Effects of fitness function in genetically auto-generated quantum feature maps

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We present and probe some improvements over the method using genetic algorithm proposed in [S. Altares-López, Automatic design of quantum feature maps, (2021)] to automatically generate quantum feature maps for quantum-enhanced support vector machine, a classifier based on kernel method, by which we can access high dimensional Hilbert space efficiently. In addition, we define a multi-objective fitness function using penalty method, which incorporates maximizing the accuracy of classification and minimizing the gate cost of quantum feature map’s circuit as the original method. Numerical results and comparisons with different kernel methods as well as the original proposed method are presented to demonstrate the efficiency of our fitness function. In particular, we reduce and optimize the gate cost of a circuit shown in [J.R. Glick, Covariant quantum kernels for data with group structure, (2022)] from 51 to 3 while remaining perfect accuracy.

Keywords: support vector machine; quantum feature map; genetic algorithm

I. INTRODUCTION

Quantum computing is a type of calculation using quantum mechanical properties, such as superposition, interference, and entanglement. It is well known that quantum computing is capable of solving certain computational problems faster than classical computers. Applying quantum mechanics on machine learning [4, 21] is expected to have a performance on speeding up calculations. As for the classifier, quantum kernel method via support vector machine [10], among other development by different research groups [5, 9, 13, 15, 16, 18, 19, 22], has been attested a powerful mean of using high dimensional quantum state space. These studies show the possibility of machine learning using quantum computers, which may have a boost in the future.

However, a suitable feature map, corresponding to a suitable kernel, plays a big role in the kernel method. A quantum circuit is employed to produce a feature map and takes the dataset from its original low dimensional real space to high dimensional quantum state space, i.e., the Hilbert space [20]. In general, the quantum circuit should be designed to increase its capacity to explore the Hilbert space and encode probability distribution more efficient but also avoid expensive gate cost and circuit size to decrease quantum noise. Taking this into account, we apply the method that automatically generates quantum circuit proposed in [3], which automatically generates quantum feature maps by using multi-objective genetic algorithm [7] [12]. The objectives of last technique are both, to maximize the accuracy in the prediction over the test set - obtaining circuits with robustness and generalization power - and to minimize the size of the circuits in order to avoid expressivity problems and effects such as barren plateaus. In this technique, not only the circuit topology is optimized, but also the circuit parameters. The proposal presented in this work focus on the optimization of the genetic fitness function and its weights.

The paper is organized as follows. A brief review of support vector machine and quantum kernel method is presented in Section II. Section III describes the genetic algorithm for generating quantum circuits in more details, including how we encode the problem into binary strings and how we optimize the multi-objective fitness function. Section IV presents the results of applying the algorithm to three datasets: moonshape data, ad hoc data and a dataset generated by a specific group structure. Experimental results and comparisons will demonstrate that the algorithm produces low gate cost circuits while maintaining high classification accuracy. Finally, we draw our conclusions and summarize our learned lessons in Section V.

II. QUANTUM KERNELS

A. Support vector machine

SVM is a widely used classical supervised classification model in machine learning. Suppose we have a set of data points \( \{(x_i, y_i) | x_i \in \mathbb{R}^n, \ y_i = \pm 1\} \). SVM finds a pair of parallel hyperplane \( w \cdot x + b = \pm 1 \) that divides the data points into two classes, where the decision boundary corresponds to the hyperplane \( w \cdot x + b = 0 \) with orientation controlled by \( w \) and offset controlled by \( b \). The goal is to differ the data points by classes as much as possible, i.e., maximize the margin (distance) between the parallel hyperplane, where we can express the problem as \( \min_{w} \frac{1}{2} \|w\|^2 \) s.t. \( y_i (w \cdot x_i + b) \geq 1 \). The optimization problem for the primal problem can be formulated into Lagrange dual problem:

\[
\min_{\alpha} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j x_i^T x_j
\]

s.t. \( \sum_{i=1}^{n} \alpha_i y_i = 0 \) and \( \alpha_i \geq 0 \) for \( i = 1, 2, \ldots, n \).
max \( L(w, b, \alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j x_i x_j \)

s.t. \( \sum_{i=1}^{n} \alpha_i y_i = 0, \alpha_i \geq 0 \) \hspace{1cm} (1)

When the data points are not linearly separable, we use a feature map \( \phi \) to map the data into high dimensional space for more features or to low dimensional space to eliminate unimportant features. The kernel trick is to offer a more efficient and less expensive way to transform data into higher dimensions, where the data can be linearly separated in the higher dimensional space. The kernel function, denoted as \( K(x_i, x_j) = \phi(x_i) \phi(x_j) \), allows us to perform SVM by just knowing how to calculate the inner product of \( \phi(x_i) \) and \( \phi(x_j) \) instead of knowing what the feature map \( \phi \) is. In particular, the RBF kernel, i.e., the Gaussian kernel is often used. Applying the kernel trick, we can rewrite the Lagrange dual problem:

max \( L(w, b, \alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(x_i, x_j) \)

s.t. \( \sum_{i=1}^{n} \alpha_i y_i = 0, \alpha_i \geq 0 \) \hspace{1cm} (2)

B. Review of quantum kernel method

A big challenge in quantum machine learning is how we encode the classical information to quantum states for quantum computing. The kernel method can be implemented to quantum computing by considering the quantum circuit as an encoding function \( \Phi \) where the quantum feature map is defined as \( |\Phi(x)\rangle = U(x)|0^n\rangle \) and the kernel is naturally defined as \( K(x_i, x_j) = |\langle \Phi(x_i) | \Phi(x_j) \rangle|^2 \). This provides the data points to be mapped into quantum Hilbert space. Where, using quantum computer will have a big advantage. Using quantum circuits, a data \( x \in \mathbb{R}^n \) is mapped to an n-qubit quantum feature state \( \Phi(x) = U(x)|0^n\rangle|0^n\rangle U^\dagger(x) \) through a unitary circuit \( U(x) \), and we can use the circuit to calculate the kernel by:

\[
K(x_i, x_j) = |\langle \Phi(x_i) | \Phi(x_j) \rangle|^2 = |0^n\rangle U^\dagger(x_i) U(x_j) |0^n\rangle|^2 \hspace{1cm} (3)
\]

The kernel can be estimated on a quantum computer by evolving the initial state \( |0^n\rangle \) with \( U^\dagger(x_i) U(x_j) \) and counting the frequency of the \( 0^n \) outcome. As long as the quantum kernel \( K(x_i, x_j) \) can be computed efficiently, we can do optimization in the Hilbert space while other optimization steps can be performed on classical computer. For more details about quantum kernel estimation, please refer to [10]. Note that the ZZFeatureMap they provided is an unitary circuit defined as \( U = \hat{U}_\Phi(x) H^\otimes 2 \hat{U}_\Phi(x) H^\otimes 2 \), where \( \hat{U}_\Phi(x) = \exp(i\Phi_1(x)ZI + i\Phi_2(x)IZ + i\Phi_1,2(x)ZZ) \), is only suitable for a specific dataset. The main challenge is to seek suitable kernel function for different datasets, which led to researches on automatically learning kernels [3-8]. Furthermore, we are going to base ourselves on the quantum machine learning technique described in the work [3], in which it is presented a way to generate the unitary circuit \( U \) is what we aim to find through the evolutionary algorithm: genetic algorithm.

III. GENETIC ALGORITHM

A. Chromosome and Population

Genetic Algorithm (GA) is an evolutionary algorithm inspired by the process of natural selection, which has extensively been used to solve optimization problems. It does not guarantee to always find the exact optimal solution; nonetheless, it may find a near-optimal solution in a limited time. The evolution starts from a population of randomly generated chromosomes, and is an iterative process, with the population in each iteration called generation. In each generation, the fitness of every chromosome in the population is calculated. The more fit chromosomes are stochastically selected from the current population, and each chromosome’s gene is modified to form a new generation, then used in the next iteration of the algorithm.

A chromosome/DNA is a candidate/potential solution to the problem being solved, consists of a set of genes/numbers. Note that encoding problems to individual genes is often the hardest, a careful analysis between the circuit and numbers is necessary. We define gates per six bits from binary strings as a gene to generate quantum circuits. As is proposed in [3], the first three bits determine whether the gate is a Rotation gate, Hadamard gate, CNOT gate or identity gate, where any unitary operation can be approximated to Rotation gate, Hadamard gate and CNOT gate. Note that it is important to implement identity gates with some probability in order to reduce the number of circuit gates as appears in our base work. If the first three bits determine to be a Rotation gate, the last three bits determine a coefficient between \( [\pi/8, \pi] \) for the rotation parameter. As for the circuit size, we use 2-qubits in order to compare with ZZFeatureMap later. The \( i \)-th gate acts on \( i \mod 2 \) qubit, CNOT gate acts on \( i \mod 2 \) and \( i+1 \mod 2 \) specifically.

A set of solutions participating in the process of optimization is called population. We use the number of CPUs in order to efficiently multi-process. The model starts by generating a binary string with the size \( M \times N \times 6 \), where \( M \) is the number of chromosomes and \( N \) is the number of genes.
FIG. 1. Modified encoding example based on [3].

B. Fitness and Matting pool

Fitness is also considered as objective function or cost function. We pass a solution to this function and it returns the fitness of that solution. In the below multi-objective fitness function (5), we aim to both maximize the accuracy and minimize the gate cost. A common strategy for multi-objective problem is to find the pareto front [1] by choosing high domination points with crowd distance techniques, however, pareto front method does not suit our situation because high-accuracy performance is usually hard to find. If we don’t give more weight to the accuracy factor, the genetic algorithm will be influenced more by gate cost, thus it tends to find low-cost circuit rather than high-accuracy circuits. A pareto front method implement is available at my Github [25].

We recast the problem into a single objective function with weights and linear combinations of the factors. The accuracy is simply the mean accuracy of the given test data and label, with the QSVM model generated by a quantum circuit/chromosome. We use the gate cost proposed in [11], by counting the sequence of basic physical operations required for implementation on a quantum computer:

\[
\text{GateCost} = R_{\text{gate}} + 2H_{\text{gate}} + 5CNOT_{\text{gate}} \quad (4)
\]

With the two ingredients, we can define the multi-objective fitness function. Our main problem is to minimize the gate cost with a constraint of maximizing the accuracy. We consider the reciprocal of square of accuracy as the penalty function and replace the problem as follows, where \( w \) is a positive constant (penalty weight) that depends on different datasets.

\[
\text{Fitness} = \text{GateCost} + \frac{w}{\text{Accuracy}^2} \quad (5)
\]

The matting pool chooses the parents for the next generation. The simplest method is to first determine a pool size and then choose the best solutions based on the pool size. Normally genetic algorithm chooses parents and generate a set of chromosomes called offspring, then compare the offspring’s fitness and parent’s fitness to decide \( M \) chromosomes for the next generation’s population. We take the \( k \)-best chromosomes as parent to produce \( M - k \) chromosomes as offspring and put them together as the next generation’s population. The reason is because calculating the fitness, i.e., accessing high dimensional Hilbert space through quantum simulator takes a long time, we tend to reduce the times of calculating fitness. Note that the same chromosome’s fitness should be calculated in every generation, due to the fact that the accuracy are encoded by probability distribution, computing in every generation guarantees the stability of the outcome by a chromosome.

IV. RESULTS

A. Moonshape dataset

First, we consider the moonshape dataset generated by Sklearn [17]. 50 data points are scaled between \([-1, 1]\) as a preprocessing step, and randomly split into a training (80%) and test (20%) sets. As illustrated in Figure 2, we optimize the circuits with 200 generations and an early stop of 24, using a population of 12 chromosomes with each 10 genes.

FIG. 2. Moonshape dataset.

We choose the weight \( w = 20 \) in equation (5) because the data here is rather simple, which we do not put much emphasize on the accuracy factor. The genetic algorithm produces the simple uncorrelated circuit with low gate cost and perfect accuracy as illustrated in Figure 3. If we choose lower weight, the algorithm will produce some circuit with only one gate cost but an accuracy of 0.8, due to the fact that this particular circuit’s fitness is lower than any other circuits with perfect accuracy. If we choose higher weight, the algorithm will eventually find the optimal solution but with more time cost. Note that the circuit can be optimized if the gates share the same rotation axis and parameter, and can be combined to a single rotation gate with additional angles. Comparing with the results presented in [3], both algorithm found perfect classification accuracy, but we have a lower gate cost due to the addition of penalty weight.
Because of the expensive cost of entangling gates makes the genetic algorithm prefer circuits that have smaller clusters of uncorrelated qubits [3]. This shows the power of individual qubits for quantum classifier [23]. As explained in [3], the circuit that can be decomposed to separate unitaries, which the kernel is also a scalar product of separate kernels, as $K(x_i, x_j) = \prod_{k=1}^{n} K_k(x_i, x_j)$. For example, we plot the decision boundary of two qubit’s kernel separately in Figure 3, with corresponding test score 0.8, 0.7. Qubit one $q_0$ shows that RZ gate’s effect cannot be seen in single qubit operation. Qubit two $q_1$ shows that large angle of RY (or RX) gives periodic separation. Together, the nonlinear combination of the two qubits give the right predictions, verifying the original technique approach [3].

We test the circuit with 150 data points and also obtain perfect accuracy, moreover, we compare the quantum kernel result with linear kernel and Gaussian kernel, which indicates a big advantage of QSVM.

B. Adhoc dataset

Secondly, we consider the ad hoc data generated by Qiskit [2]. Again, 50 data points are randomly split into a training (80%) and test (20%) sets. As illustrated in Figure 5, we optimize the circuits with 200 generations and an early stop of 20, using a population of 12 chromosomes with each 20 genes.

We choose the weight $w = 40$ in equation 4 because the data here is more complex, which we need to put more emphasis on the accuracy factor. Again, we obtain perfect accuracy and we compare the circuit with ZZFeatureMap [10], though ZZFeatureMap will always get perfect accuracy because the Ad hoc dataset is generated by ZZFeatureMap. We have an advantage by gate cost 11 in compare with ZZFeatureMap’s gate cost is 34 as illustrated in Figure 6. With lots of experiments, we observe that with perfect accuracy circuits, more gate cost circuit makes the QSVM model more over fitting. If we compare the results here with pareto front method implement, it is clear that without defining the importance of the two objectives, pareto front method’s model is highly influenced by gate cost while high accuracy solutions are hard to find. More details are available at my Github [25].
TABLE I. Comparing classification methods.

| Method                  | Moonshape | Ad hoc |
|-------------------------|-----------|--------|
|                         | Accuracy  | Gate cost | Accuracy  | Gate cost |
| SVM linear              | 73.3%     | 30.0%   |           |           |
| SVM Guassian            | 76.6%     | 70.0%   |           |           |
| QSVM ZZFeatureMap       | 73.3%     | 34      | 100%      | 34        |
| QSVM multi-objective    | 100%      | 4       | 100%      | 11        |
| QSVM pareto-front       | 100%      | 4       | 70.0%     | 5         |

C. Covariant quantum kernel dataset

Thirdly, due to the fact that our model is an algorithm "finding" a suitable kernel, we compare our model with quantum kernel training [9], which is also designed to find a proper kernel via trainable parameters. Because our dataset does not fit the group structure with the circuit they designed, we try to compare by implementing our model to their dataset [2] with 14 features generated by specific group cosets.

Table II. Comparison with covariant kernel.

| Quantum covariant kernel | QSVM multi-fitness |
|-------------------------|---------------------|
| Accuracy                | 100%                |
| Gate cost               | 51                  |
|                        | 41 → 3              |

After experiments, we found a circuit with the gate cost of 41 and perfect accuracy, the rotation gates on the left side of the barrier are identity gates and can be ignored. It is obvious that the 4 Hadamard gates at the last qubit does not effect and can be removed to decrease the gate cost to 33. The circuit has already outperformed covariant quantum kernel’s circuit, due to the fact that their circuit is with the gate cost of 51 (21 R gates and 6 CZ gates). Moreover, the circuit can be optimized as shown in Figure 7, we test the necessity of each rotation gate where only 3 are essential, 2 among them can be added on the same qubit in order to decrease the size of circuit. As a result, we optimized the circuit to a simple uncorrelated circuit with the gate cost of 3 and perfect classification accuracy. More details are available at my Github [26].

V. CONCLUSION

In this work, we optimize the quantum feature map of QSVM using multi-objective genetic algorithm. Based on the technique proposed in [3], this work, has focused on improvements over the fitness function and the objectives weights. A quantum circuit is generated by modifying the technique proposed in [3] as a feature map that maps the data points into Hilbert space, and then classified with quantum kernel method applied QSVM. The algorithm modified in this study [3], aims to maximize the accuracy of QSVM while minimizing the gate cost of quantum circuit with a multi-objective fitness function. We have improved the fitness function that the original technique uses, shown improvements on three different datasets, a simpler moonshape dataset, a more complex ad hoc dataset and a specifically generated dataset for comparison. We all found perfect accuracy of classification through modifying this fitness function on the Anitares-López et al. 2021 algorithm [3], where more complex dataset is needed to increase the penalty weight w to decrease the influence of gate cost. Moreover, all circuits are with low-cost gate and without correlations as stated in [3], which we believe single qubits or linear combination of single qubits are powerful for generating quantum feature maps.

There are many more things to explore, including testing the circuit by variational quantum classifier (VQC), quantum neural network (QNN) or quantum distance-based classifier. Adding trainable parameters θi to the circuit that can be optimized using SPSA is also another strategy. We believe it is possible to find suitable feature maps that classification can be well-performed in the Hilbert space.
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