

### Introduction to Quantum Machine learning

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### **Overview**



# <span id="page-2-0"></span>Introduction---IBM Quantum Computer





IBM has ambitious pursuits:

- 433-qubits IBM Quantum Osprey
- Three times larger than the Eagle processor (127-qubits)
- Going up to 10k-100k qubits.

### Credited to Thomas Prior for **TIME**<br>Now, IBM provides up to 127 qubits for free.



#### 2024/8/4 Qiyu Sha qsha@cern.ch 3

# Introduction---Origin Quantum Computer





Origin wuyuan:

- The first "practical quantum computer" in China.
- 24-qubits with own control system.

#### Origin wuyuan provide up to 6 qubits for free.



### **Overview**



# Outline of today

### **Applications of quantum computing in HEP**

- Simulation
	- Parton shower correlations
	- Lattice QCD
- Reconstruction
	- Particle tracking
- Analysis
	- Higgs analyses
	- SUSY search
	- $^{\circ}$  …

### Progress has been very rapid here.

### **Simulation**



#### Reconstruction



**Analysis** 



# Outline of today

## **Theory**



## **Experiment**



# Outline of today

### **Theory**





## Introduction---SVM

[SVM](http://luojinping.com/2018/04/14/Stanford-Machine-Learning-7-SVM/): Max margin

Usually done using the dual(think Lagrangian multipliers)

Results in building a kernel matrix.  $f(K_{1,2})$ 





### Introduction---SVM feature map



### Introduction---SVM code

import numpy as np from sklearn import datasets from sklearn.model selection import train test split from sklearn.preprocessing import StandardScaler from sklearn.svm import SVC from sklearn.metrics import classification report, accuracy score

#### # 加载数据集

 $iris = datasets.load iris()$  $X = iris.data$  $y = iris.target$ 

# 数据集拆分 X train, X test, y train, y test = train test split(X, y, test size=0.3, random state=42)

#### # 数据标准化

scaler = StandardScaler()  $X train = scalar.fit transform(X train)$  $X$  test = scaler.transform $(X$  test)

# 训练SVM模型  $model = SVC(kernel='linear', C=1.0)$ model.fit(X train, y train)

# 预测  $y$  pred = model.predict(X\_test)

# 评估模型

print(classification\_report(y\_test, y\_pred)) print('Accuracy:', accuracy\_score(y\_test, y\_pred))

### What we can do?



### What we can do?

#### <https://arxiv.org/abs/2212.07279>



### **Classical**

### Quantum

#### 2024/8/4 Qiyu Sha qsha@cern.ch 13



➢ Env: source /hpcfs/cepc/higgsgpu/shaqy/miniconda/etc/profile.d/conda.sh Conda activate Qiskit

### [SVC](https://scikit-learn.org/stable/modules/svm.html#custom-kernels):

1. use your own defined kernels by passing a function to the kernel parameter.

2. You can pass pre-computed kernels by using the kernel='precomputed' option. You should then pass Gram matrix instead of X to the fit and predict methods. The kernel values between all training vectors and the test vectors must be provided:

```
>>> import numpy as np
>>> from sklearn import svm
>>> def my kernel(X, Y):
       return np.dot(X, Y.T)>>> clf = svm.SVC(kernel=my kernel)
```

```
>>> import numpy as np
>>> from sklearn.datasets import make classification
>>> from sklearn.model selection import train test split
>>> from sklearn import svm
>>> X, y = make classification(n samples=10, random state=0)
>>> X train, X test, y train, y test = train test split(X, y, random state=0)
>>> clf = svm.SVC(kernel='precomputed')
>>> # linear kernel computation
>>> gram train = np.dot(X train, X train.T)
>>> clf.fit(gram train, y train)
SVC(kernel='precomputed')
>>> # predict on training examples
>>> gram_test = np.dot(X_test, X_train.T)
>>> clf.predict(gram test)
array([0, 1, 0])
```
# Data encoding and processing



Operator

 $Gate(s)$ 

Matrix

 $\blacklozenge$  Encoding the  $e^+e^-$  →  $ZH \rightarrow q\bar{q}\gamma\gamma$  (signal) and  $e^+e^ \rightarrow$   $(\frac{Z}{\gamma^*})\gamma\gamma$  (background)

◆ Six variables are passed through preliminary mapping and then passed to a quantum circuit for evaluation.

◆The Quantum support-vector machines kernel (QSVM-Kernel) is evaluated for each data point and the rest.

## Feature map and quantum kernel estimation

Quantum feature map determines the QSVM-Kernel:

- ➢ Identical layers
- $\triangleright$  Single-qubit rotation gates
- $\triangleright$  Two-qubits CNOT entangling gates







QSVM-Kernel estimation:

- ➢ Using 6 variables mapped to 6-qubit
- $\triangleright$  The expectation of each data point

$$
k(\vec{x_i}, \vec{x_j}) = \left| \left\langle 0^{\otimes N} \right| \mathcal{U}_{\Phi(\vec{x_i})}^{\dagger} \mathcal{U}_{\Phi(\vec{x_j})} \left| 0^{\otimes N} \right\rangle \right|^2
$$

## AUCs as function of the event

- ➢ The QSVM-Kernel and classical SVM classifiers with different dataset size from 1000 to 12500 events.
- ➢ The quoted errors are the standard deviations for AUCs calculated from several shuffles of the dataset.





# Performance of the quantum simulator

- ➢ The performance of the QSVM-Kernel using State-vector-simulator from IBM and the classical SVM.
- ➢ Use 12500 events for both signal and backgrounds.



## Performance of the real quantum computers

- ➢ IBM Nairobi & Origin Wuyuan quantum computer hardware
- $\triangleright$  Use 100 events for both signal and backgrounds.
- $\triangleright$  Use 6 qubits.



IBM Nairobi quantum

Origin Wuyuan quantum



Set up:  $\triangleright$  pip install Linux pyqpanda software version GCC  $>= 5.4.0$ Python  $>= 3.7.0 \& 6 = 3.9.0$ 

### Requirements:  $\triangleright$  [Official Tutorial: pyQPanda](https://pyqpanda-toturial.readthedocs.io/zh/latest/index.html)

- ➢ Code path: /cefs/higgs/shaqy/Quantum/QC\_HEP/For\_tutorial
- ➢ Env: source /hpcfs/cepc/higgsgpu/shaqy/miniconda/etc/profile.d/conda.sh conda activate QT\_re (conda deactivate)

### $\triangleright$  Everything is similar as IBM:

Different: Wuyuan don't have enough built-in functions like QSVM. We need to do by ourself.

➢ Only three steps: Use IBM Qiskit to generate QSVM kernel (gen\_qasm.py shown in the [next page](#page-20-0).)



#### <span id="page-20-0"></span>Same as IBM tutorial:

f.close()

### Create a feature map and kernel using Qiskit Different part: (In red frame.)

def gen\_qasm():  $seed = 2022$ backend = BasicAer.get backend("statevector simulator") feature map cus = customised feature maps.FeatureMap(num qubits=6, depth=1, degree=1, entanglement='full', inverse=False) for  $i$  in range $(1)$ :  $seed = 2022$ algorithm\_globals.random\_seed = seed data = pd.read  $\text{csv}$  "sample %d.csv" % i) train =  $data[0:100]$ test =  $data[100:200]$  $train\_label = train.pop('tag')$  $test\_label = test.pop('tag')$ train data = train. to numpy()  $test_data = test.to_number()$ X\_train = train\_data  $X_test = test_data$ q\_backend = QuantumInstance(backend, shots=10, seed\_simulator=None, seed\_transpiler=None) q\_kernel = QuantumKernel(feature\_map=feature\_map\_cus, quantum\_instance=q\_backend) qsvm\_kernel\_matrix\_train = q\_kernel.evaluate(x\_vec=X\_train) qsvm\_kernel\_matrix\_test = q\_kernel.evaluate(x\_vec=X\_test, y\_vec=X\_train) kernel\_train\_IBM = np.asmatrix(qsvm\_kernel\_matrix\_train) kernel\_test\_IBM = np.asmatrix(qsvm\_kernel\_matrix\_test)  $x =$  ParameterVector('x', length=6)  $y = ParameterVector('y', length=6)$  $circuit = q_kernel.comstruct_circuit(x,y)$  $circuit = q_backend.trainspile(circuit)[0]$ for  $i$  in range $(100)$ : for  $j$  in range $(100)$ :  $f = open("all_qasm_train/qasm_Md_M.txt"$(i,j), 'w')$ cirtemp = circuit.assign\_parameters({x:X\_train[i], y:X\_train[j]}, inplace=False)

2024/8/4 Qiyu Sha shaqiyu@ihep.ac.cn 21

- $\triangleright$  Save the dataset into a file(txt or .csv)
- $\triangleright$  For different (i,j) in train/test dataset:
	- ➢ Generate a QASM file.
	- $\triangleright$  One file represent a feature map for one point in kernel matrix.

```
OPENOASM 2.0:
include "gelib1.inc";
qreg q[6];
creg C[6];u2(0, pi) q[0];
rz(0.522150994) q[0];u3(0.261075497, 0.0, 0.0) q[0];
u3(0.658964753, 0.0, 0.0) q[0];
rz(1.317929506) q[0];
u2(0, pi) q[0];u2(0, pi) q[1];rz(0.845885038) q[1];u3(0.422942519,0.0,0.0) q[1];
u3(0.0224528909,0.0,0.0) q[1];
rz(0.0449057818) q[1];u2(0, pi) q[1];
```
- $\triangleright$  Apply a key in the OriginQ website. (One key can run 1000 jobs in one day.)
- ➢ Apply X qubits and classical bits which used to save the result.
- ➢ Convert QASM to program.
- ➢ Use real\_chip\_type:origin\_wuyuan\_d5 to run. (Only d4 and d5 can use, d5 is better)
- $\triangleright$  The value with  $[′00000′]$  is the point of  $\cdot$ kernel matrix. Save it.

```
from pygpanda import *
def run(i, j):
    QCM = QCIoud()QCM.init_qvm("58DCD70A14814A4DB73ACF5C8F854FA2"
    glist = QCM.qAlloc_many(5)clist = QCM.cAlloc_max(5)qvm = init_quantum_machine(QMachineType.CPU)
   qvm.init_qvm()
    prog_trans, qv, cv = convert_gasm_to_gprog("all_gasm_train/gasm_%d_%d.txt"%(i,j), qvm)
      result = QCM.read chip measure (prog trans, 10000, real chip_type.cright_wuyuan_d5)except:
      print("job %d %d failed" % (i,j))
     return
    value = result['00000']f = open("results_train_try/result_%d_%d.txt" %(i,j),'w')
    f.write(str(value))
    f.close()
if name ==" main ":
 for i in range(19,20):
    for j in range(i+1, 100):
      run(i, j)
```
#### $\triangleright$  Import the kernel matrix.

```
score = []for i in range(1):
  data = pd.read_csv("sample_Md.csv" % i)train = data[0:100]test = data[100:200]train\_label = train.pop('tag')test\_label = test.pop('tag')train_label_oh = label_binarize(train_label, classes=[1,-1])
   test label oh = label binarize(test label, classes=[1,-1])
   test kernel = [1]for i in range(100):
    test kernel line = [1]for j in range(100):
      value = get_{\text{general}(i, j, 'test')}test kernel line.append(value)
     test_kernel.append(test_kernel_line)
   test_kernel_array = np.array(test_kernel, np.float32)
   train_kernel = [1]for i in range(100):
    train_{\text{general}_\text{line}} = []for j in range(100):
       if i = i:
         train_kernel_line.append(1.0)
       else:
         if i > j:
           value = get_{\text{general}(j,i,'train')}train_kernel_line.append(value)
         else:
           value = get_{\text{general}(i,j,'train')}train_kernel_line.append(value)
   | train_kernel.append(train_kernel_line)                 Qiyu Sha shaqiyu@ihep.ac.cn                         23<br>train_kernel_array = np.array(train_kernel, np.float32)         Qiyu Sha shaqiyu@ihep.ac.cn
```
➢ Then use the classical svc to get the final results, generate AUC value and draw plots.

#QSVM svc = SVC(C=30, probability=True, kernel="precomputed") csvc = svc.fit(train\_kernel\_array, train\_label) predictions = csvc.predict\_proba(test\_kernel) fpr, tpr,  $=$  sklearn.metrics.roc\_curve(test\_label\_oh, predictions[:, 0])

### Quantum transformer

### ➢ Quantum Transformer:

- ➢ At the core of any Transformer sits the so-called *Multi-Headed Attention.*
- We apply three different linear transformations  $W_Q$ ,  $W_K$ , and  $W_V$ , to each element of the input sequence to transform each element embedding into some other internal representation states called Query (Q), Key (K) and Value (V). These states are then passed to the function that calculates the attention weights, which is simply defined as:

$$
Attention(Q, K, V) = softmax_k(\frac{QK^T}{\sqrt{d_k}})V
$$

➢ To promote the Transformer from the classical to quantum real, one can simply replace the linear transformations  $W_0$ ,  $W_K$ , and  $W_V$  with variational quantum circuits.



### Code detail

#### [Quantum transformer](https://github.com/shaqiyu/Quantum_transformer/blob/main/Qtransformer.py): (This code following [here](https://arxiv.org/pdf/2110.06510.pdf))

- [The MultiHeadAttentionQuantum](class MultiHeadAttentionQuantum(MultiHeadAttentionBase):) block
- Change the linear transformations.

class MultiHeadAttentionClassical(MultiHeadAttentionBase):

def \_init\_(self,

embed\_dim: int,

num\_heads: int,  $droput=0.1$ ,

mask=None,

use\_bias=False):

super(MultiHeadAttentionClassical, self). init (embed\_dim=embed\_dim, num\_heads=num\_heads, dropout=dropout, mask=mask, use\_bias=use\_bias)

self-k\_linear = nn.Linear(embed\_dim, embed\_dim, bias=use\_bias) self.q\_linear = nn.Linear(embed\_dim, embed\_dim, bias=use\_bias) self.v\_linear = nn.Linear(embed\_dim, embed\_dim, bias=use\_bias) self.combine\_heads = nn.Linear(embed\_dim, embed\_dim, bias=use\_bias) elf.head\_dim = embed\_dim // num\_heads

def forward(self, x, mask=None):

batch\_size, seq\_len, embed\_dim = x.size() assert embed\_dim == self.embed\_dim, f"Input embedding ({embed\_dim}) does not match layer embedding size ({self.embed\_dim})"

 $K = self.k_1 \in (x)$ 

 $Q = self.q_1 \text{linear}(x)$ 

 $V = self.v_linear(x)$ 

x = self.downstream(Q, K, V, batch\_size, mask)  $output = self.compile\_heads(x)$ return output

 $self.n_qubits = n_qubits$  $self.n$  glayers = n glayers  $self.q$  device =  $q$  device  $self. head$  dim = embed dim // num heads if 'qulacs' in a device: self.dev = qml.device(q\_device, wires=self.n\_qubits, gpu=True) elif 'braket' in q device: self.dev = qml.device(q\_device, wires=self.n\_qubits, parallel=True) else: self.dev = qml.device(q device, wires=self.n qubits) def circuit(inputs, weights): for i in range(n qubits): aml.Hadamard(wires=i) qml.AngleEmbedding(inputs, wires=range(n qubits)) qml.BasicEntanglerLayers(weights, wires=range(n qubits)) return [qml.expval(qml.PauliZ(wires=i)) for i in range(n\_qubits)]

self.qlayer = qml.QNode(\_circuit, self.dev, interface="torch") self.weight\_shapes = {"weights": (n\_qlayers, n\_qubits)}

#draw plots

weights = np.random.random([n\_qlayers, n\_qubits])

 $X = np.random.randn(6)$ 

print(qml.draw(self.qlayer, expansion\_strategy="device")(X,weights))

print(f"weight\_shapes = (n\_qlayers, n\_qubits) = ({n\_qlayers}, {self.n\_qubits})")

self\_k\_linear = qml.qnn.TorchLayer(self.qlayer, self.weight shapes) self.q\_linear = qml.qnn.TorchLayer(self.qlayer, self.weight\_shapes) self.v\_linear = qml.qnn.TorchLayer(self.qlayer, self.weight\_shapes) self.combine\_heads = qml.qnn.TorchLayer(self.qlayer, self.weight\_shapes)

### Quantum transformer model

- We make use of Xanadu's PennyLane quantum machine learning library to add quantum layers.
	- Add a function to the class and performs the quantum calculation (with a circuit).
	- Wrap this circuit with a "QNode" to tell TensorFlow how to calculate the gradient with the [parameter-shift](https://pennylane.ai/qml/glossary/parameter_shift)



- Finally, we create a KerasLayer to handle the I/O within the hybrid neural network.( $W_0$ ,  $W_K$ , and  $W_V$ )
- Other part is same as the classical transformer.
- [https://github.com/shaqiyu/Quantum\\_transformer](https://github.com/shaqiyu/Quantum_transformer)

### How to work

#### ➢ Download miniconda

➢ conda create -n env\_name(Change the name as you want) root==6.24.00 python=3.8.6 -c conda-forge

 $\rho$  pip install -r requirment/\*

Or:

source /hpcfs/cepc/higgsgpu/shaqy/miniconda/etc/profile.d/conda.sh

conda activate QT\_re

 $\triangleright$  Python train test.py (Change the option)

#### $if __name__ == '__main__':$



#### Num\_dataset = 20000

if args.n\_qubits\_transformer > 0: Type\_model = "Quantum" else: Type\_model = "Classical"

### Quantum transformer

- $\triangleright$  The dataset we used now is the CEPC MC sample
	- $e^+e^-$  → ZH →  $q\bar{q}$ γγ (signal) and  $e^+e^-$  →  $(Z/\gamma^*)\gamma\gamma$  (background)
- Simulator: Pennlylane default device.
	- Time consuming:  $O(n)$ , ~80 mins in CPU for 10k dataset with one epoch and one block(Q layer).
- ➢ Current results (Use CPU): ~76% acc on validation dataset both in Quantum transformer and classical transformer in 20k dataset (10k train, 10k val).

Quantum: Epoch 8/30 Info in <TCanvas::Print>: pdf file ./plot/ROCs/ROC 10000 train.pdf has been created Info in <TCanvas::Print>: pdf file ./plot/ROCs/ROC 10000 val.pdf has been created Epoch: 08 | Epoch Time: 140m 18s Train Loss: 0.510 | Train Acc: 76.24% Val. Loss: 0.500 | Val. Acc: 76.52%

Classical:

Epoch  $10/10$ 

Info in <TCanvas::Print>: pdf file ./plot/ROCs/ROC 10000 train Classical.pdf has been created Info in <TCanvas::Print>: pdf file ./plot/ROCs/ROC 10000 val Classical.pdf has been created Epoch: 10 | Epoch Time: 0m 50s Train Loss: 0.485 | Train Acc: 76.39% Val. Acc: 77.66% Val. Loss: 0.467 |

