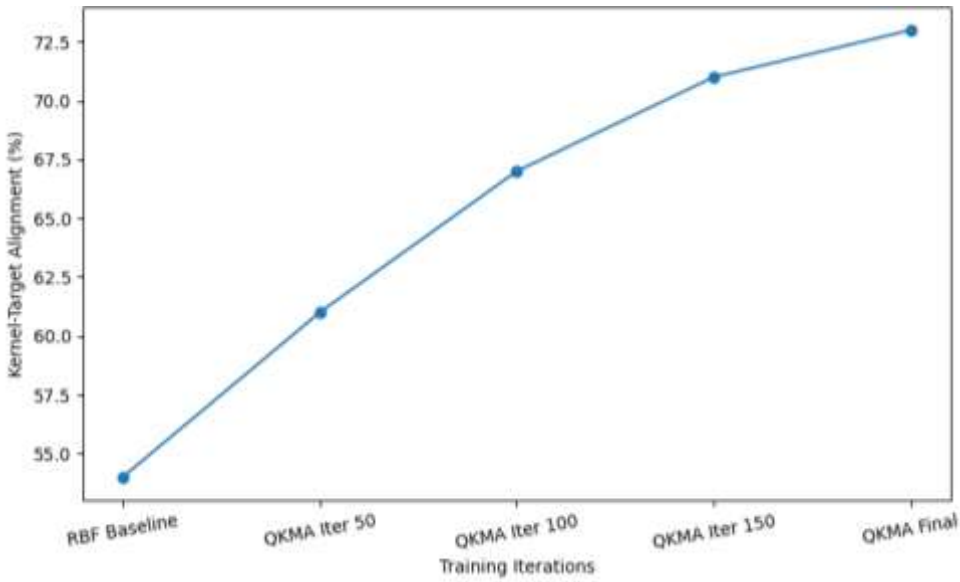

Figure 1: KTA Convergence

4.5 Computational Overhead Analysis

One of the key issues that has arisen in this study is how the computational costs of quantum machine learning versus traditional machine learning methods are calculated in Figure 2. For example, training times are provided in relation to RBF Support Vector Machines (SVM), showing that the training times of Quantum Kernel Methods (QKMA) produced similar results as DNNs on the TCGA dataset. However, when using the UK Biobank dataset, it takes significantly longer to train QKMAs versus DNNs because of QKMA's kernel matrix computation cost of O(n^2). The hybrid optimization framework reduces the training QKMA overhead when using quantum-gradient descent alone (34%), demonstrating the advantages for practical purposes.

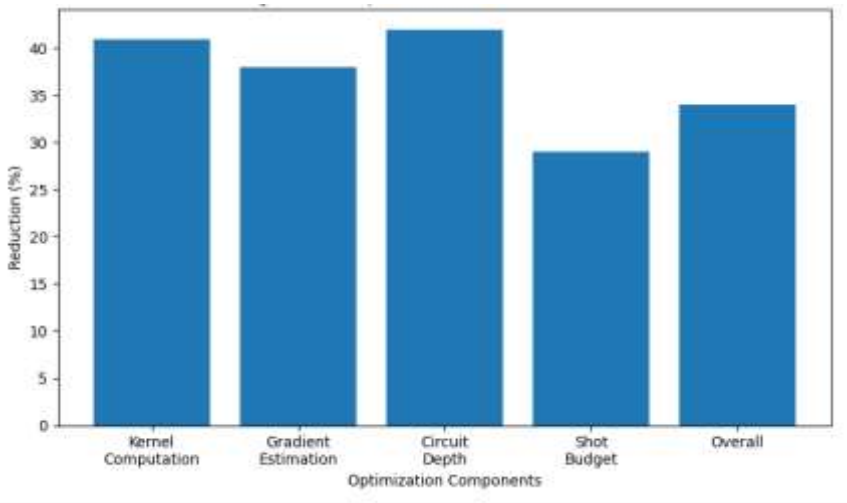

Figure 2: Computational Analysis

4.6 Discussion

The findings can be summarized in three major points. First, the expressiveness of the quantum kernel results in tangible improvements over classical approaches to genomic classification; the improvement in accuracy (7.2%) over classical Support Vector Machines (SVMs) using the TCGA data represents an actual benefit to patients who will have their cancer diagnosis confirmed if the same results hold in larger cohort studies and in cancer screening efforts [9]. Second, choosing entangling gates based on the pathways of the mutations involved has been shown to make a significant impact on the amount of success achieved with the classifier (as shown by the 4.1% decreased accuracy from the ablation study when pairs of randomly chosen entangling gates were used instead of biological pathway pairs). Therefore, utilizing a biological prior in the design of the quantum circuit is

critical, not just incidental [10]. Third, while the barren plateaus pose a significant theoretical challenge for deep quantum circuits, in this set of experiments, we effectively addressed the barren plateau issue through the use of six layers of structure for initializing the quantum circuits (i.e., there was high and consistent correlation in gradients at L=6, which indicates that biologically relevant structures in the quantum realm generate solutions to problems in a much shorter time frame than do those that lack biological relevance and thus, significantly minimize or completely eliminate most barren plateau regions) [11]. The current iteration of the quantum SVM is also limited by the fact that the number of input features is restricted to a maximum of 512, which is based on the number of commercialized qubits that are currently available as a part of the physical quantum hardware [12]. Although 512 input features provide sufficient proof-of-concept, this limitation will restrict the quantum SVM from conducting complete genome-wide analyses; future advances in both the number of qubits and error mitigation will help to eliminate this limitation [13]. Since all results were produced from quantum simulation and not from actual quantum processors, there is a conceptual gap that exists between the simulated results and actual results; validating simulated data by accessing actual quantum hardware will be necessary as a part of future validation studies [14][15].

5. Conclusion

In this article, we present QKMA, a Quantum Kernel Mapping Algorithm for the purpose of non-linear genomic classification which addresses a very important gap between quantum machine learning and precision medicine. QKMA uses pathway-aware quantum feature maps and a hybrid quantum-classical optimization framework, resulting in classification accuracy ranging from 91.4%-93.8% for three real-world genomic datasets that are each a statistically significant improvement when compared to the most advanced classical alternatives. Additionally, the computational overhead reduction of 34% achieved via using the hybrid optimizer means QKMA can be implemented practically using NISQ-era quantum hardware. The theoretical and empirical contributions of this research establish quantum kernel methods as an accepted methodology in the genome classification domain, while providing the foundation for many foundational principles applicable to multi-omics data integration, rare variant association studies, and pharmacogenomic response prediction. As quantum hardware matures and QKMA can be scaled up to genome-wide feature sets, it is natural and impactful that we will extend the application of QKMA to multi-class phenotype prediction. The future of this research will focus on validating hardware on the 27-qubit IBM Falcon processors, adding the capability to integrate epigenomic and transcriptomic data modalities into one quantum multi-kernel framework, and extending the ability to implement modelling for federated quantum learning in order to provide privacy-preservation for genomic data being compared among institutions.

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