

Quadratic speed-ups in quantum kernelized binary classification

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I. INTRODUCTION

Recent advancements in quantum hardware and simulation frameworks have led to the rise of quantum machine learning (QML), which merges machine learning (ML) with quantum information processing (QIP). This integration offers the potential to overcome the limitations of classical ML methods. A prominent approach within QML is the quantum kernel method (QKM) [1–4], which leverages quantum computing to enhance the performance of kernel-based algorithms.

In ML, the kernel is a function that quantifies the similarity between two data points, enabling the learning of patterns within a dataset for effective classification or prediction. The computational advantages of the QKM stem from the state and measurement postulates of quantum mechanics, which allow for efficient computation of certain kernel functions on a quantum computer. In particular, the Hadamard or swap test can exponentially expedite the computing of fidelity between two quantum states compared to its classical counterpart [5, 6]. Therefore, they have been harnessed in several quantum kernelized binary classifiers (QKCs) for exponential speed-ups with respect to the number of features (dimensions) in the data when evaluating the classification score in supervised classification. These algorithms are known as the Hadamard classifier (HC) [7] and swap test classifier (SC) [8], respectively, and represent one of the simplest QML protocols with potential quantum speed-up.

The original QKCs prepare an initial quantum state containing entire data samples in a quantum superposition, which is a distinct feature of what quantum computers can do. This state preparation routine is implemented at the cost of increasing the circuit depth linearly and its width logarithmically with the number of data samples. However, QKCs do not utilize this unique property of quantum computing. Thus, there is no quantum advantage with respect to the number of data samples. In other words, previous QKCs failed to utilize the capability of placing training data in superposition and therefore merely increased the size of the quantum circuits without yielding any computational advantages.

In this work, as a minor result, we propose simplified QKCs (SQKCs) by modifying the encoding and measurement processes. These modifications allow SQKCs to provide the same work as QKCs while using one less qubit and linear reduction in circuit depth concerning the number of training data. Then, as the main result, we present a protocol for integrating Quantum Amplitude Estimation (QAE) [9] into SQKCs (hence, QKCs), resulting in a quadratic speed-up with respect to the number of data samples used in superposition.

II. RESULT

A. Simplified quantum kernelized binary classifiers

As QKCs are supervised classification algorithms, they should be able to identify the class of the data after initial quantum state preparation. The original QKCs encode the class information into an extra qubit by linearly increasing the depth of the circuit to training data. However, this can be simplified by the class-ordered encoding, shown in the green dashed box in Fig. 1, i.e. encode class 1 data after class 0 data are encoded. With this strategy, the class information is implicitly encoded into one of the qubits making the quantum superposition, $|m\rangle$. Thus, labeling the class of the data points can be achieved without increasing extra circuit width or depth by data size. Moreover, the Clifford transformation shown in the red dotted box in Fig. 1 can further reduce the measurement process from two-qubits to a single-qubit. This reduces the application of QAE by a factor of two, as the new measurement scheme allows classification with a single probability.

B. Main protocols

The main protocol of this work is to verify whether SQKCs with QAE (SQKCs-QAE) have the potential to get any quantum speed-up compared with normal SQKCs. Thus, it is crucial to establish a clear and rigorous evaluation criterion for comparing the performance of SQKCs-QAE and SQKCs. In this regard, we compare the rate at which the

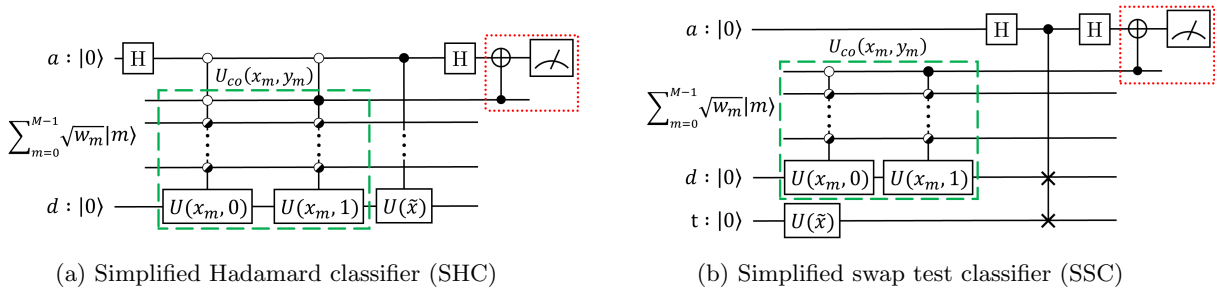


FIG. 1: Quantum circuit diagrams for (a) Simplified Hadamard classifier (SHC) and (b) Simplified swap test classifier (SSC). The green dashed box, $U_{co}(x_m, y_m)$, indicates that the class-ordered encoding and the red dotted box is the measurement with the Clifford transformation.

	Number of samples	Estimation error
SQKCs-QAE	$2^{t+1} N_{shot}^q := 2^{t+1}$	The 81% largest value among all errors, $ a - \tilde{a}_i $, $i = 1, 2, \dots, I$. I is the number of repetitions for a given number of samples.
SQKCs	$N_{shot}^c := 2^{t+1}$	

TABLE I: An overview of variables used for comparing the performance of SQKCs-QAE and SQKCs.

estimation errors decrease in SQKCs-QAE and SQKCs as the number of samples increases. Two variables, namely the number of samples and the estimation error, whose relationship is analyzed and compared in the subsequent section, are summarized in Table I. Here “sample” is prepared by querying the circuit Fig. 1a or 1b. Thus, the “number of samples” corresponds to the instances of applying the circuit. The estimator of QAE satisfies the absolute error that is upper bounded by $\mathcal{O}(1/N_q)$ with a probability of at least $8/\pi^2 (\approx 81\%)$, where N_q is the number of applications of the Grover operator (see Section 4 in [9] for more detail). Considering the success probability of QAE, “estimation error” is defined as the 81st percentile largest error value for each sample on both SQKCs-QAE and SQKCs. If, for instance, we generated 1000 error results on both SQKCs and SQKCs-QAE, respectively, the comparison is based on the 810th largest error. Note that, in this scenario, I in Table I is 1000, where a and \tilde{a}_i denote the real value we want to estimate and its i th estimator, respectively. For a more concise comparison, we fitted each error result to a linear curve using the \log_2 function. The slope of the fitted line for SQKCs-QAE and SQKCs indicates how fast the estimation error decreases. Thus, we can verify the speed-up quantitatively by investigating the ratio between two slopes: (slope of the linear fit for SQKCs-QAE estimation error)/(slope of the linear fit for SQKCs estimation error).

C. Numerical simulation results

Numerical simulations were conducted on the IBM quantum simulator using the first and last classes, *setosa* and *virginica*, based on two features of the Iris dataset: *sepal width* and *petal length*. The error curves in Fig. 2a represent the mean value computed from a total of 12 results, with 6 for SHC and 6 for SSC. A total of 11 subsets from the Iris dataset are utilized, comprising one set used in both SHC and SSC, along with five independent random sets for each SHC and SSC. Fig. 2b displays the linear fitting results of Fig. 2a, and the ratio between two slopes is approximately 1.9185 (≈ 2). Comparative simulation results between SQKCs-QAE and SQKCs indicate that, for a given level of precision, the estimation speed of SQKCs can be quadratically enhanced by leveraging data superposition via QAE.

III. FUTURE WORK

Since the classification score over the full dataset is computed entirely coherently on a quantum computer, the protocols we discussed are fully quantum algorithms. This work primarily focuses on achieving quantum speed-up in computing the classification score, expressed as a weighted kernel sum between new input and data samples. However, QAE can also expedite estimating a single kernel function, an element of the kernel matrix or Gram matrix (typically given by quantum state fidelity), by integrating QAE into the Hadamard or swap test. Thus, QAE is beneficial in quantum-classical hybrid ML, where the quantum kernel matrix is utilized in classical ML algorithms, such as the support vector machine (SVM). Therefore, estimating the kernel function faster through QAE could pave the way for

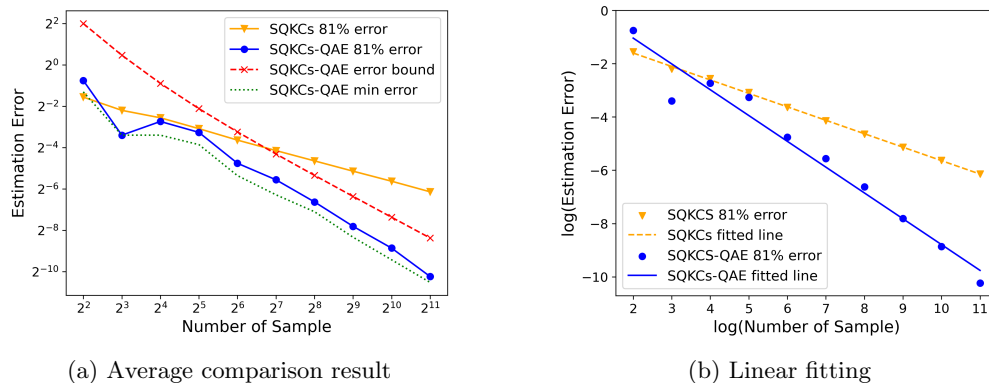


FIG. 2: (a) Comparison of average error scaling between SQKCs with QAE (SQKCs-QAE) and standard SQKCs. The results are derived from a total of 12 measurements, with 6 for SHC and 6 for SSC. (b) Linear fitting of (a) shows a slope ratio of approximately 1.9185, indicating a quadratic speed-up.

interesting future work, since many near-term and fault-tolerant quantum models can be replaced or formulated by a general SVM with a quantum kernel [10].

While QKCs and SQKCs introduced in this paper focus on binary problems, they can also address multi-class classification problems using heuristic strategies such as one-vs-rest or one-vs-one. Moreover, we emphasize that QKCs can apply to any datasets, as long as they are supplied as quantum states that can be handled by a quantum computer, either by an inherently quantum-mechanical system or through quantum feature mapping. Therefore, extending our method to multi-class QKCs or investigating it on other datasets remains an interesting avenue for future research.

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