

Introduction to Quantum Machine learning

<u>Qiyu Sha</u>

IHEP

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Overview



Introduction---IBM Quantum Computer



Credited to Thomas Prior for TIME

Development Roadmap IBM Quantum 2024 Beyond 2026 Prototype quantum software applications Ouantum software applications Machine Learning | Optimization | Natural Science | Financ \bigcirc Quantum algorithm and application modules Quantum Serverless Machine Learning | Natural science | Optimization | Finance Qiskit Runtime 🛛 🕢 Dynamic Circuits 🛛 🕢 Threaded Primitive Error suppression and mitigation Eagle 127 gubits System Modularity Falcon \odot Hummingbird 📿 \bigcirc Osprey Condor Flamingo Kookaburra \bigcirc 27 aubits 65 aubits 433 aubits 1.121 aubits 1.386+ aubits 4.158+ aubits Crosshill Heron 133 aubits x p 408 aubits

IBM has ambitious pursuits:

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

Now, IBM provides up to 127 qubits for free.



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Qiyu Sha qsha@cern.ch

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
 - •

Progress has been very rapid here.

Simulation



Reconstruction



Analysis



Outline of today

Theory



Experiment



Outline of today

Theory





Introduction---SVM

<u>SVM</u>: Max margin

Usually done using the dual(think Lagrangian multipliers)

Results in building a kernel matrix.





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

数据集标分 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 = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)

训练SVN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

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QSVM

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

<u>SVC</u>:

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

◆Encoding the $e^+e^- \rightarrow ZH \rightarrow q\bar{q}\gamma\gamma$ (signal) and $e^+e^- \rightarrow (Z/\gamma^*)\gamma\gamma$ (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
- Single-qubit rotation gates
- > Two-qubits CNOT entangling gates

Rotation	Depth	Events	Best AUC	Variation
$R_z(2\cdot\vec{x_i}) + R_y(\vec{x_i})$	2	5000	0.935	0.009
$R_z(\vec{x_i}) + R_y(\vec{x_i})$			0.933	0.015
$R_y(\vec{x_i}) + R_x(\vec{x_i})$			0.932	0.015
$R_z(\vec{x_i}) + R_z(\vec{x_i})$			0.932	0.014
$R_y(\vec{x_i})$			0.928	0.008
$R_z(\vec{x_i})$			0.928	0.008





QSVM-Kernel estimation:

- Using 6 variables mapped to 6-qubit
- The expectation of each data point

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

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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
- > Use 100 events for both signal and backgrounds.
- Use 6 qubits.



IBM Nairobi quantum Origin Wuyuan quantum



Set up: Requirements: > pip install pyqpanda
Linux
GCC >= 5

Official Tutorial: pyQPanda

- 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)

> Everything is similar as IBM:

Python

version

>= 5.4.0

>= 3.7.0 && <= 3.9.0

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 <u>next page</u>.)



Same as IBM tutorial:

f.close()

Create a feature map and kernel using Qiskit

rng = np.random.RandomState(0) def gen_qasm(): seed=2022 backend = BasicAer.get_backend("statevector_simulator") feature_map_cus = customised_feature_maps.FeatureMap(num_gubits=6, depth=1, degree=1, entanglement='full', inverse=False) seed = 2022algorithm_globals.random_seed = seed data = pd.read_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_numpy() 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, guantum_instance=q_backend) gsvm_kernel_matrix_train = q_kernel.evaluate(x_vec=X_train) gsvm_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(gsvm_kernel_matrix_test) x = ParameterVector('x', length=6) y = ParameterVector('y', length=6) circuit = q_kernel.construct_circuit(x,y) circuit = q_backend.transpile(circuit)[0] for i in range(100): f = open("all_gasm_train/gasm_%d_%d.txt"%(i,j),'w') cirtemp = circuit.assign_parameters({x:X_train[i], y:X_train[j]}, inplace=False) f.write(cirtemp.qasm()) cn

Different part: (In red frame.)

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

OPENQASM 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];

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> Apply a key in the OriginQ website.(One key can run 1000 jobs in one day.) from pygpanda import * def run(i, j): QCM = QCloud()Apply X qubits and classical bits which used QCM.init_qvm("58DCD70A14814A4DB73ACF5C8F854FA2" to save the result. glist = QCM.qAlloc_many(5) clist = QCM.cAlloc_many(5) qvm = init_quantum_machine(QMachineType.CPU) Convert QASM to program. qvm.init_qvm() prog_trans, qv, cv = convert_gasm_to_gprog("all_gasm_train/gasm_%d_%d.txt"%(i,j), qvm) > Use real chip type:origin wuyuan d5 to result = QCM.real_chip_measure(prog_trans, 10000, real_chip_type.origin_wuyuan_d5) run. (Only d4 and d5 can use, d5 is better) except: print("job %d %d failed" % (i,j)) return value = result['00000'] f = open("results_train_try/result_%d_%d.txt" %(i,j),'w') The value with ['00000'] is the point of. f.write(str(value)) kernel matrix. Save it. f.close() if __name =="__main__": for i in range(19,20): for j in range(i+1,100): run(i,j)

> Import the kernel matrix.

score = [] for i in range(1): data = pd.read_csv("sample_%d.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 = [] for i in range(100): test_kernel_line = [] for j in range(100): value = get_kernel(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 = [] for i in range(100): train_kernel_line = [] for j in range(100): train_kernel_line.append(1.0) if i>j: value = get_kernel(j,i,'train') train_kernel_line.append(value) value = get_kernel(i,j,'train') train_kernel_line.append(value) train_kernel.append(train_kernel_line) train_kernel_array = np.array(train_kernel, np.float32)

Then use the classical svc to get the final results, generate AUC value and draw plots.

vvm svc = SVC(C=30, probability=True, kernel="precomputed") #svc = QSVC(C=5, probability=True, quantum_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_Q , W_K , and W_V with variational quantum circuits.



Code detail

Quantum transformer: (This code following here)

- The MultiHeadAttentionQuantum block
- Change the linear transformations.

class MultiHeadAttentionClassical(MultiHeadAttentionBase):

def __init__(self,

embed_dim: int,

num_heads: int, dropout=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)
self.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_linear(x)

Q = self.q_linear(x)

V = self.v_linear(x)

x = self.downstream(Q, K, V, batch_size, mask)
output = self.combine_heads(x)
return output

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self.n_qubits = n_qubits self.n_qlayers = n_qlayers self.q device = q device self.head_dim = embed_dim // num_heads if 'qulacs' in q_device: self.dev = qml.device(q_device, wires=self.n_qubits, gpu=True) elif 'braket' in g 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): qml.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.rand(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



- Finally, we create a KerasLayer to handle the I/O within the hybrid neural network.(W_Q , W_K , and W_V)
- Other part is same as the classical 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

pip install -r requirment/*

Or:

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

conda activate QT_re

Python train test.py (Change the option)

if __name__ == '__main__':

parser = argparse.ArgumentParser()	
parser.add_argument('-D', 'q_device', default='default.qubit', type=str) #Fix
<pre>parser.add_argument('-B', 'batch_size', default=32, type=int)</pre>	#Fix for now.
parser.add_argument('-E', 'n_epochs', default=10, type=int)	#Fix for now, change after fix all hyperparameters
parser.add_argument('-C', 'n_classes', default=2, type=int)	#Fix
parser.add_argument('-1', 'lr', default=0.001, type=float)	#Changeable
parser.add_argument('-v', 'vocab_size', default=6, type=int)	
parser.add_argument('-e', 'embed_dim', default=6, type=int)	
parser.add_argument('-f', 'ffn_dim', default=2048, type=int)	#hidden layer dimension of feedforward networks. Changeable
<pre>parser.add_argument('-t', 'n_transformer_blocks', default=2, type=int)</pre>	#Changeable
parser.add_argument('-H', 'n_heads', default=2, type=int)	
<pre>parser.add_argument('-q', 'n_qubits_transformer', default=0, type=int)</pre>	#6 for Quantum
parser.add_argument('-Q', 'n_qubits_ffn', default=0, type=int)	#6 for Quantum
parser.add_argument('-L', 'n_qlayers', default=1, type=int)	# For Quantum
parser.add_argument('-d', 'dropout_rate', default=0.1, type=float)	#Changeable, but for few events, 0.1 is good
args = parser.parse_args()	

Num_dataset = 20000

if args.n_qubits_transformer > 0: Type_model = "Quantum" else: Type_model = "Classical"

Quantum transformer

- The dataset we used now is the CEPC MC sample
 - $\blacktriangleright e^+e^- \rightarrow ZH \rightarrow q\bar{q}\gamma\gamma$ (signal) and $e^+e^- \rightarrow (Z/\gamma^*)\gamma\gamma$ (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. Loss: 0.467 | Val. Acc: 77.66%

