Generating quantum feature maps for SVM classifier

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We present and compare two methods of generating 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. The first method is a genetic algorithm with 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. The second method uses variational quantum circuit, focusing on how to construct the ansatz based on unitary matrix decomposition. Numerical results and comparisons are presented to demonstrate how the fitness function reduces gate cost while remaining high accuracy and conducting circuit through unitary matrix obtains even better performance. In particular, we propose some thoughts on reducing and optimizing the gate cost of a circuit 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 [3,27] 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 [5,9,16,18,20,22,24,28], 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 [25]. 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 first modified the method proposed in [3], which automatically generates quantum feature maps by using multi-objective genetic algorithm [7,15] both to maximize the accuracy and to minimize the size of the circuits. Then, we proposed another method learning through parameterized variational circuit [12] with different ansatz constructed by unitaty decomposition [11,13,23,29].

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 in more details, including how we encode the problem and how we optimize the multi-objective fitness function. Section IV explains the variational method we proposed, using hardware efficient ansatz and unitary decomposition ansatz. Section V presents the results of applying the algorithm to three datasets: moonshape data, ad hoc data and a dataset generated by a specific group structure. Finally, we draw our conclusions and summarize our learned lessons in Section VI.

II. QUANTUM KERNELS

A. Support vector machine

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

\[
\max \frac{1}{2} \|w\|^2 \text{ s.t. } y_i(w \cdot x_i + b) \geq 1.
\]

The optimization problem for the primal problem can be formulated into Lagrange dual problem:

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

s.t. \( \sum_{i=1}^{n} \alpha_i y_i = 0, \; \alpha_i \geq 0 \) (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. 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 \cite{25}, 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 $\Phi(x) = U(x)(0^n)(0^n)^\dagger U(x)$ through a unitary circuit $U(x)$, and we can employ the circuit to evaluate the kernel by:

$$K(x_i, x_j) = |\langle \Phi(x_i) | \Phi(x_j) \rangle|^2 = |\langle 0^n | U^\dagger(x_i) U(x_j) | 0^n \rangle|^2$$ \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 \cite{10}. Note that the ZZFeatureMap they provided is an unitary circuit defined as $U = \tilde{U}_\Phi(x) H^{\otimes 2} \tilde{U}_\Phi(x) H^{\otimes 2}$, where $\tilde{U}_\Phi(x) = \exp(i\Phi_1(x)ZI + i\Phi_2(x)IZ + i\Phi_{1,2}(x)ZZ)$, 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 \cite{3,8}.

III. GENETIC ALGORITHM

Genetic Algorithm is a evolutionary algorithm inspired by the process of natural selection, which has extensively been used to solve optimization problems. The evolution starts from a population of randomly generated chromosomes, with the population in each iteration called generation. The fitness of every chromosome in the population is calculated, selected from the current population, and each chromosome’s gene is modified to form a new generation for the next iteration of the algorithm.

A. Chromosome and Population

A chromosome is a 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 modified the encoding method \cite{4} as follows, 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. 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. We added more bits to determine the rotation angle for more precisely results. 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.

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 \cite{7}, 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 \cite{1} by choosing high domination points with crow 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 model will be influenced more by gate cost, thus it tends to find low-cost circuit rather than high-accuracy circuits. The accuracy is simply the mean accuracy of the given test data and label, with the QSVM model generated by a quantum circuit. We use the gate cost proposed in [14], 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.

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

The mating 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. Note that the same chromosome’s fitness should be calculated in every generation, due to the fact that the accuracy is encoded by probability distribution, computed in every generation guarantees the stability of the outcome by a chromosome. For the mutation operation, we set a probability at 80% to randomize a chromosome outcome by a chromosome. For the mutation operation, putting in every generation guarantees the stability of the accuracy are encoded by probability distribution, computed in every generation, due to the fact that the size. Note that the same chromosome’s fitness should be encoded more by gate cost, thus it tends to find low-cost circuit rather than high-accuracy circuits. The accuracy is simply the mean accuracy of the given test data and label, with the QSVM model generated by a quantum circuit. We use the gate cost proposed in [14], by counting the sequence of basic physical operations required for implementation on a quantum computer:

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### IV. VARIATIONAL ANSATZ

In quantum mechanics, every quantum circuit is equivalent to an unitary matrix. Because that the feature map is calculated by a quantum circuit, it is also calculated by a specific unitary matrix, which our goal is to find the unitary matrix corresponding to a feature map that suits the dataset. We propose two ways to construct a variational quantum circuit with learnable parameters in order to find the unitary matrix.

#### A. Hardware Efficient Ansatz

We use the hardware efficient ansatz, which is spanned by special unitaries andentangle layers, proposed in [12]. This ansatz is often used as the parameterized circuit for variational quantum eigensolver [19], consisting of a RY gate layer, RZ gate layer, then a CNOT gate layer. One can simply add the depths by repeating the layers where the ansatz usually ends with the rotation layer. We encode the linear combination of the data points as the parameter of each rotation gate. An one depth 2-qubit feature map can be formulated as follow:

\[
(e^{I\phi_1 Z} \otimes e^{I\phi_2 Z})(e^{I\phi_3 Y} \otimes e^{I\phi_4 Y})
\]

\[
\phi_j = a_j x_1 + b_j x_2
\]

\[
\text{FIG. 2. Hardware efficient ansatz.}
\]

After the circuit is constructed, we set the accuracy of the QSVM model as the cost function and update the parameters through classical optimizer COBYLA (constraint optimization by linear approximation). Note that COBYLA only performs one objective function evaluation per optimization iteration.

#### B. Unitary Decomposition Ansatz

Due to the fact that quantum circuits are equivalent to unitary matrices, we use the unitary decomposition ansatz proposed in [23] in order to produce arbitrary unitaries. Given an even size unitary matrix \( M \), which the matrix we want to encode to a quantum circuit is always the size of \( 2^k \), it can be decomposed to smaller unitaries \( L_1, L_2, R_1, R_2 \) and diagonal matrices \( C, S \) with the size of \( 2^{k-1} \) by Cosine-Sine Decomposition such that \( C^2 + S^2 = I_{2^{k-1}} \), as below:

\[
M = \begin{bmatrix} L_1 & 0 \\ 0 & L_2 \end{bmatrix} \begin{bmatrix} C & -S \\ S & C \end{bmatrix} \begin{bmatrix} R_3 & 0 \\ 0 & R_2 \end{bmatrix}
\]

(7)

The cosine-sine matrix is in the form of multiplexor gate, while the left and right factor can further be decomposed. Given an unitary matrix \( X \) with the form of \( X_1 \oplus X_2 \), it can be decomposed to \( (I \otimes V)(D \oplus D^\dag)(I \otimes W) \) where \( D^2, V \) are the eigenvalues and eigenvectors of the marix \( X_1 X_2^\dag \), that is,

\[
\begin{bmatrix} X_1 & 0 \\ 0 & X_2 \end{bmatrix} = \begin{bmatrix} V & 0 \\ 0 & V \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & D^\dag \end{bmatrix} \begin{bmatrix} W & 0 \\ 0 & W \end{bmatrix}
\]

(8)

\( V, W \) are now smaller unitary matrices and the diagonal matrix is also in the form of multiplexor gate. The whole process is called the Quantum Shannon Decomposition, please refer to [23] for more details. At last, the single qubit unitary matrices can be decomposed by Euler Decomposition (ZYX Decomposition). Again, We encode the linear combination of the data points as the parameter of every rotation gates. A 2-qubit feature map can be formulated as follow:
\[ U_{\phi_1,2,3} M_{R_Z \phi_4,5} U_{\phi_{6,7,8}} M_{R_Y \phi_{9,10}} U_{\phi_{11,12,13}} M_{R_Z \phi_{14,15}} U_{\phi_{16,17,18}} \]
\[ U_{\phi_{j,j+1,j+2}} = \exp(i\phi_j I_Z + i\phi_{j+1} I_Y + i\phi_{j+2} I_Z) \]
\[ \phi_j = a_j x_1 + b_j x_2 \]  

(9)

FIG. 3. Unitary decomposition ansatz.

V. RESULTS

A. Moonshape dataset

First, we consider the moonshape dataset generated by Sklearn [21]. By using genetic algorithm, we choose the weight \( w = 20 \) in equation (5) because the data here is rather simple, which we do not put much emphasis on the accuracy factor. The genetic algorithm produces the simple uncorrelated circuit with low gate cost and perfect accuracy as illustrated in Figure 4. If we choose lower weight, the algorithm will produce some circuit with only one gate cost but a lower accuracy, 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.

FIG. 4. Moonshape data using genetic algorithm.

By using variational circuits, both hardware efficient ansatz and unitary decomposition produce perfect accuracy. For hardware efficient ansatz, we choose to use only one depth such that the circuit’s gate cost is only 4, again the data here is rather simple. A disadvantage of unitary decomposition ansatz is its high gate cost, unlike hardware efficient ansatz, the circuit is fixed.

FIG. 5. Moonshape data using hardware efficient ansatz.

FIG. 6. Moonshape data using unitary decomposition ansatz.

B. Adhoc dataset

Secondly, we consider the ad hoc data generated by Qiskit [2]. For genetic algorithm, we choose the weight \( w = 80 \) in equation 4 because the data here is more complex, which we need to put more emphasize on the accuracy factor. We obtain 90\% 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 is 23 in compare with ZZFeatureMap’s gate cost is 34 as illustrated in Figure 7. From lots of experiments, we observe that with high accuracy circuits, more gate cost circuit makes the QSVM model more over fitting.

For variational circuits, hardware efficiency ansatz has produced an accuracy of 92.5\%, while unitary decomposition ansatz has reached almost perfect accuracy with 97.5\%. We choose to use four depths of hardware efficient ansatz in order to have similar numbers of parameters with unitary decomposition ansatz, and it turns out that with more complex datasets, unitary decomposition ansatz have better performance in general.

We compared different kernels and quantum feature map generating methods together, the RBF (Gussian) kernel can already obtain well performance with simple datasets and using ZZFeatureMap for the quantum kernel is only suitable for the ad hoc dataset. Comparing genetic algorithm (GA), hardware efficient ansatz (HE) and unitary decomposition ansatz (UD), genetic algorithm works well with simple datasets and can efficiently
FIG. 7. Ad hoc dataset using genetic algorithm (left) and ZZFeatureMap (right).

FIG. 8. Ad hoc dataset using hardware efficient ansatz.

decrease the gate cost, but with more complex datasets, it is hard to find global solution and consumes a lot of time. Hardware efficient ansatz is flexible with gate cost by choosing suitable depths, and have slightly better accuracy than genetic algorithm. Unitary decomposition ansatz has the best accuracy overall, but has the disadvantage of high fixed gate cost.

FIG. 9. Ad hoc dataset using unitary decomposition ansatz.

TABLE I. Comparing classification methods.

| Method      | Moonshape acc | Ad hoc acc | gate cost | time | gate cost | time  |
|-------------|---------------|------------|-----------|------|-----------|-------|
| SVM-linear  | 80.0%         | 60.0%      |           |      |           |       |
| SVM-RBF     | 100% ($\gamma = 0.5$) | 80.0% ($\gamma = 8$) |           |      |           |       |
| QSVM-ZZ     | 50.0%         | 34         | 100%      | 34   | 100%      | 34    |
| QSVM-GA     | 100%          | 3          | 66.30s    | 90.0%| 23        | 2067.96s |
| QSVM-HE     | 100%          | 4          | 33.51s    | 92.5%| 31        | 197.68s |
| QSVM-UD     | 100%          | 38         | 209.61s   | 97.5%| 38        | 220.06s |

C. Covariant quantum kernel dataset

Thirdly, we compare our genetic algorithm 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                 |

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 11, we test the necessity of each rotation gate in order to check if every feature is useful, and it turns out that only 4 features are essential here. Again, it is trivial to remove qubits without feature parameters involved, the last qubit without any gates and the two qubits with only a Hadamard gate and CNOT gate can be removed. We repeat the steps before, as we found that the two Hadamard gates and CNOT gates can also be
removed, that leaves 4 rotation gates. Again, 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 [30].

FIG. 11. Optimizing circuit.

VI. CONCLUSION

In this work, we optimize the quantum feature map of QSVM using genetic algorithm and quantum variational circuit. A quantum circuit is generated as a feature map that maps the data points into Hilbert space, and then classified with quantum kernel method applied QSVM. The genetic 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. The variational circuit learns through parameters with a given ansatz, based on special unitary groups and unitary matrix decomposition. We test our models on three different datasets, a simpler moonshape dataset, a more complex ad hoc dataset and a specifically generated dataset for comparison. We all found high accuracy of classification, where more complex dataset is needed to increase the penalty weight $w$ to decrease the influence of gate cost or increase the circuit depth in order to have more learnable parameters.

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 $\theta_i$ 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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