中国科学院高能物理研究所
Institute of High Energy Physics Chinese Academy of Sciences

Introduction to Quantum Machine learning

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IHEP

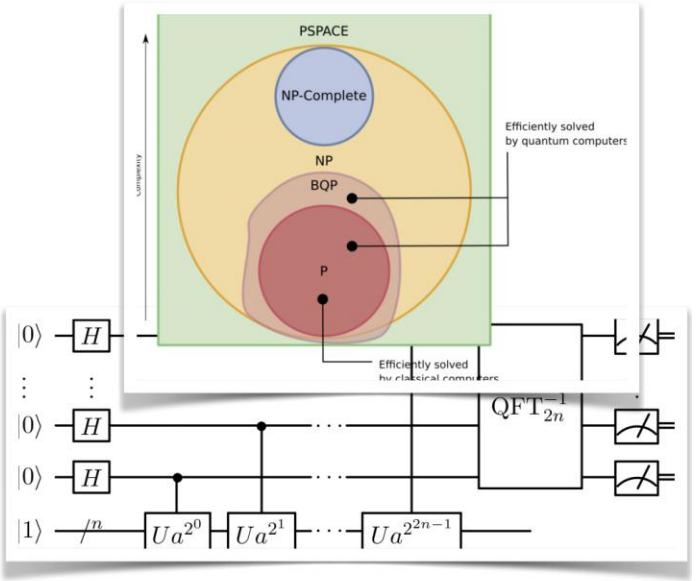
1st Machine Learning and Quantum Computing Winter School

Overview

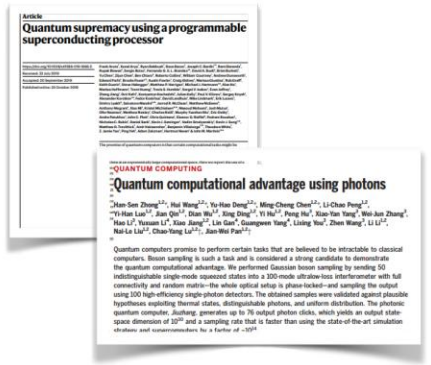
Qubit Type	Pros/Cons	Select Players
Superconducting	***Pros***: High gate speeds and fidelities. Can leverage standard lithographic processes. Among first qubit modalities so has a head start.	rigetti, Google, IBM Q, QuTech, OQC, IQM, qci Quantum Circuits, Inc, 本源量子 Origin Quantum
	Cons: Requires cryogenic cooling; short coherence times; microwave interconnect frequencies still not well understood.	
Trapped Ions	***Pros***: Extremely high gate fidelities and long coherence times. Extreme cryogenic cooling not required. Ions are perfect and consistent.	IONQ, AQT, QUANTINUUM, oxford ionics, Universal Quantum
	Cons: Slow gate times/ operations and low connectivity between qubits. Lasers hard to align and scale. Ultra-high vacuum required. Ion charges may restrict scalability.	
Photonics	***Pros***: Extremely fast gate speeds and promising fidelities. No cryogenics or vacuums required. Small overall footprint. Can leverage existing CMOS fabs.	PsiQuantum, XANADU, QUIX QUANTUM, ORCA Computing
	Cons: Noise from photon loss; each program requires its own chip. Photons don't naturally interact so 2Q gate challenges.	
Neutral Atoms	***Pros***: Long coherence times. Atoms are perfect and consistent. Strong connectivity, including more than 2Q. External cryogenics not required.	ColdQuanta, QuEra Computing Inc., atom computing, PASQAL
	Cons: Requires ultra-high vacuums. Laser scaling challenging.	
Silicon Spin/Quantum Dots	***Pros***: Leverages existing semiconductor technology. Strong gate fidelities and speeds.	intel, Silicon Quantum Computing, diraq, QUANTUM MOTION, QUANTUM BRILLIANCE
	Cons: Requires cryogenics. Only a few entangled gates to-date with low coherence times. Interference/cross-talk challenges.	

Computers

Algorithms

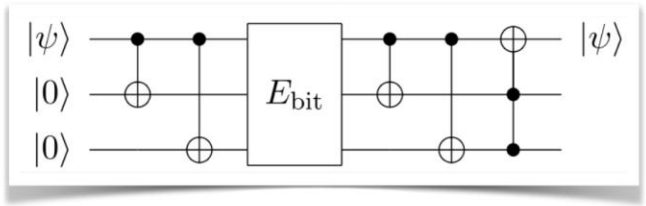


Advantage

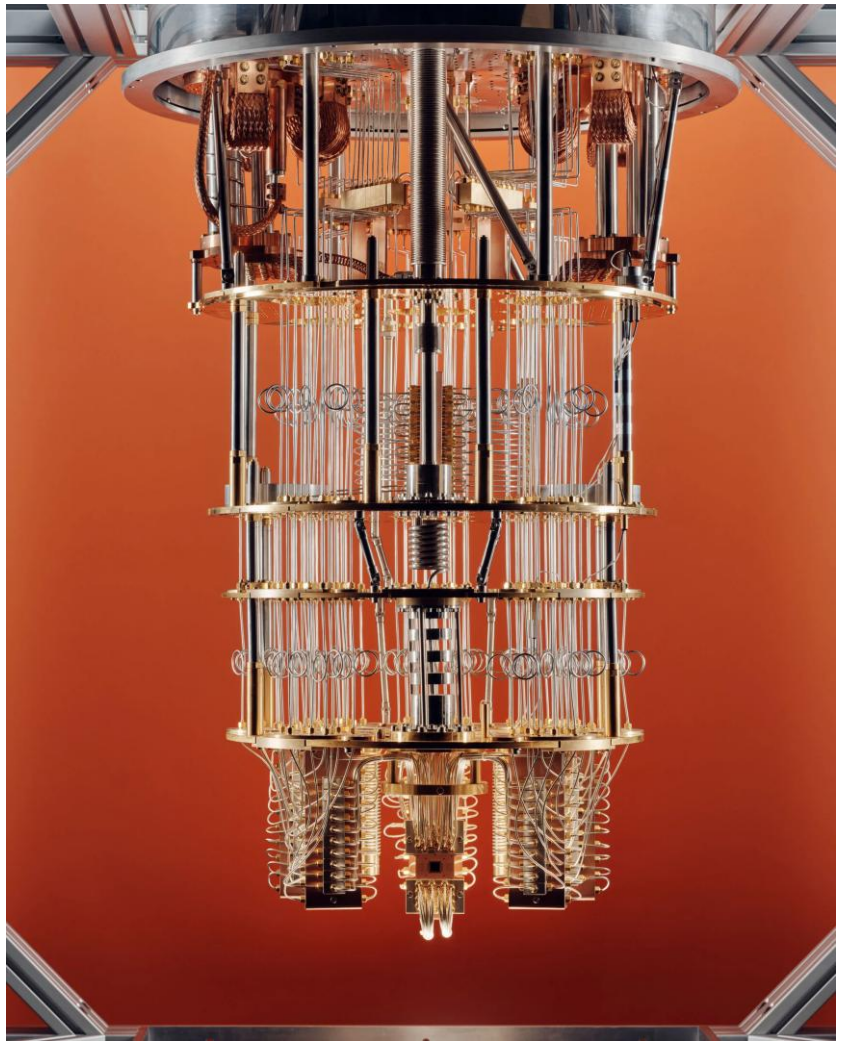


Programming

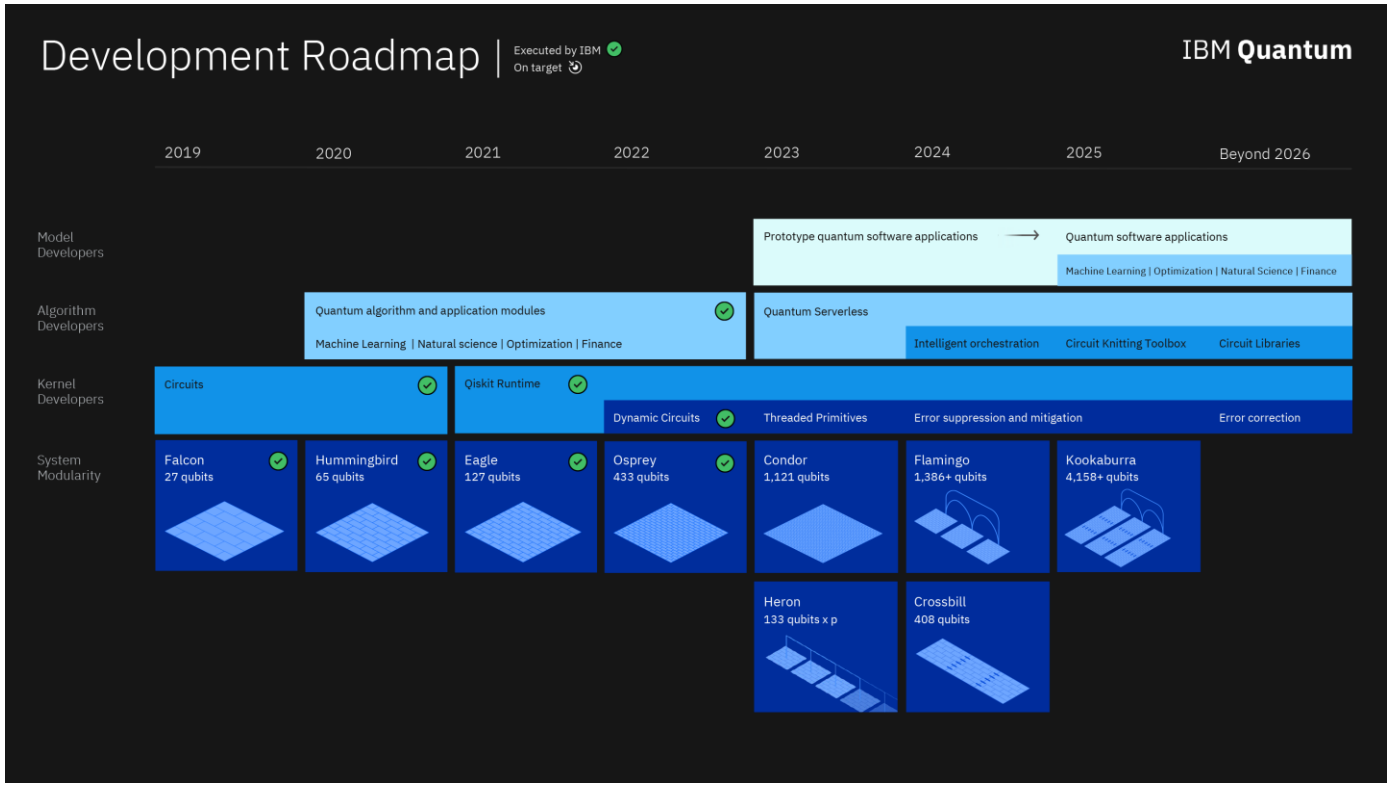
Error Correction



Introduction---IBM Quantum



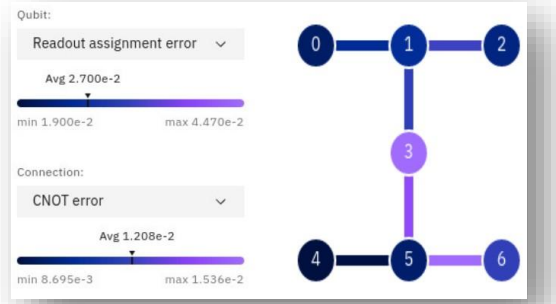
Credited to Thomas Prior for TIME



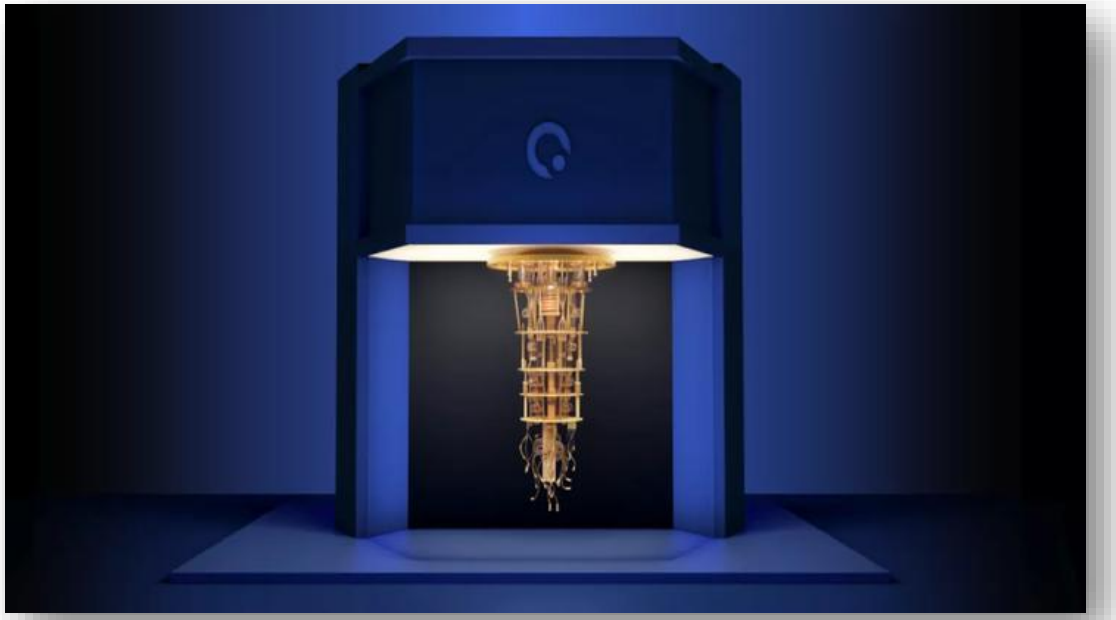
IBM has ambitious pursuits:

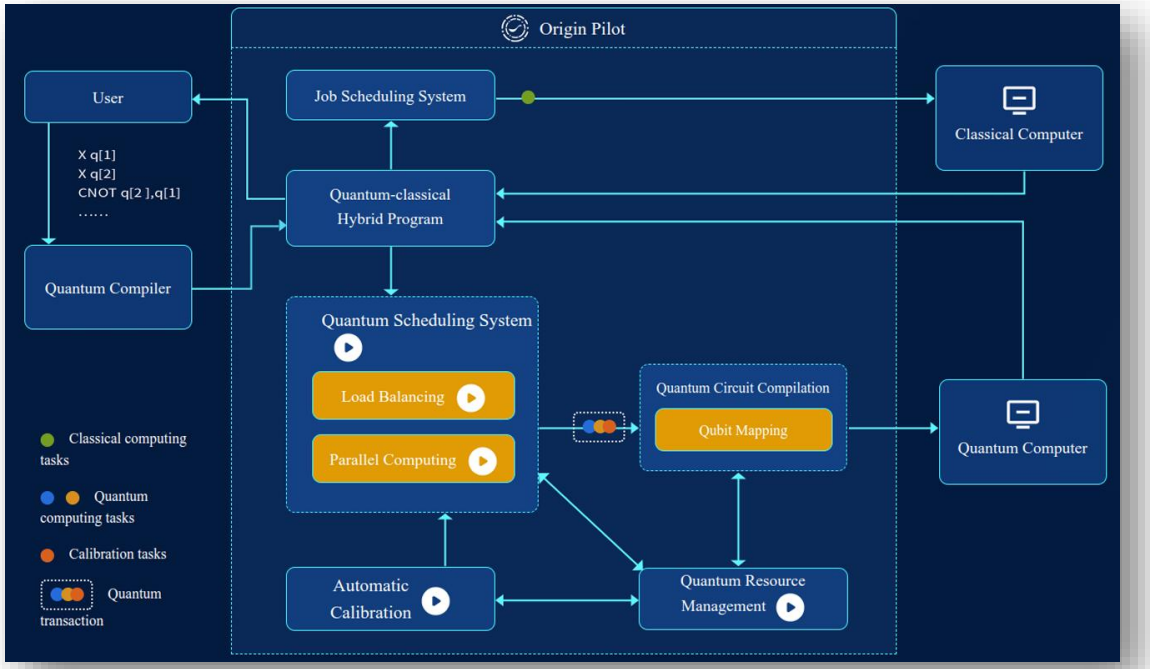
- 433-qubits IBM Quantum Osprey
- Three times larger than the Eagle processor (127-qubits)
- Going up to 10k-100k qubits.

Now, IBM provides up to 127 qubits for free.



Introduction---Origin Quantum Computer



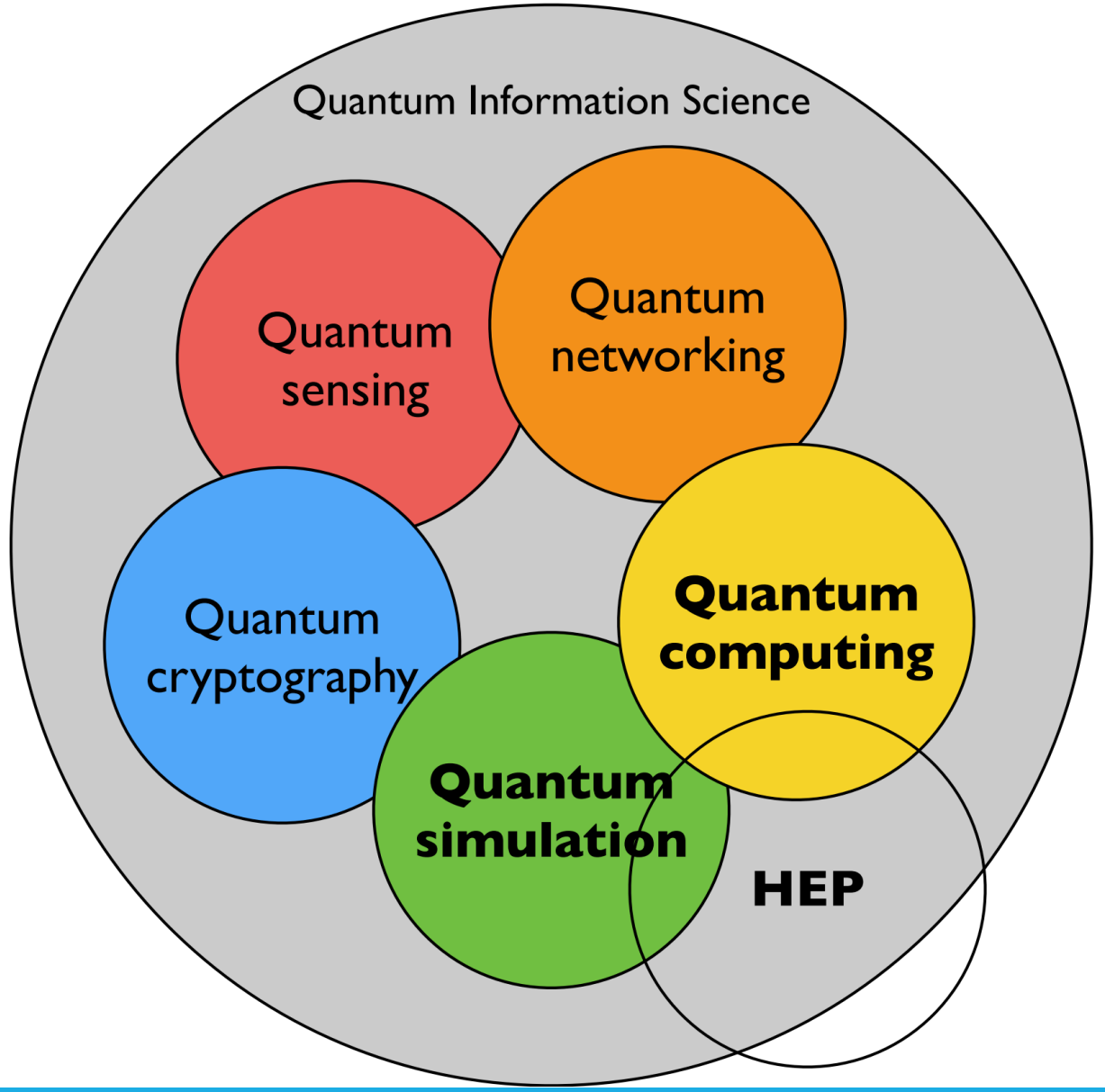


Origin wuyuan:

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

Origin wuyuan provide up to 6 qubits for free.

Overview


Quantum Information Science
Quantum sensing
Quantum networking
Quantum cryptography
Quantum computing
Quantum simulation
HEP

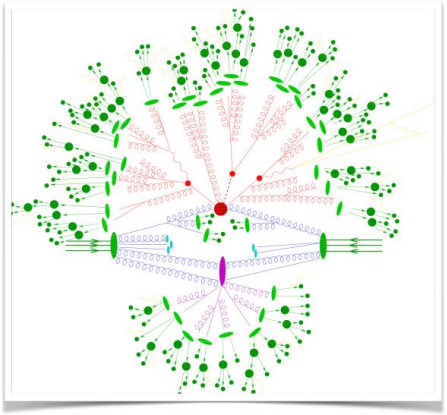
Outline of today

Applications of quantum computing in HEP

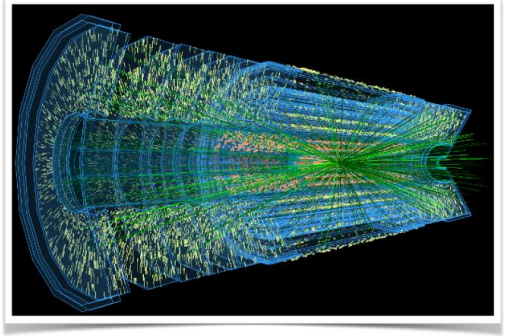
- Simulation
  - Parton shower correlations
  - Lattice QCD
- Reconstruction
  - Particle tracking
- Analysis
  - Higgs analyses
  - SUSY search
  - …

Progress has been very rapid here.

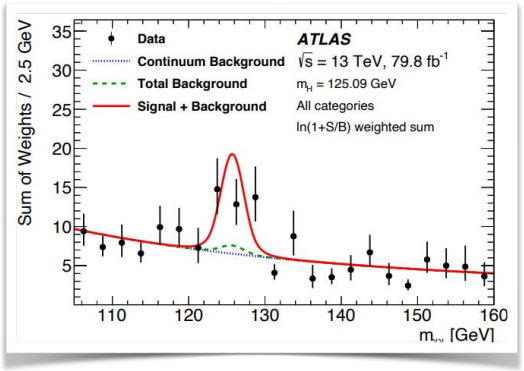
Simulation



Reconstruction

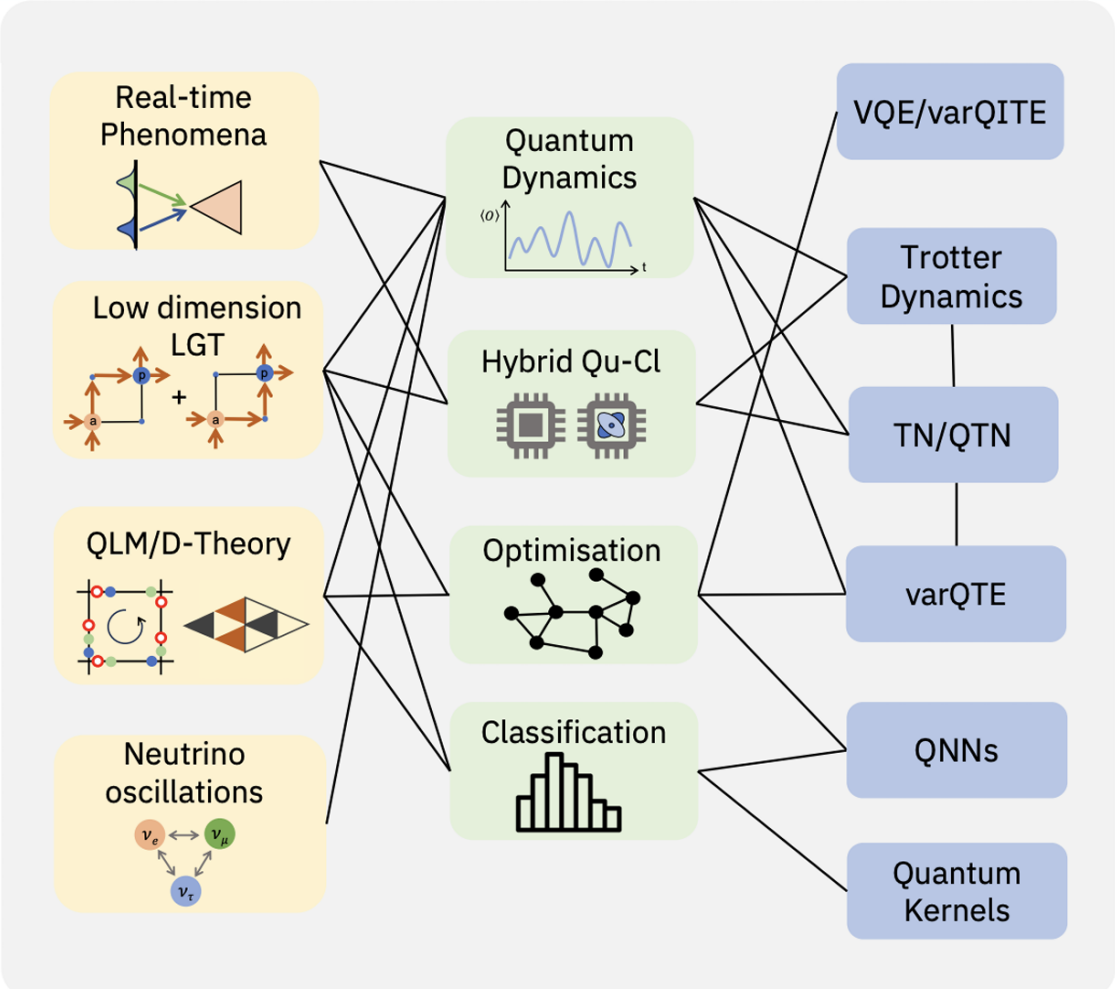


Analysis

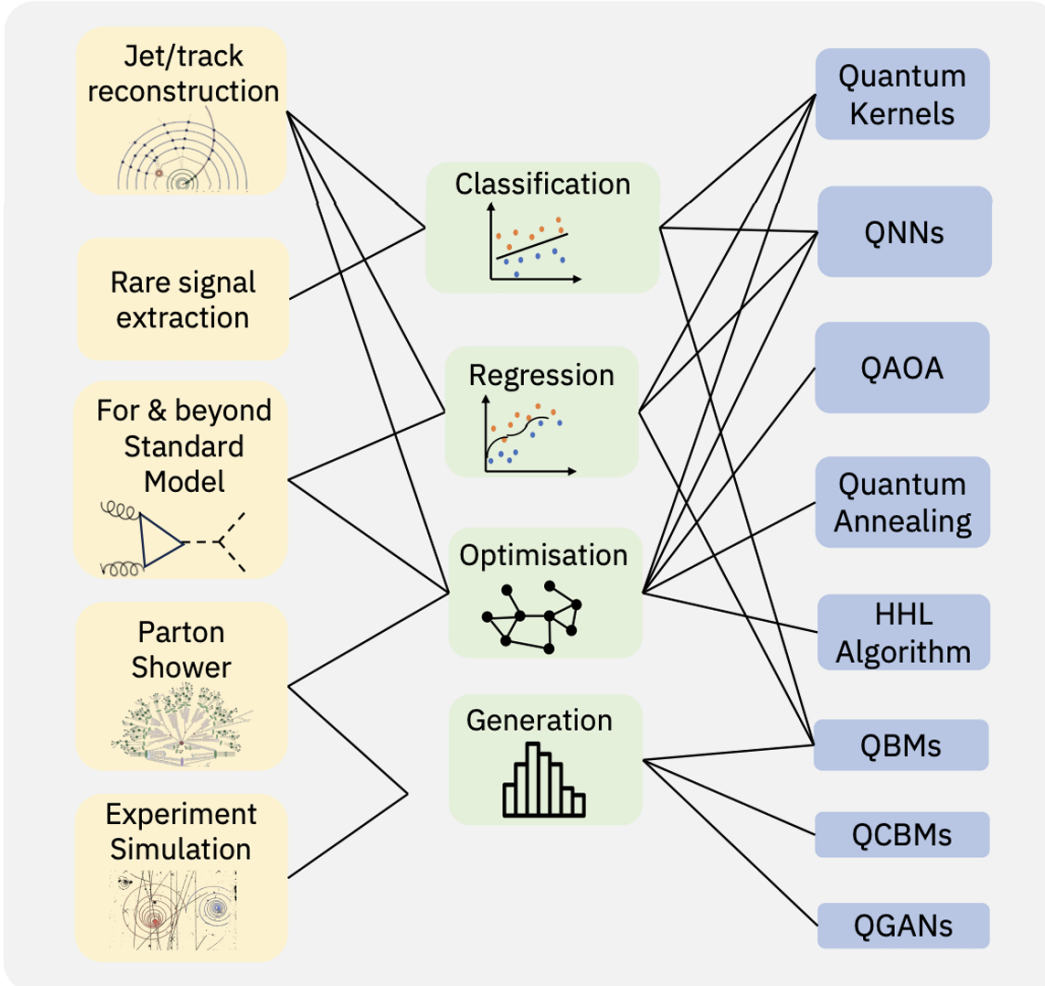


Outline of today

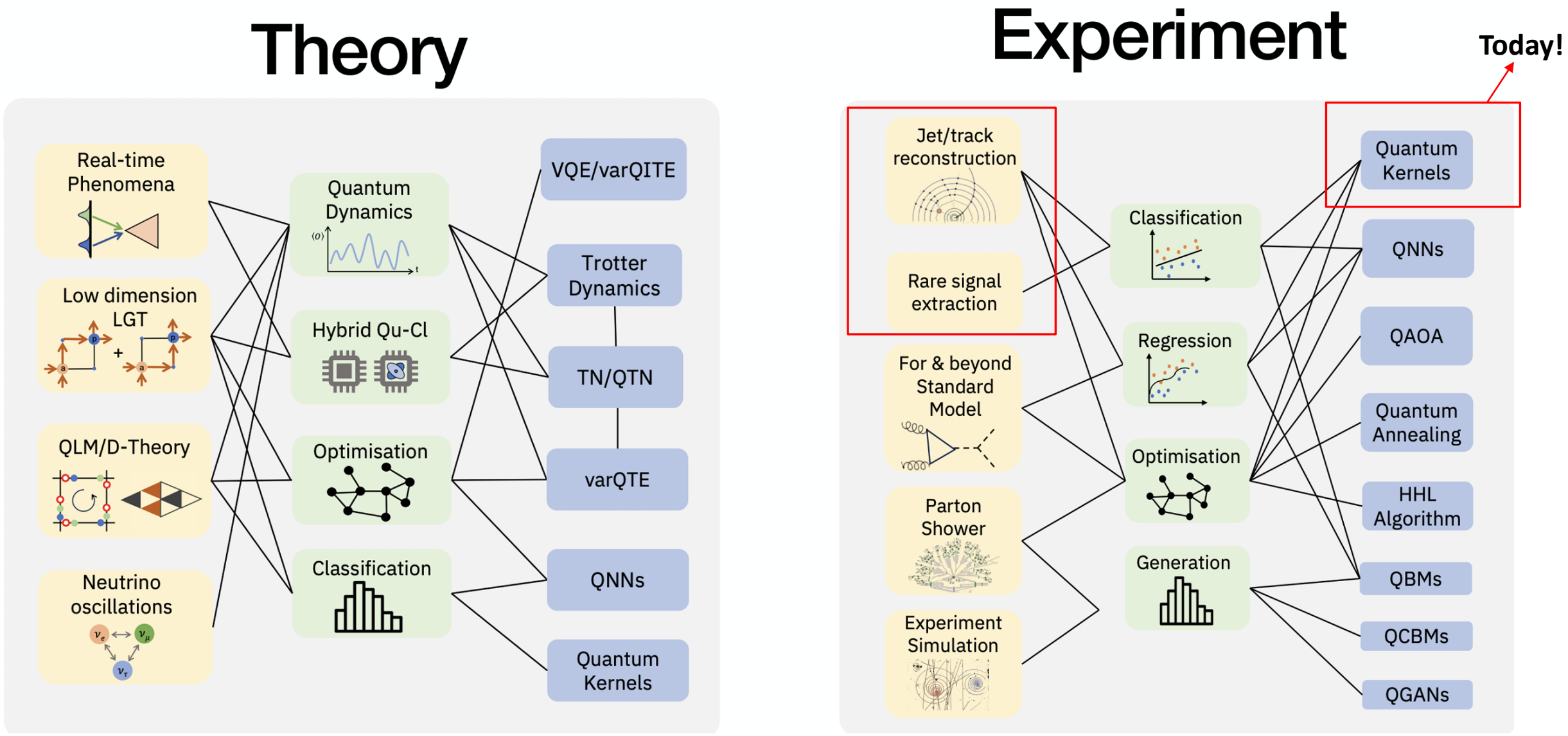
Theory



Experiment



Outline of today



Introduction---SVM

SVM: 将分类间隔最大化——用于分类/回归问题

通过寻找一个最优的超平面对数据进行分类。

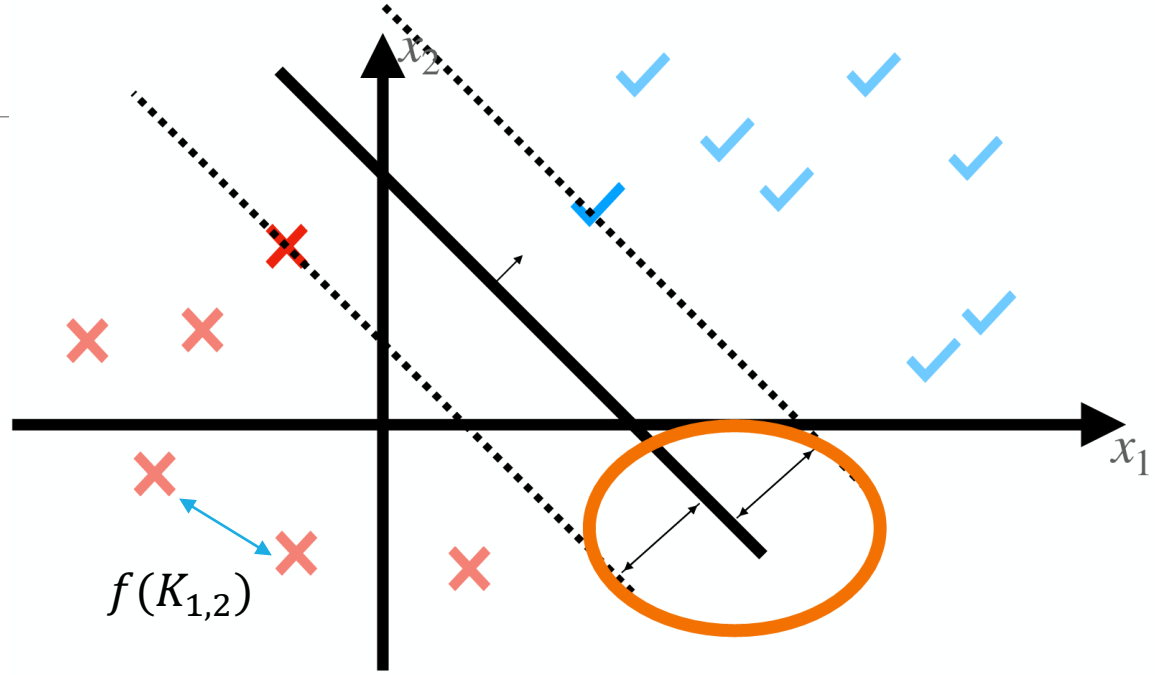
- 给定一组数据$\{\{x_i, y_i\}\}$，x_i为特征向量，y_i为样本标签。
- SVM的决策函数为：

$$f(x) = \omega^T x + b$$

其中ω为超平面的法向量，b为偏置

- 最大化间隔：约束优化问题，满足优化：

$$y_i(\omega^T x_i + b) \geq 1$$



Maximise this

通过拉格朗日对偶函数（Lagrangian Dual Function）解决该约束优化问题：

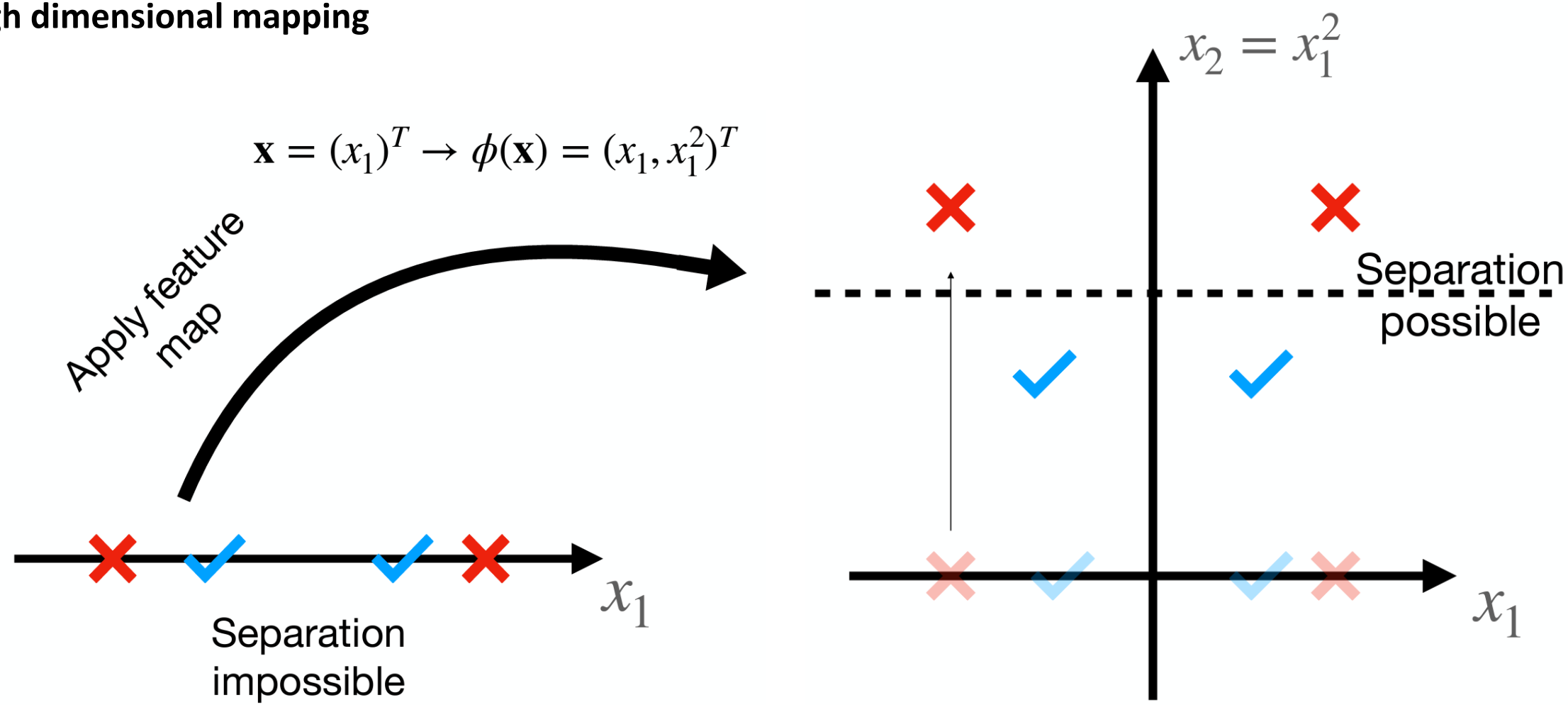
$$D(\alpha) = \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j x_i^T x_j$$

用核函数$(K_{i,j})$替代内积的计算（kernel trick）：
避免了直接计算高维的映射，提高计算效率。

$K_{1,1}$	$K_{1,2}$	$K_{1,3}$
$K_{2,1}$	⋱	
		⋱

Introduction---SVM feature map

High dimensional mapping



Introduction---SVM code

```python
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 = scaler.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))
```

线性核：

$$K(x_i, y_i) = x_i^T x_j$$

多项式核：

$$K(x_i, y_i) = \left(x_i^T x_j + \mathrm{c}\right)^d$$

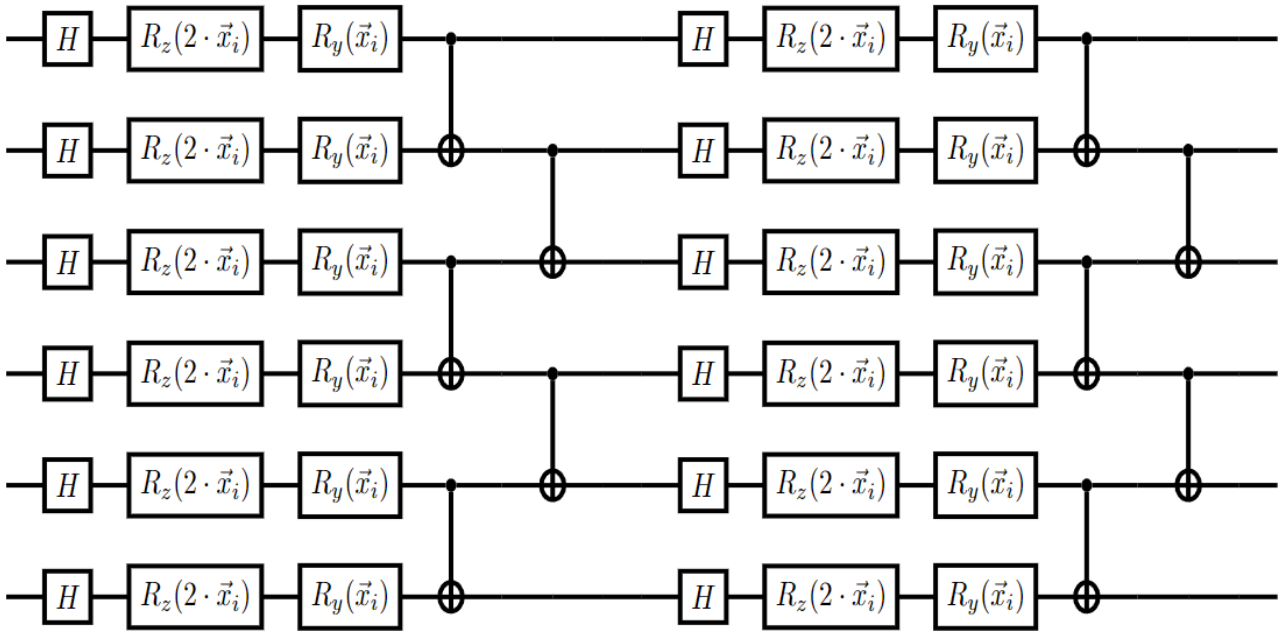
model = SVC(kernel='poly', degree=3)

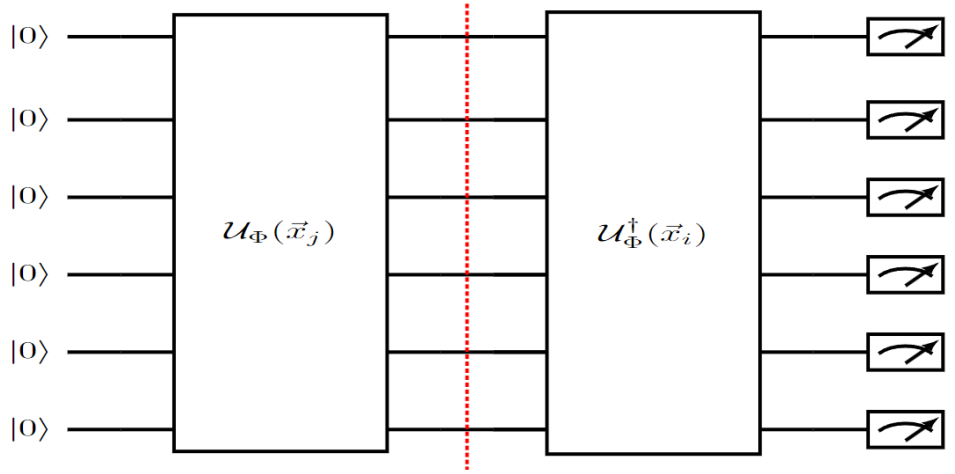
高斯径向基核：

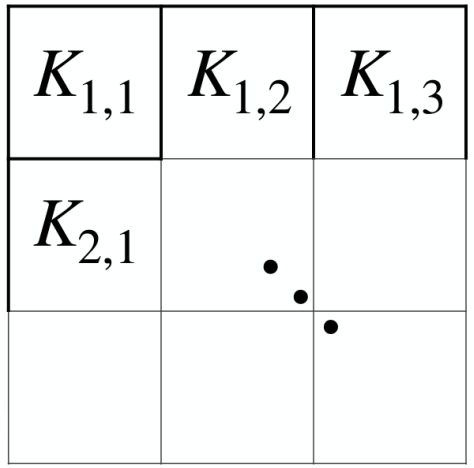
$$K(x_i, y_i) = -\frac{\|x_i - x_j\|^2}{2\sigma^2}$$

model = SVC(kernel='rbf', gamma='scale')

What we can do?





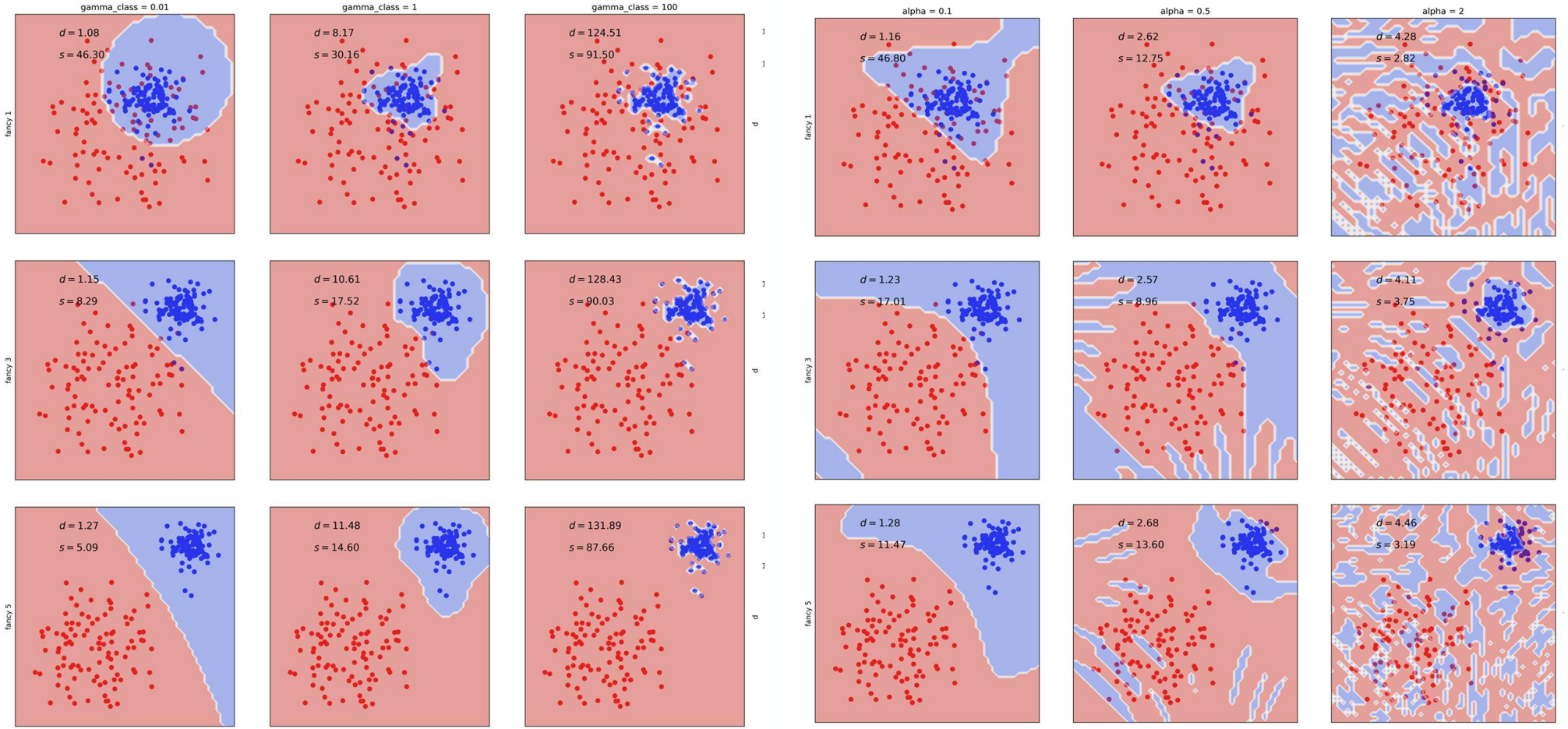


The only Quantum part in the QSVM!

$$k(\vec{x}_i, \vec{x}_j) = \left| \left\langle 0^{\otimes N} \right| \mathcal{U}^\dagger_{\Phi(\vec{x}_i)} \mathcal{U}_{\Phi(\vec{x}_j)} \left| 0^{\otimes N} \right\rangle \right|^2$$

What we can do?

https://arxiv.org/abs/2212.07279



Classical **Quantum**

QSVM

- Code path: /cefs/higgs/shaqy/Quantum/QC_HEP/For_tutorial/QSVM
- Env: source /hpcfs/cepc/higgsgpu/shaqy/miniconda/etc/profile.d/conda.sh
  Conda activate Qiskit

SVC(支持向量分类器):

1. 使用自定义的kernel矩阵

```
>>> 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)
```

2. 也可以通过kernel='precomputed' 选项去传递预计算的kernel（通常为Gram矩阵）。该方法可以在训练/预测的时候用Gram矩阵替代原始的特征数据X作为输入。

- 适用于已有核函数的情况

```
>>> 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])
```

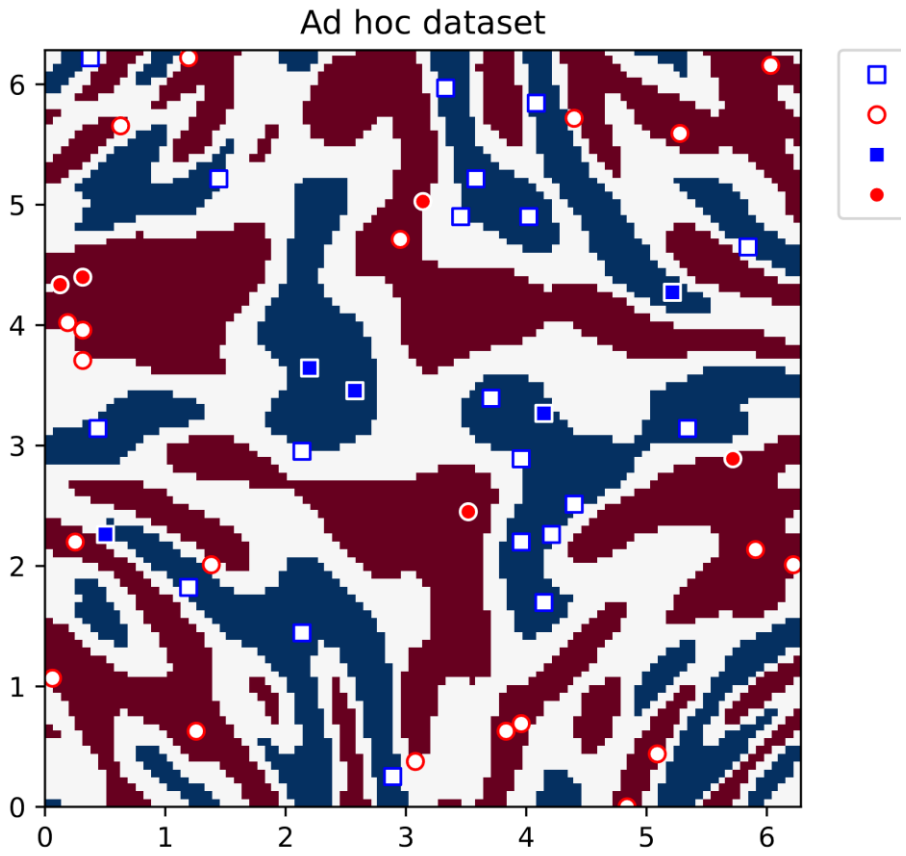
Coding-QSVM

- Code path: /cefs/higgs/shaqy/Quantum/QC_HEP/For_tutorial/QSVM
- Env: source /hpcfs/cepc/higgsgpu/shaqy/miniconda/etc/profile.d/conda.sh
  Conda activate Qiskit
  Or: source env.sh

第一步：
捏一个数据集（step1_dataset_pre.py)

```
#algorithm_globals.random_seed = 2025
adhoc_dimension = 2
train_features, train_labels, test_features, test_labels, adhoc_total = ad_hoc_data(
    training_size=20,
    test_size=5,
    n=adhoc_dimension,
    gap=0.3,
    plot_data=False,
    one_hot=False,
    include_sample_total=True,
)
```

One-hot :用于将分类变量转换为二进制向量形式。
适用于神经网络/多分类问题。但在feature数量很大时，会导致高维且稀疏的向量，增大计算/存储开销。



Coding-QSVM

第二步：（打开step2_QSVM.py）

```
adhoc_feature_map = ZZFeatureMap(feature_dimension=adhoc_dimension, reps=2, entanglement="linear")
```

建立一个量子特征映射——用来将经典数据映射到量子态

这里使用了Qiskit自带的ZZFeaturemap作为量子电路：（可以自行优化调整）

其核心构造为：

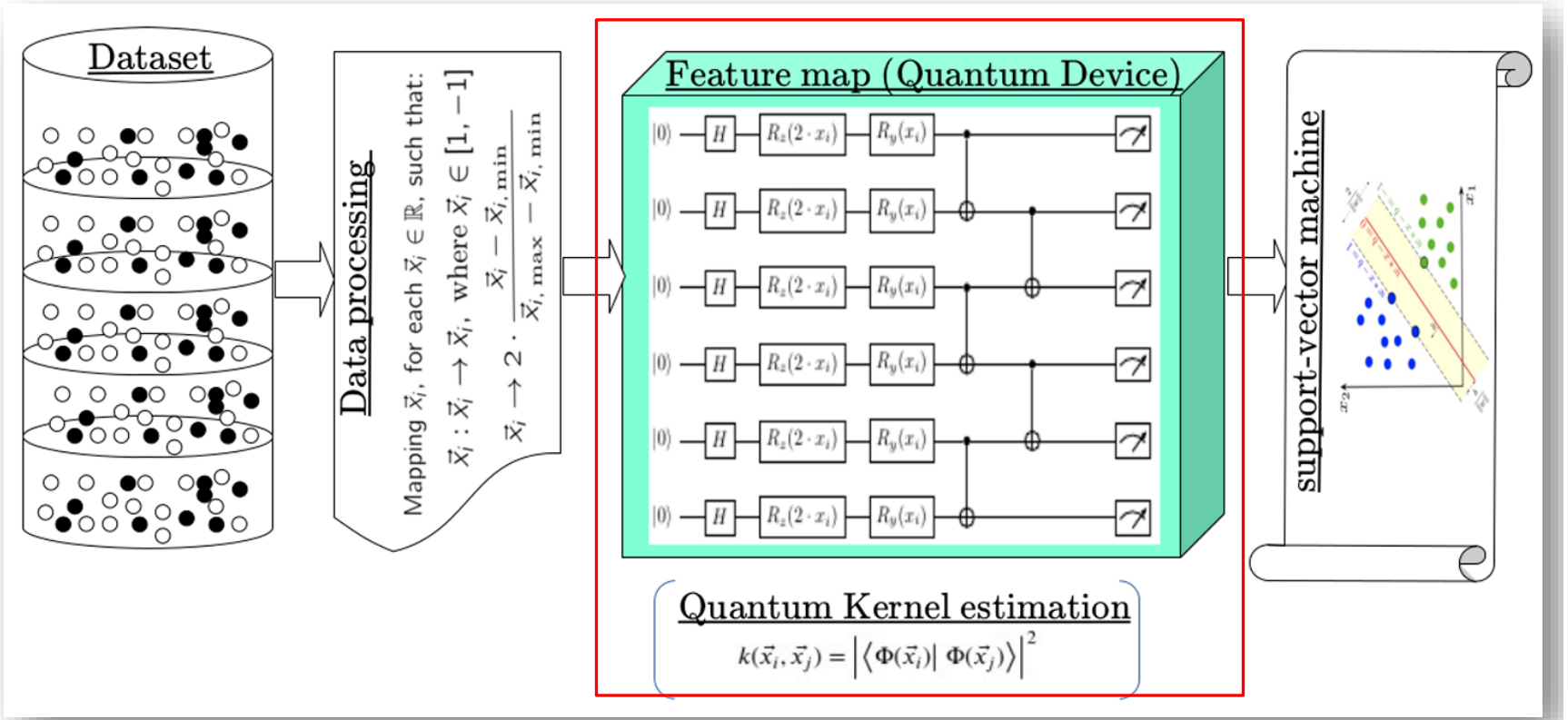
1. H gate
2. RZ旋转门
3. 纠缠门（通过CX与RZ实现双量子比特交互）

reps:重复n次该特征映射；entanglement：对量子比特进行纠缠，此处为每个量子比特与相邻的进行线性纠缠。

第三步：初始化量子核并计算Kernel ——最后放入Qiskit.qsvc or 作为预计算核输入SVC。

```
sampler = Sampler()
fidelity = ComputeUncompute(sampler=sampler)

###Use fidelity
adhoc_kernel = FidelityQuantumKernel(fidelity=fidelity, feature_map=adhoc_feature_map)
```

Data encoding and processing



Operator	Gate(s)	Matrix
Pauli-X (X)	X	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	Z	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)		$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$

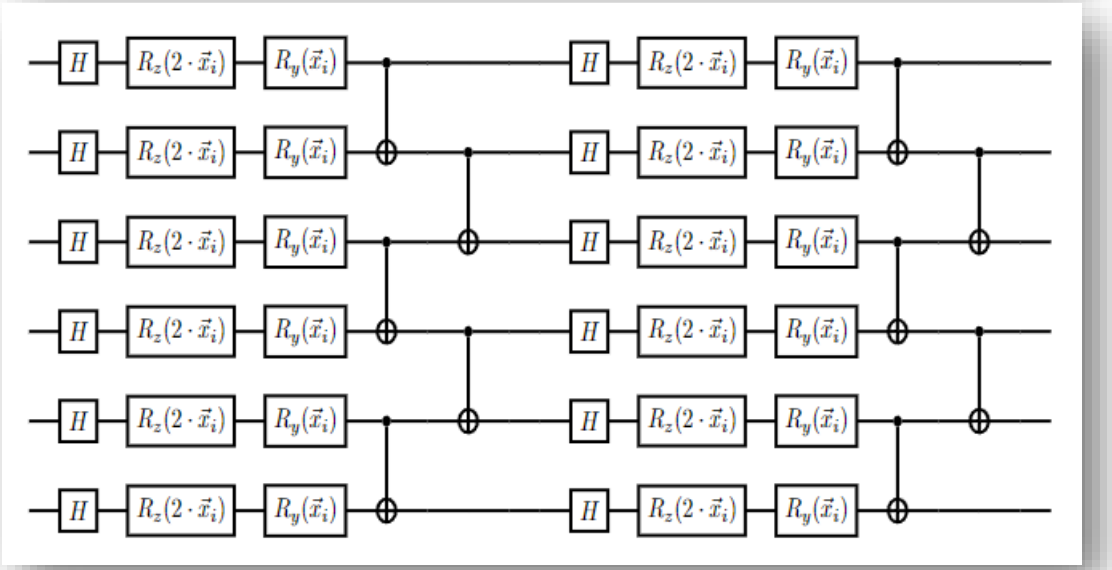
- Encoding the $e^+e^- \to ZH \to q\bar{q}\gamma\gamma$ (signal) and $e^+e^- \to (Z/\gamma^*)\gamma\gamma$ (background)
- Six variables are passed through preliminary mapping and then passed to a quantum circuit for evaluation.
- The Quantum support-vector machines kernel (QSVM-Kernel) is evaluated for each data point and the rest.

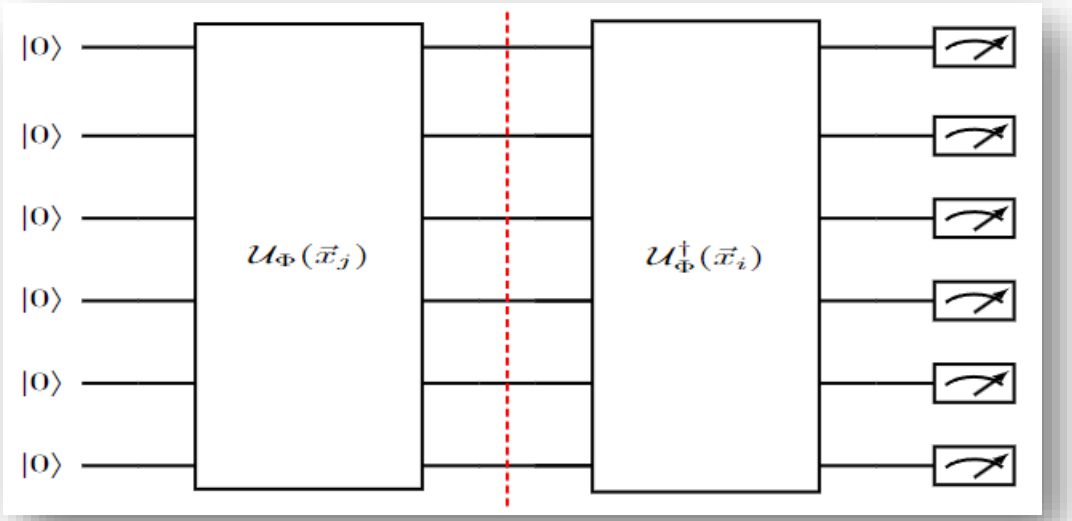
Feature map and quantum kernel estimation

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





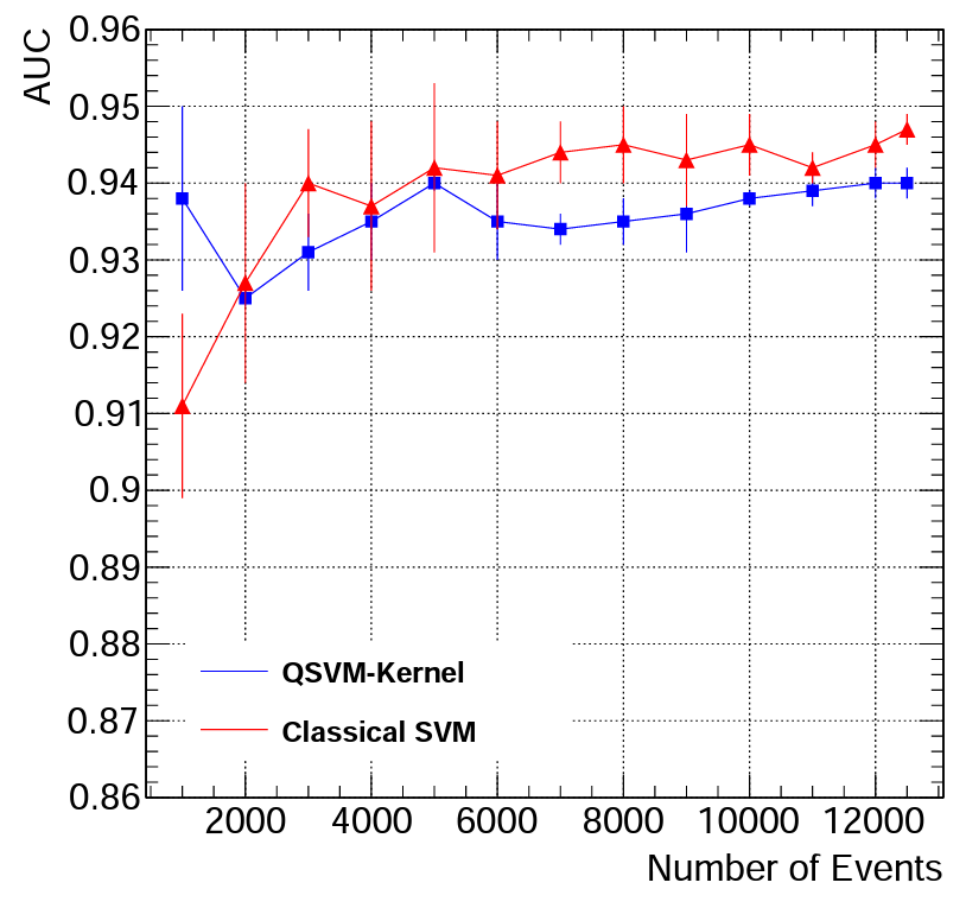
QSVM-Kernel estimation:

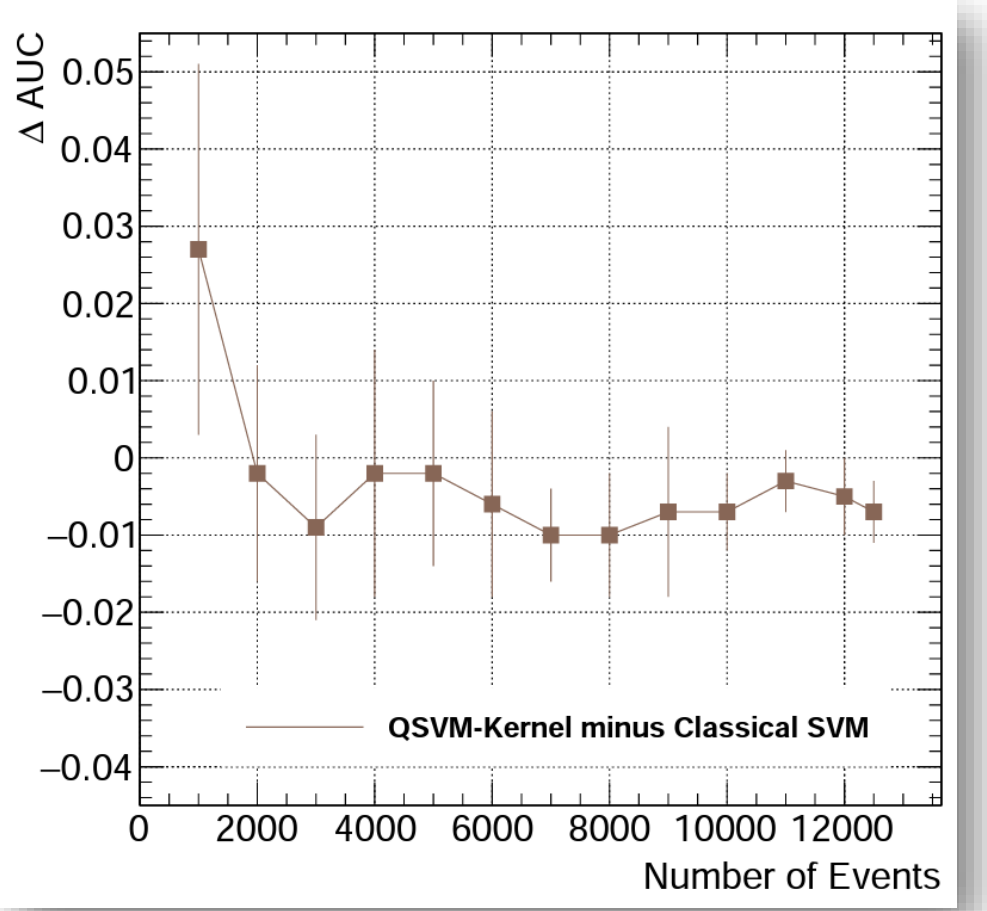
- Using 6 variables mapped to 6-qubit
- The expectation of each data point

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

AUCs as function of the event

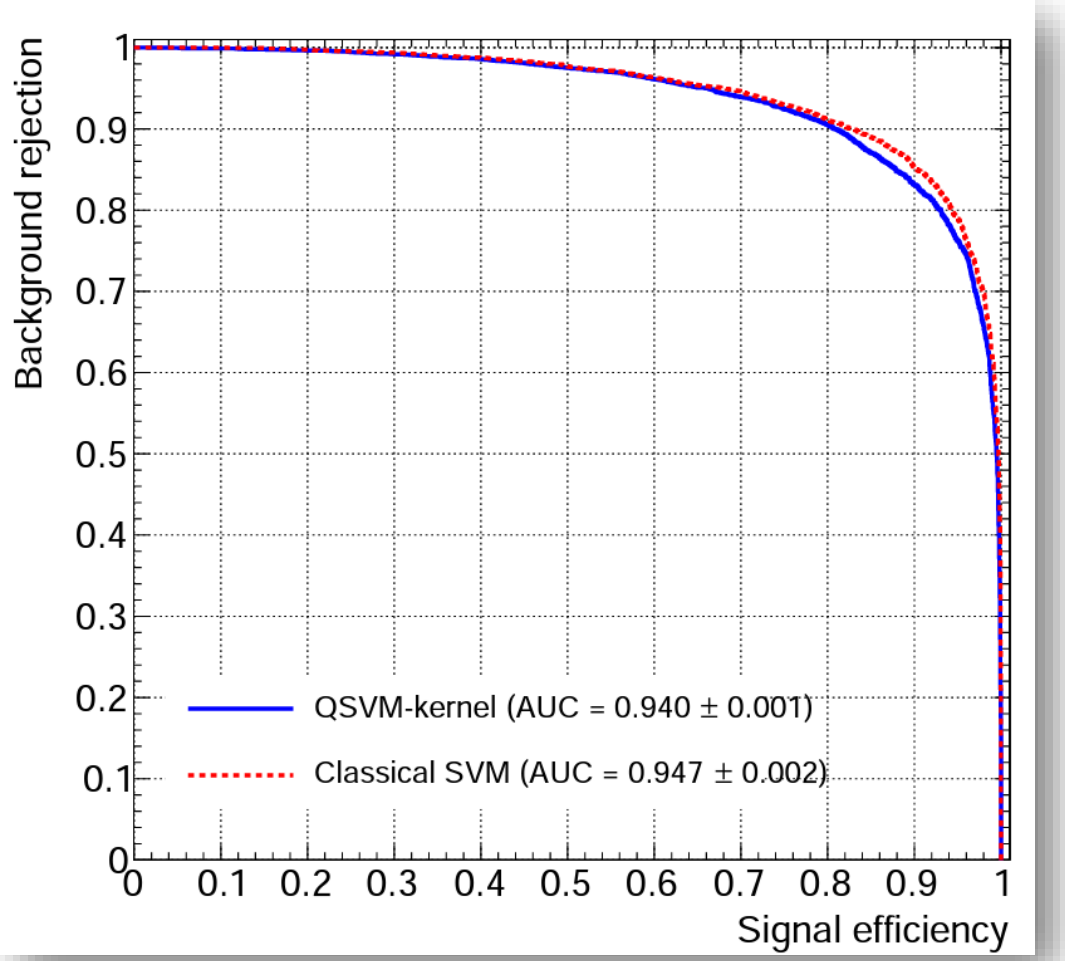
- The QSVM-Kernel and classical SVM classifiers with different dataset size from 1000 to 12500 events.
- The quoted errors are the standard deviations for AUCs calculated from several shuffles of the dataset.





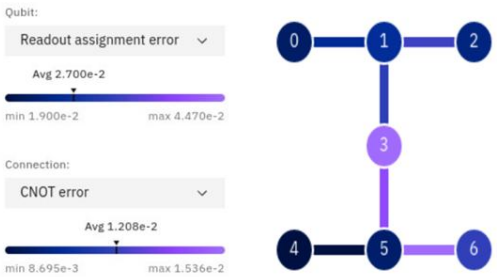
Performance of the quantum simulator

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



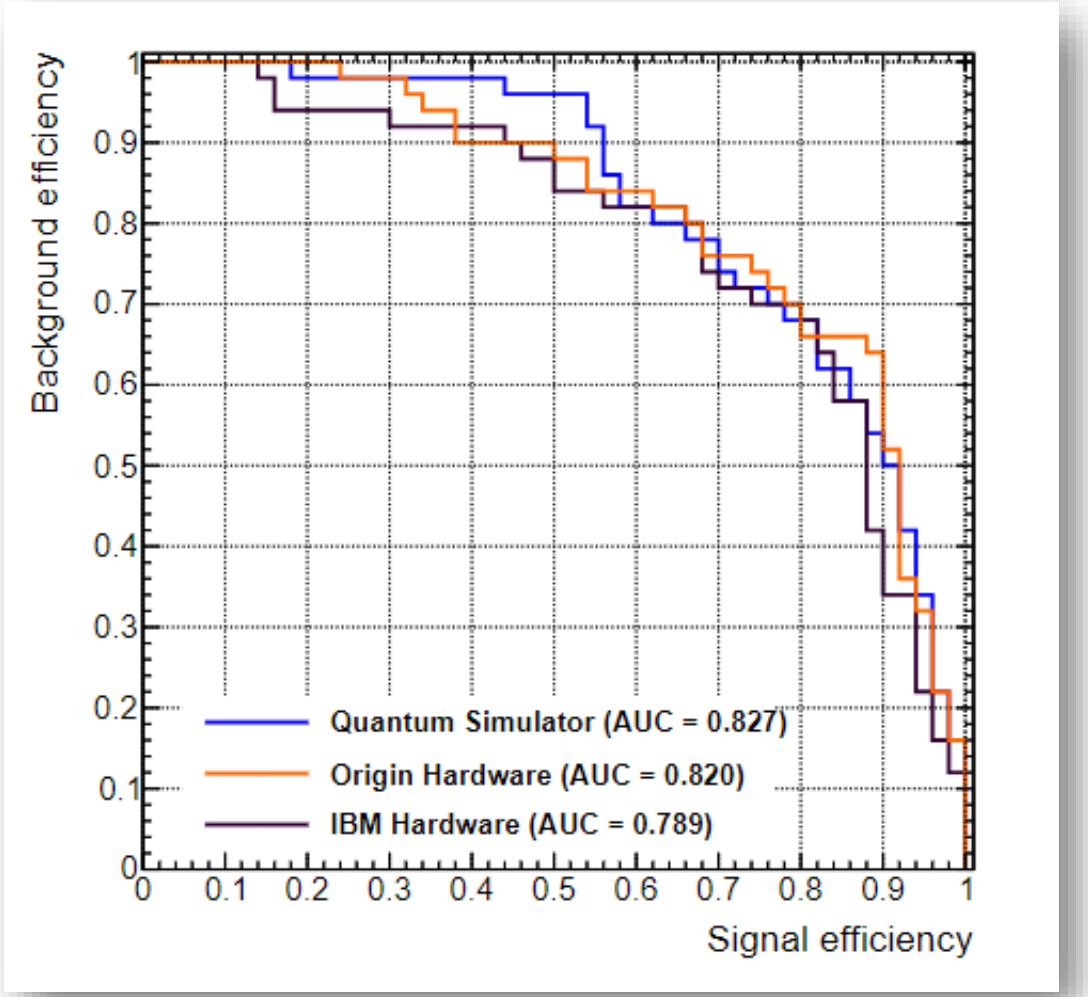
Performance of the real quantum computers

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



IBM Nairobi quantum

Origin Wuyuan quantum



How to do it

Set up:

- pip install pyqpanda

Requirements:

Linux

software	version
GCC	>= 5.4.0
Python	>= 3.7.0 && <= 3.9.0

- Official Tutorial: pyQPanda
- Code path: /cefs/higgs/shaqy/Quantum/QC_HEP/For_tutorial/QSVM_hardware
- Env: source /hpcfs/cepc/higgsgpu/shaqy/miniconda/etc/profile.d/conda.sh
  conda activate QT_re (conda deactivate)

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.)

QASM(Quantum Assembly Language):

Convert QASM to program in wuyuan
Get the kernel matrix.

The same way as IBM:
Use classical way to get results.

```
OPENQASM 2.0;
include "qelib1.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];
```

How to do it

Same as IBM tutorial:

- 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_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_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, 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.construct_circuit(x,y)
    circuit = q_backend.transpile(circuit)[0]

    for i in range(100):
      for j in range(100):
        f = open("all_qasm_train/qasm_%d_%d.txt"%(i,j),'w')
        cirtemp = circuit.assign_parameters({x:X_train[i], y:X_train[j]}, inplace=False)
        f.write(cirtemp.qasm())
        f.close()
```

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 "qelib1.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];
```

How to do it

- 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.
- The value with [‘00000’] is the point of kernel matrix. Save it.

```
from pyqpanda import *

def run(i,j):
    QCM = QCloud()
    QCM.init_qvm("58DCD70A14814A4DB73ACF5C8F854FA2")

    qlist = QCM.qAlloc_many(5)
    clist = QCM.cAlloc_many(5)

    qvm = init_quantum_machine(QMachineType.CPU)
    qvm.init_qvm()

    prog_trans, qv, cv = convert_qasm_to_qprog("all_qasm_train/qasm_%d_%d.txt"%(i,j), qvm)
    try:
      result = QCM.real_chip_measure(prog_trans, 10000, real_chip_type.origin_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)
```

How to do it

- 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):
      if i == j:
        train_kernel_line.append(1.0)
      else:
        if i>j:
          # the matrix is symmetric
          # switch i and j as j is always greater than i in data
          value = get_kernel(j,i,'train')
          train_kernel_line.append(value)
        else:
          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.

```
#QSVM
    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.

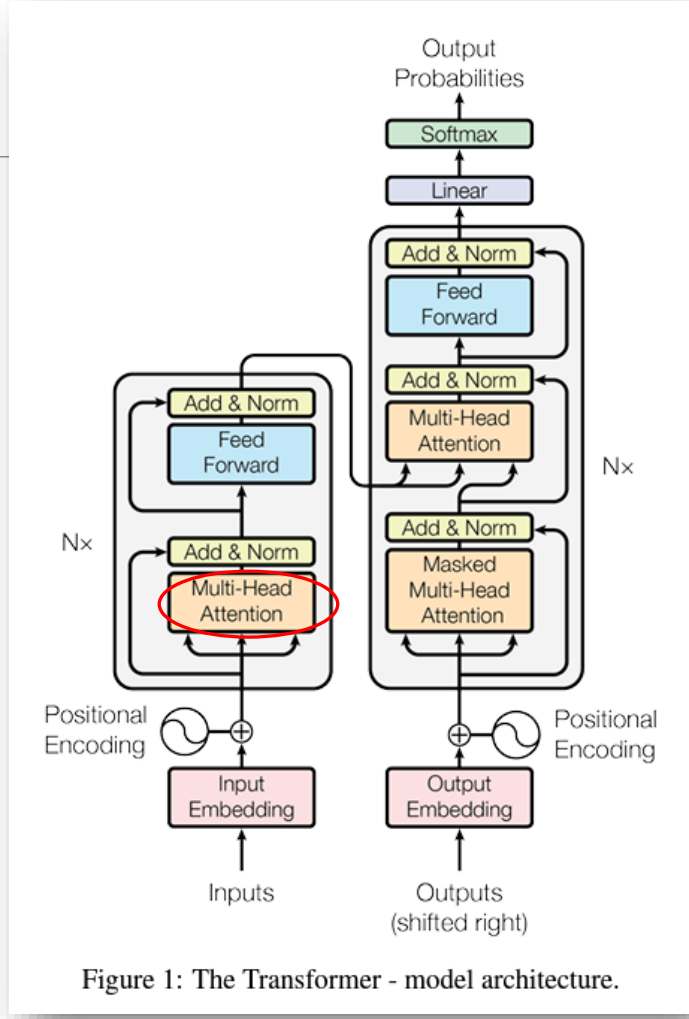


Figure 1: The Transformer - model architecture.

Code detail

Quantum transformer: (This code following here)

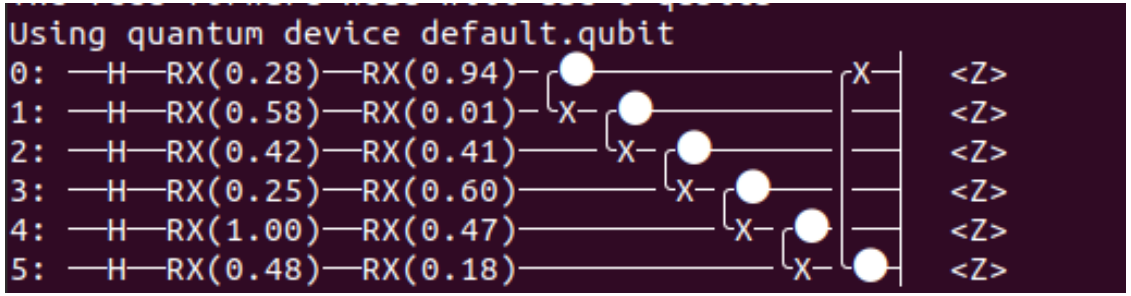
- The MultiHeadAttentionQuantum block
- Change the linear transformations.

```
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
```

```
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 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):
        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

- 使用Xanadu's PennyLane 类去创建量子电路，然后通过TensorFlow进行计算.
  - 建立量子电路
  - 用Qnode将量子电路与TensorFlow连接，方便TensorFlow可使用参数偏移规则（ parameter-shift ）去计算梯度：
    - 量子电路的参数是量子门，无法使用经典反向传播计算梯度。
    - 参数偏移规则适用于可调参的量子门



- 用KerasLayer将量子电路封装为一个神经网络层整合到TensorFlow里，实现一个量子-经典混合的Transformer结构的神经网络，其中$W_Q, W_K,$ and W_V涉及量子计算，其余部分为经典结构。
- https://github.com/shaqiyu/Quantum_transformer

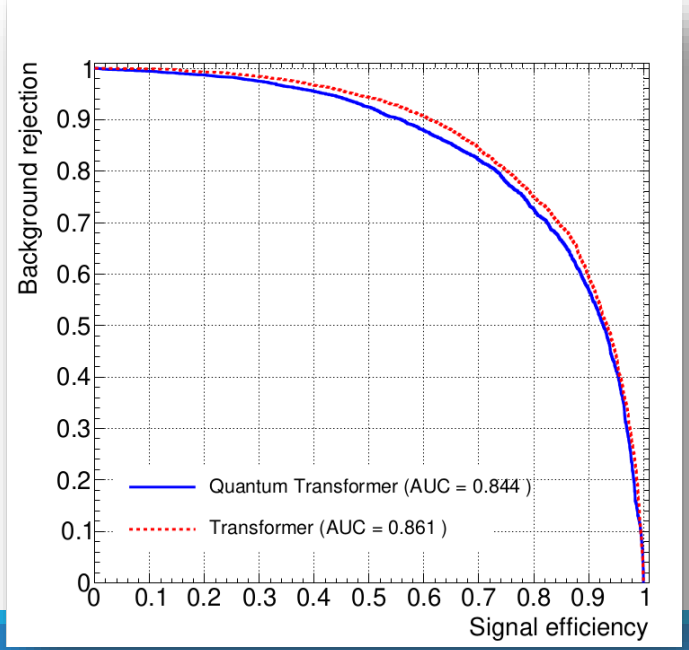
Quantum transformer ——测试

- The dataset we used now is the CEPC MC sample
  - $e^+e^- \to ZH \to q\bar{q}\gamma\gamma$ (signal) and $e^+e^- \to (Z/\gamma^*)\gamma\gamma$ (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%
```



Quantum transformer——实际研究

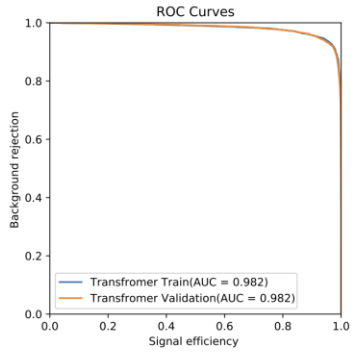
研究过程与成果

- 利用BESIII数据进行了$Zc(3900)$的物理分析
- 经过预筛选后选择了26个变量进行Transformer和Quantum transformer的训练：

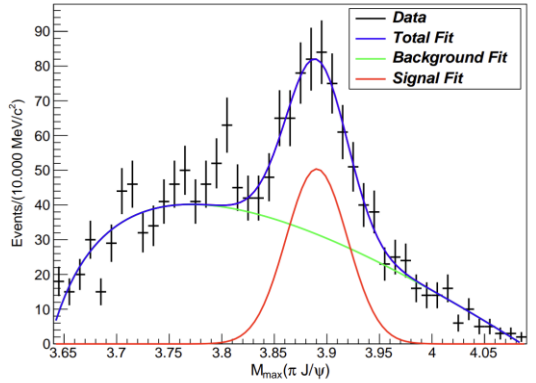
Zc(3900) decay chain

$$e^+e^- \to Zc(3900)^\pm\pi^\mp$$
$$Zc(3900)^\pm \to J/\psi\pi^\pm$$
$$J/\psi \to e^+e^-(\mu^+\mu^-)$$

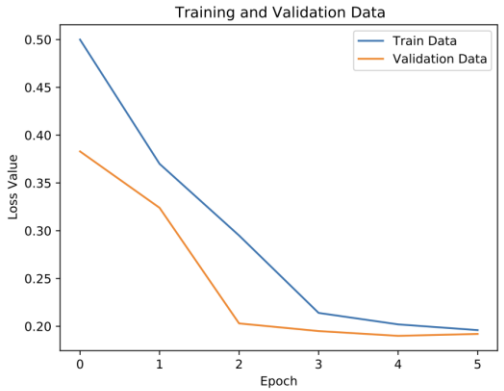
Transformer 训练结果：

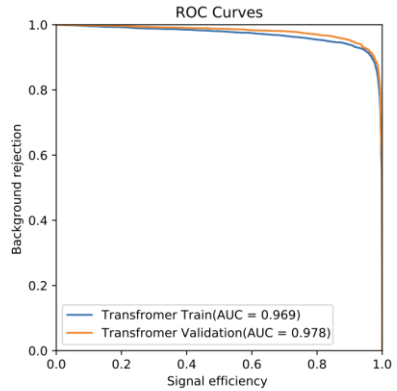


将训练结果apply到data上，在对信号与本底的分布进行拟合：



Quantum Transformer 训练结果（量子模拟，受限于GPU运行时间限制无法运行更多的epochs）：

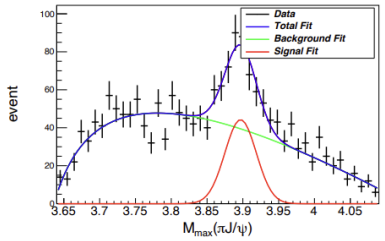




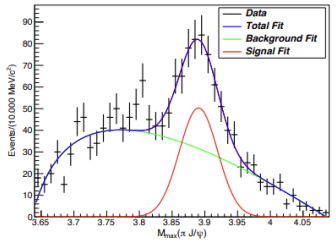
Quantum transformer ——实际研究

研究过程与成果

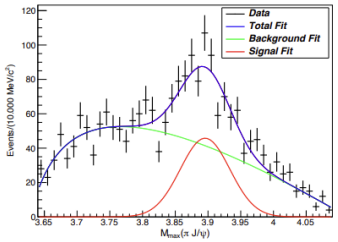
- Quantum transformer与transformer均优于传统cut-based的效果
- 仍在进行迭代优化。
- 在真实量子计算机上运行限制较大，目前难以得到很好的结果。



classical cut



Transformer



Quantum Transformer

	classical cut	Transformer	Quantum
Signal	243.1	367.6	434.4
Background	1526.9	1197.0	1644.4
Total	1770.1	1546.7	2078.8
s	232.1	350.9	414.6
b	344.0	363.6	617.8
$\varepsilon = \frac{s}{\sqrt{s+b}}$	9.67	13.13	12.90

Here, s and b are obtained by fitting the data.

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.py (Change the option)

```
if __name__ == '__main__':
    parser = argparse.ArgumentParser()
    parser.add_argument('-D', '--q_device', default='default.qubit', type=str)      #Fix
    parser.add_argument('-B', '--batch_size', default=32, type=int)                 #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('-l', '--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
    parser.add_argument('-t', '--n_transformer_blocks', default=2, type=int)       #Changeable
    parser.add_argument('-H', '--n_heads', default=2, type=int)
    parser.add_argument('-q', '--n_qubits_transformer', default=0, type=int) #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"
```