Application of the Quantum Kernel Algorithm on the Particle Identification at the BESIII Experiment

Teng Li[1], Zhipeng Yao[1], Jiaheng Zou[2], Tao Lin[2], Weidong Li[2], Xingtao Huang[1]

[1] Shandong University, Qingdao

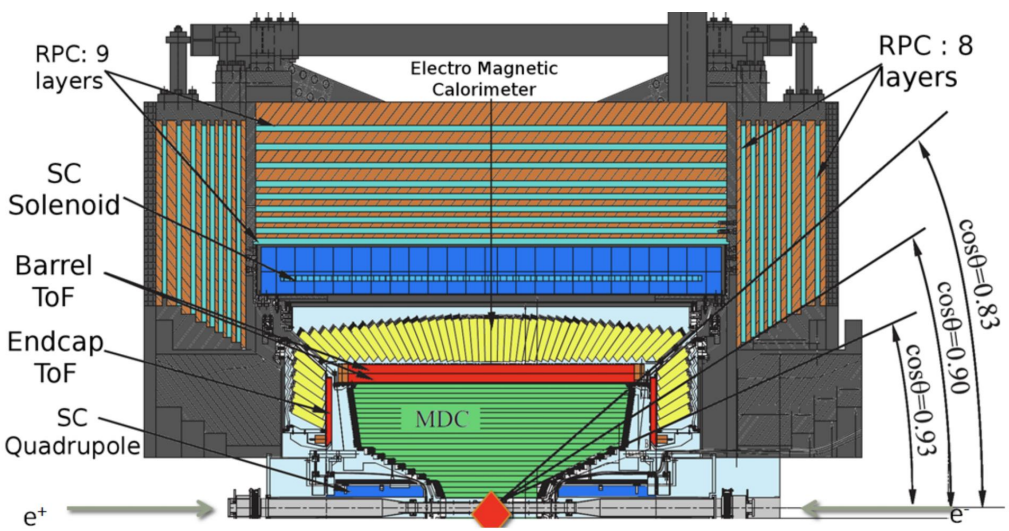
[2] Institute of High Energy Physics, CAS, Beijing

Outline

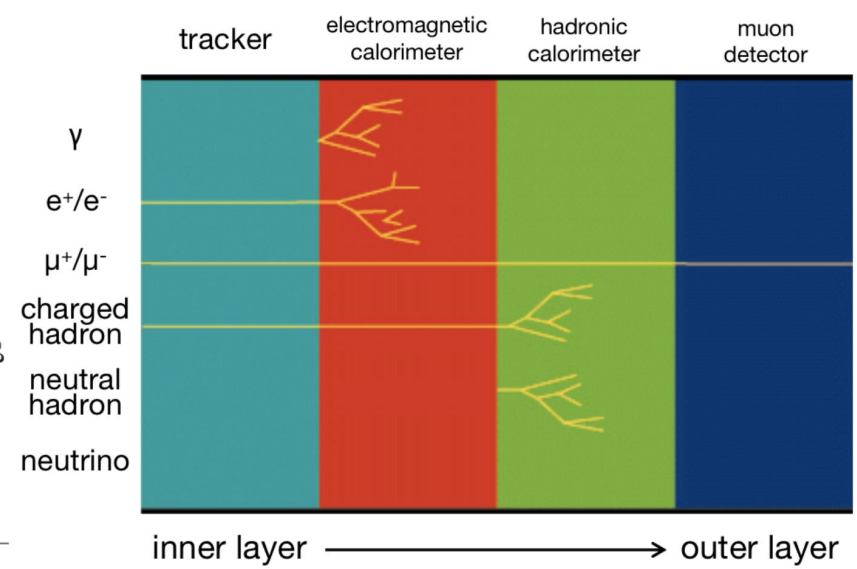
- Motivation
- Working principle of Quantum SVM
- Results obtained from quantum simulator
- Results obtained from OriginQ Wuyuan hardware
- Summary

Motivation: Particle Identification at BESIII

- PID performance is critical for various physics studies at BESIII
- Machine learning has armed PID with a powerful toolbox
  - Frequently used models include deep NN and tree based models
  - Good at combining information of multiple sub-detectors, especially for hard PID tasks (such as, μ/π separation in this study)



BESIII detector (upper half)



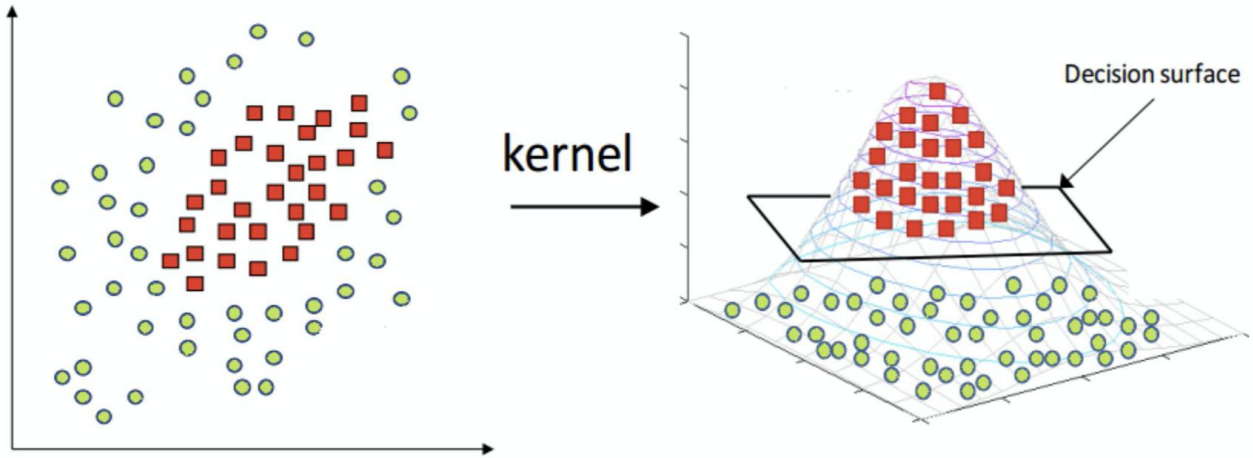
Characters of particles in sub-detectors

Motivation: Quantum Machine Learning

- Quantum computer provides a new set of tools for ML
  - Serve as a valuable alternative for classical ML models
- Potential quantum advantage for ML problems
  - Potential speed-up for training [1]
  - Data is processed in a high dimensional Hilbert spaces that is intractable on classical computers [2]
- Study quantum computing as a proof of concept
  - Test Under Noisy Intermediate-Scale Quantum (NISQ) device
  - Explore and demonstrate of the potential of quantum computer in HEP experiments [3-5]
  - Pave the way for future applications (e.g. PID, tracking, ...)

Classical Support Vector Machine

- Support Vector Machine (large margin classifier)



- The heavy part of training SVM is the computation of the kernel matrix

$$maximize \quad L(\vec{\alpha}) = \sum_{i=1}^{N} y_i \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \boxed{K(\vec{x}_i, \vec{x}_j)}$$

$$subject\ to \quad \sum_{i=1}^{N} \alpha_i y_i = 0 \ and \ \alpha_i \geq 0, \forall i = 1, 2, ..., N$$

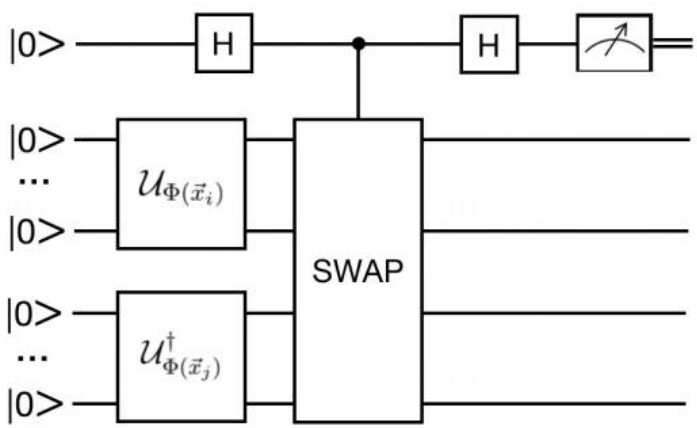
- Quantum device provides an extension of the kernel methods

Quantum Support Vector Machine

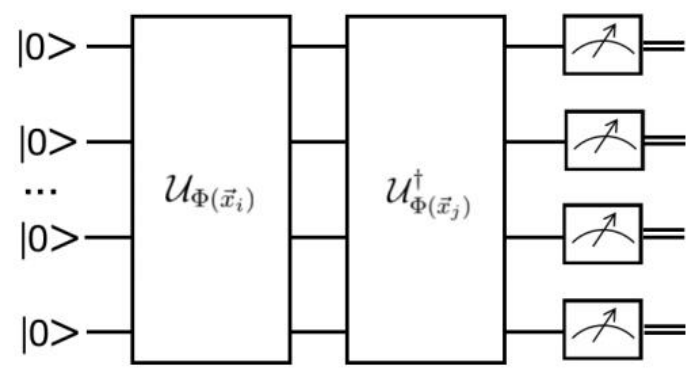
- The inner product of two quantum states representing two data points can be seen as the kernel [6]

$$K(\vec{x}_i, \vec{x}_j) = |\langle \Phi(\vec{x}_i) | \Phi(\vec{x}_j) \rangle|^2 = \left| \left\langle 0^{\otimes n} \middle| \mathcal{U}^{\dagger}_{\Phi(\vec{x}_j)} \mathcal{U}_{\Phi(\vec{x}_i)} \middle| 0^{\otimes n} \right\rangle \right|^2$$

- The quantum circuits that can estimate the kernel values:



(a)



(b)

Quantum Feature Map

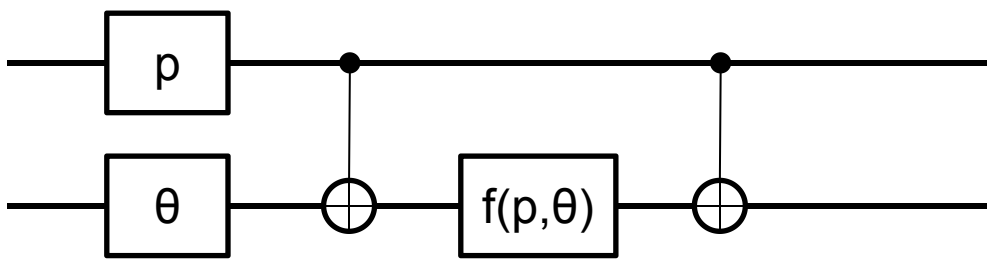
- The core part of QSVM is the encoding circuit (feature map) [7]

$$|\Phi(\vec{x}_i)\rangle = \mathcal{U}_{\Phi(\vec{x}_i)} \left| 0^{\otimes n} \right\rangle = H^{\otimes n} U_{\Phi(\vec{x}_i)} H^{\otimes n} U_{\Phi(\vec{x}_i)} \left| 0^{\otimes n} \right\rangle$$

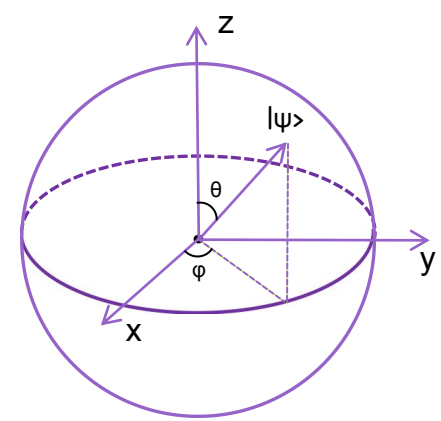
- The feature map encodes data points into the amplitude of quantum states based on Pauli rotation operators

$$U_{\Phi(\vec{x})} = exp(i \sum_{S \in [n]} \Phi_s(\vec{x}) \prod_{i \in S} P_i) \qquad \Phi_s(\vec{x}) = \begin{cases} x_i & \text{for the i-th qubit} \\ (\pi - x_i)(\pi - x_j) & \text{for the i-th and the j-th qubits} \end{cases}$$

Z,ZZ



x : rotate x angle around z axis



Training Sample and Baseline Models

- BESIII MC Sample:
  - Single $\mu^{\pm}$ and $\pi^{\pm}$ tracks from MC, 20000 training tracks and 10000 test tracks per dataset
  - Cross validation on 20 datasets
  - Nine selected features:
    - Reconstructed momentum and direction
    - PID likelihood from TOF and dE/dX
    - Shower shape in EMC
    - Penetration depth in MUC
- Baseline models are carefully tuned as control group
  - Classical SVM: scikit-learn 0.24.1
  - BDT: py-xgboost 0.90
  - MLP: tensorflow 2.4.1

Scan of Various Encoding Circuits

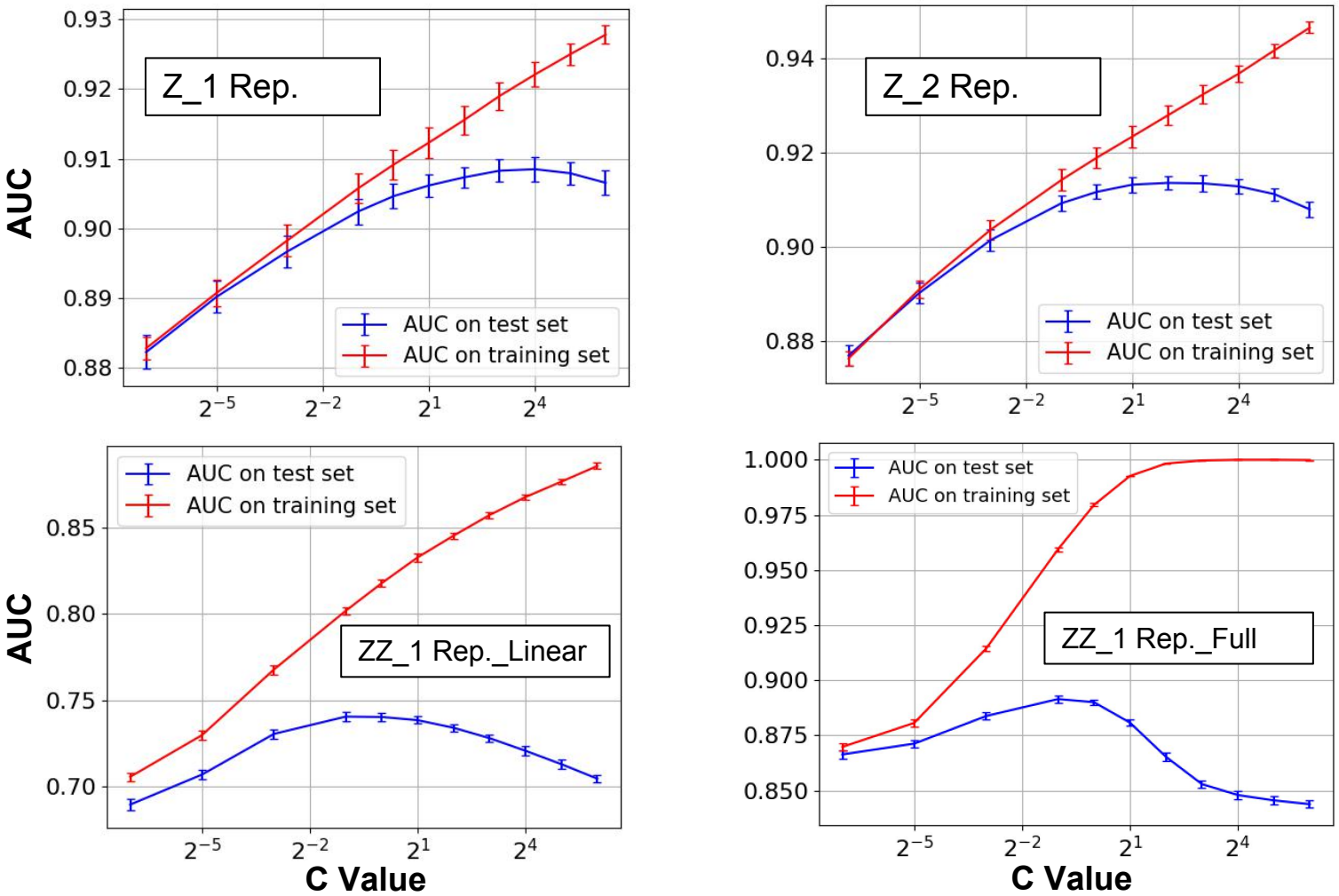
- Various types of encoding circuits are simulated using qiskit
  - A few simple circuits show comparable performance
  - Complicated circuits are prone to overfitting

Classical Model	AUC
SVM	0.91234±0.0030
BDT	0.91292±0.0024
MLP neural network	0.90651±0.0058

Circuit	Rep.	Entanglement	Test set AUC	Training set AUC
X	2	none	0.90834±0.0030	0.91658±0.0021
	3		0.91238±0.0036	0.93055±0.0027
Z	1	none	0.90834±0.0030	0.91658±0.0020
	2		0.91238±0.0036	0.93055±0.0027
	3		0.89240±0.0036	0.90949±0.0009
XX	2	linear	0.73146±0.0037	0.84744±0.0017
		full	0.86332±0.0052	0.99887±0.0001
	3	linear	0.73198±0.0048	0.93766±0.0009
		full	0.72999±0.0047	0.99970±0.0002
ZZ	1	linear	0.73146±0.0037	0.84744±0.0025
		full	0.86332±0.0052	0.99887±0.0002
	2	linear	0.73198±0.0048	0.93767±0.0009
		full	0.72999±0.0047	0.99970±0.0002
	3	linear	0.67960±0.0040	0.88481±0.0004
		full	0.62707±0.0035	0.99964±0.0001
X, XX	2	linear	0.87201±0.0043	0.97902±0.0012
		full	0.88359±0.0021	0.99974±0.0001
	3	linear	0.84779±0.0010	0.99364±0.0002
		full	0.80892±0.0020	1.00000±0.0000
X, ZZ	1	linear	0.73145±0.0037	0.84745±0.0034
		full	0.86332±0.0052	0.99886± 0.0011
	2	linear	0.84441±0.0029	0.99136±0.0013
		full	0.82086±0.0029	1.00000±0.0000
	3	linear	0.84892±0.0029	0.99551±0.0002
		full	0.70668±0.0031	1.00000±0.0000
Z, ZZ	1	linear	0.87423±0.0024	0.97972±0.0004
		full	0.88378±0.0039	0.99974±0.0001
	2	linear	0.84675±0.0022	0.99253±0.0010
		full	0.80875±0.0032	1.00000±0.0000
	3	linear	0.83464±0.0030	0.99512±0.0003
		full	0.69984±0.0026	1.00000±0.0000

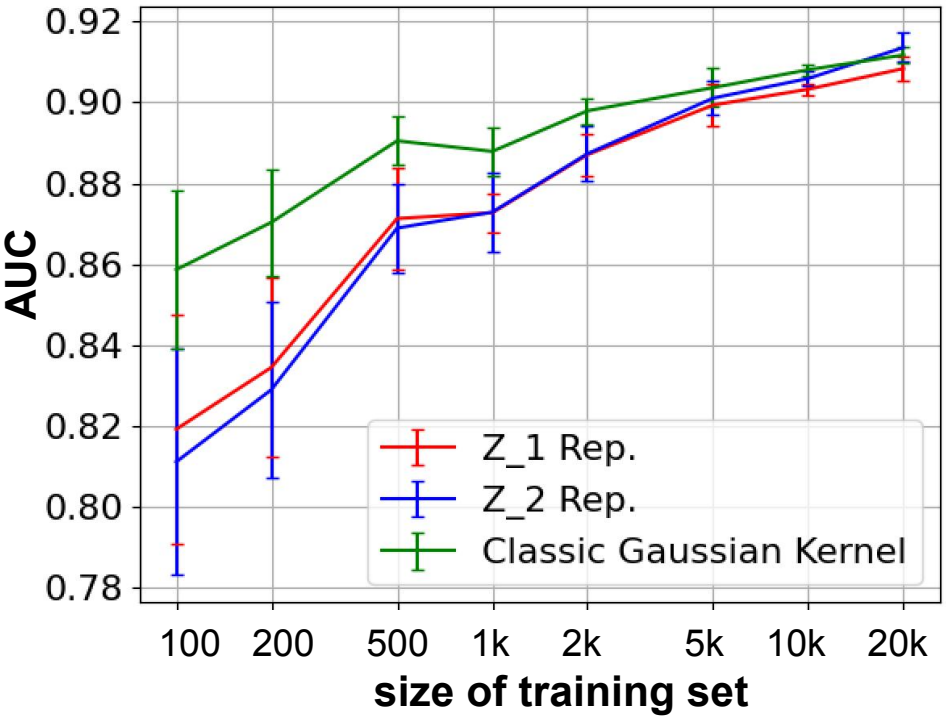
Influence of the Regularization Parameter

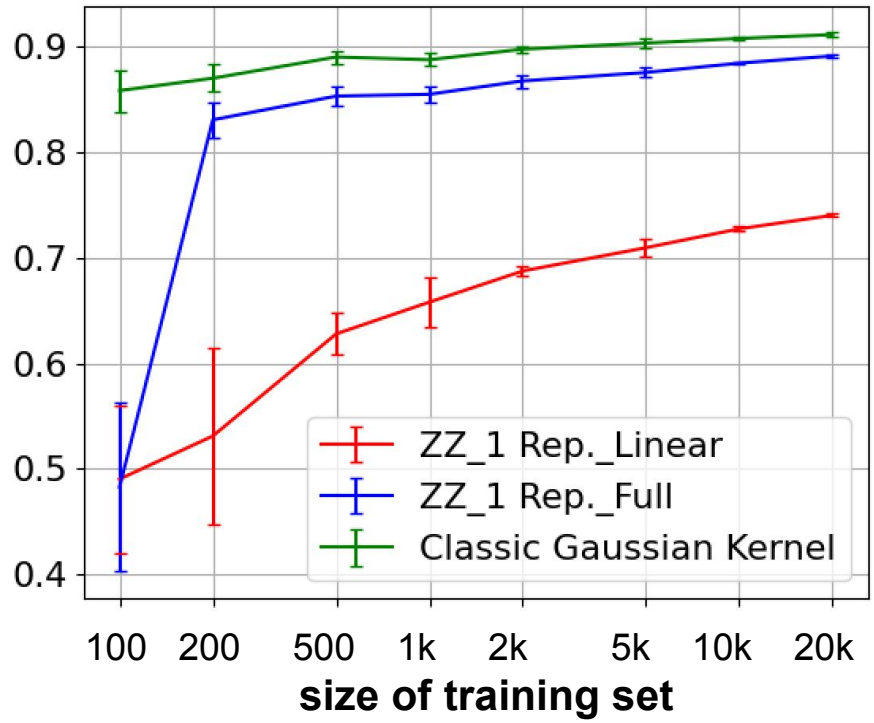
- The influence of the SVM regularization parameter can be carefully tuned to handle the overfitting/underfitting trade-off



Influence of the training size

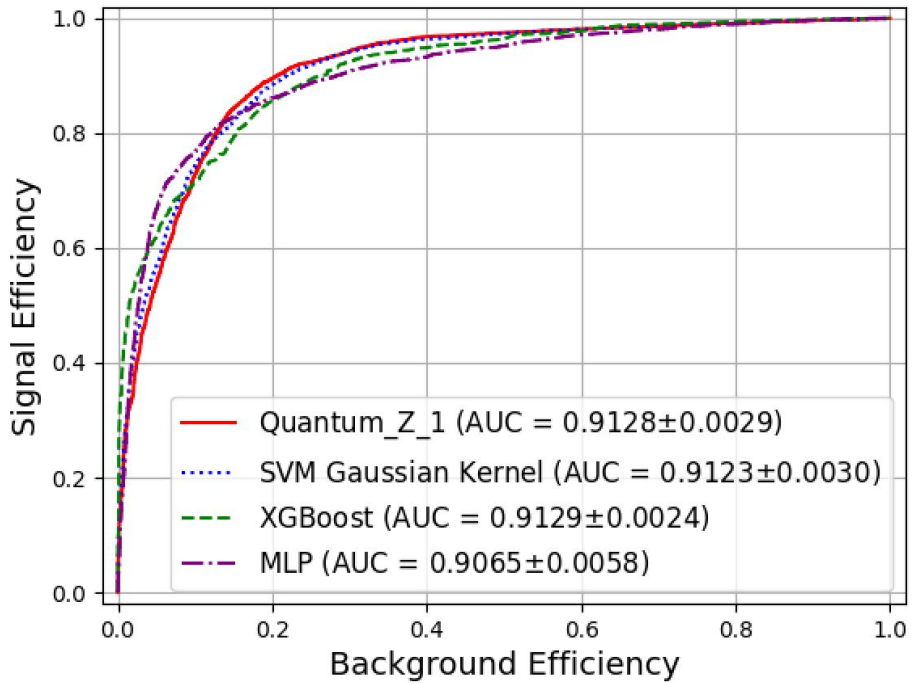
- Different size of the training set are tested
  - The quantum SVM usually shows unstable performance when the training size is small
  - Some circuits start to overtake Gaussian kernel with larger training sets

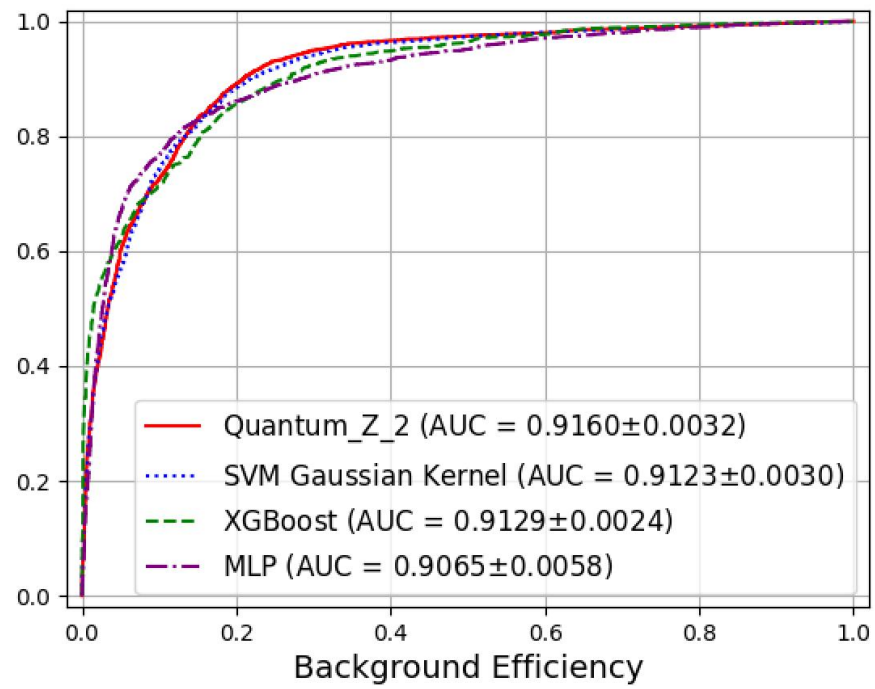




Comparison with Traditional Models

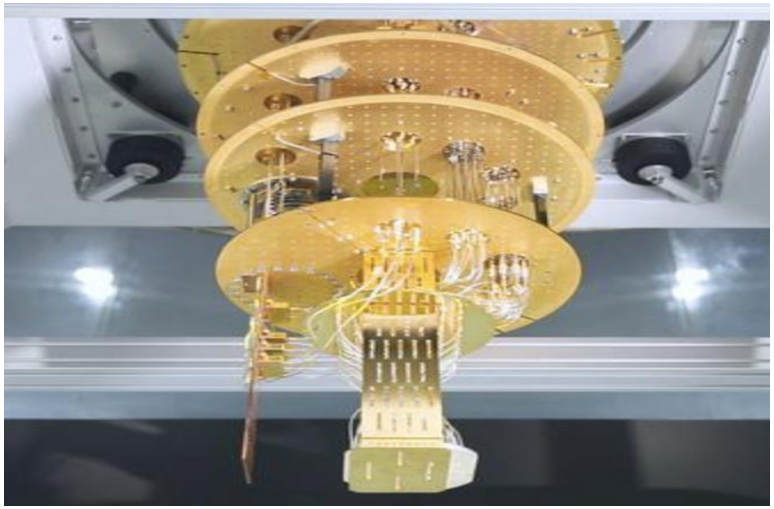
- The discrimination power is compared with the baseline models
  - After the fine tuning of hyper-parameters
  - Similar discrimination power can be achieved





Run on the Quantum Hardware

- It's interesting to see how the noise from real hardware affects the performance
- The OriginQ Wuyuan system based at Hefei, China [8]
  - Based on super-conducting technology
  - 6 qubits, controlled by QPanda API
- Procedure of running QSVM model
  - Design quantum circuits
  - Generate Qpanda code
  - Submit jobs to calculate the Kernel Matrix
  - Train and evaluate the models



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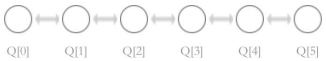
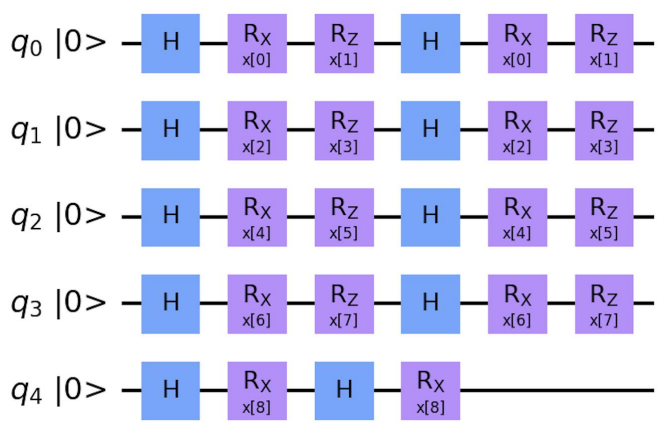


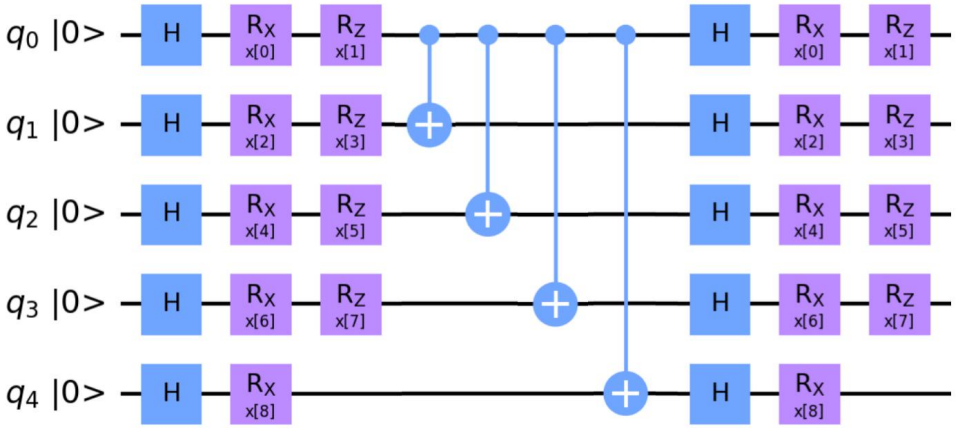
芯片详细参数

量子比特编号	工作频率(MHz)	T1(μs)/T2(μs)	读取保真度F0/F1	平均单比特门 保真度
Q0	5442	17/12.6	0.989/0.965	0.9993
Q1	4470	30/2.3	0.95/0.859	0.9990
Q2	5319	20/2.6	0.975/0.951	0.9990
Q3	4696	32/6.6	0.958/0.923	0.9991
Q4	5214.995	36/3.3	0.984/0.967	0.9992
Q5	4579.685	28/5.4	0.914/0.845	0.9992

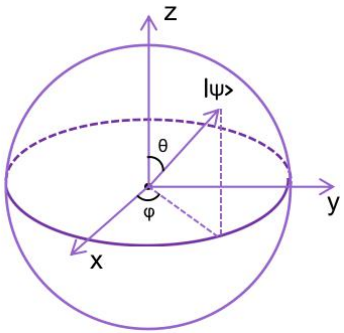
Compressed Feature Map on Quantum Hardware

- Two feature maps are re-designed to meet the limited number of qubits on the Wuyuan system
  - Two features are encoded into each qubit, based on the R_X and R_Z rotations



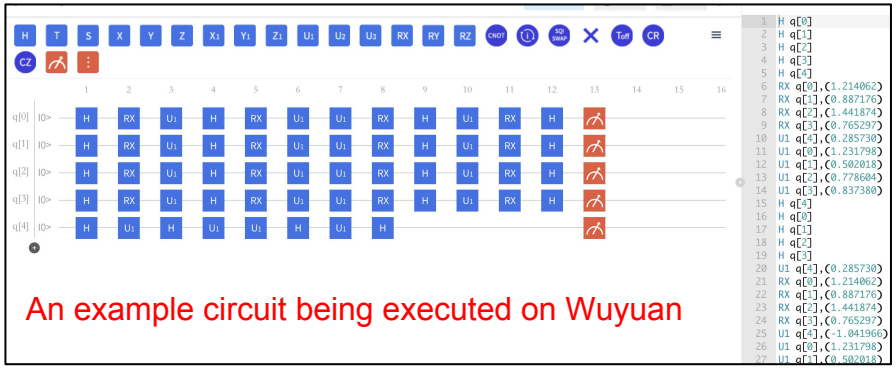


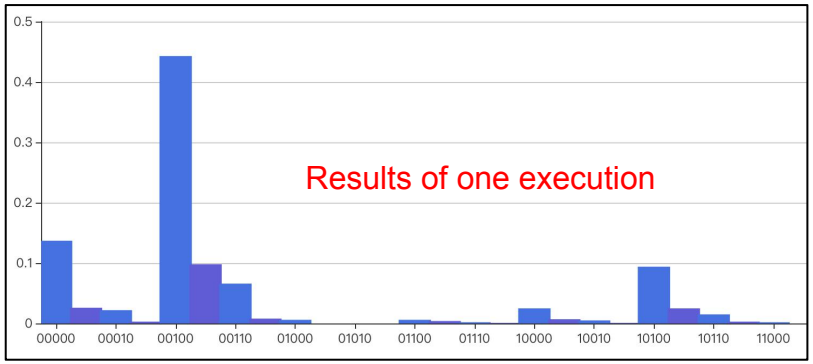
  - The feature map structure is carefully tuned for the best simulation results
    - AUC (1): 0.90373±0.0024
    - AUC (2): 0.91029±0.0023



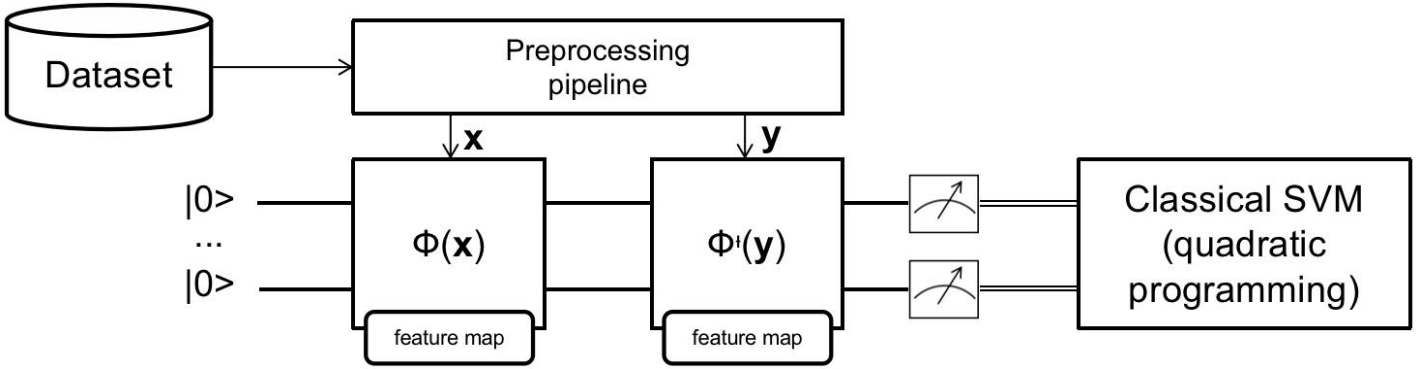
Job Execution on the Wuyuan System

- The quantum circuits are generated based on the dataset, then uploaded to the Wuyuan system via QPanda
  - Quantum circuits are automatically optimised against the Wuyuan system



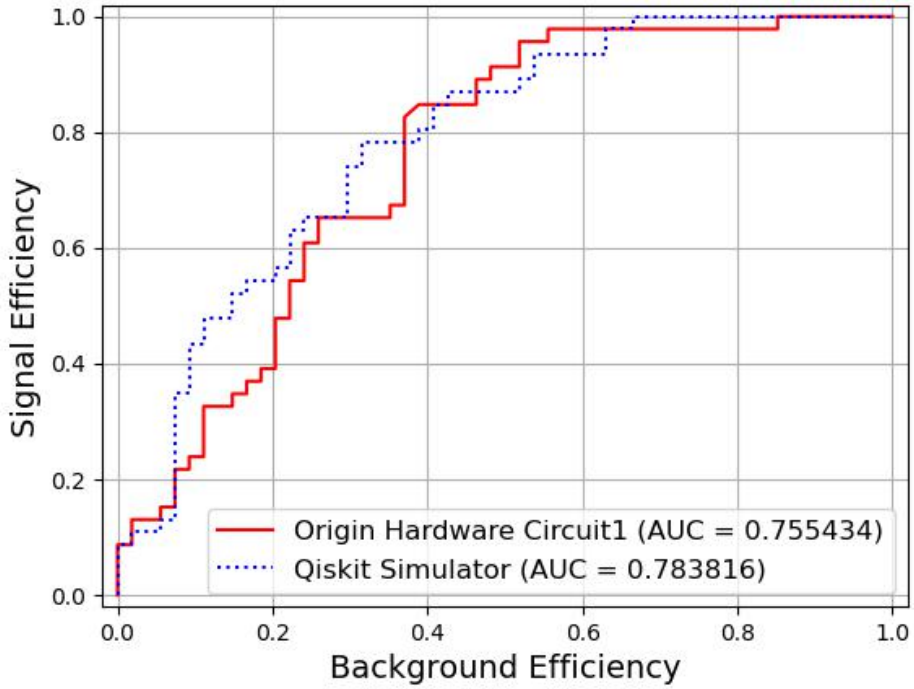


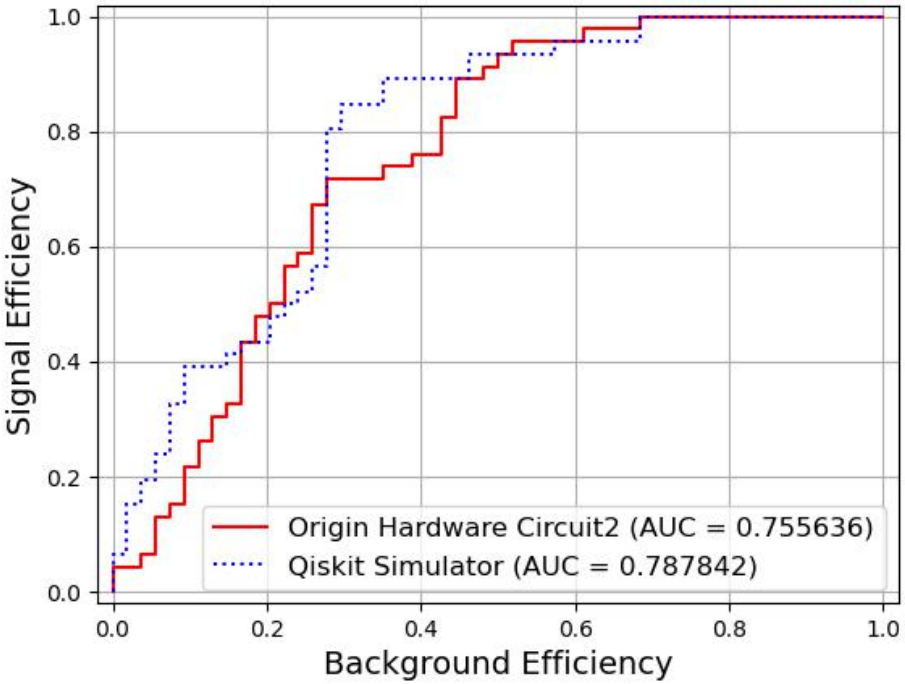
  - Results are transferred back to the classical computer for downstream computations



Results from the Hardware

- Results from Origin Wuyuan
  - Results obtained from 100 training tracks and 100 test tracks, averaged from three runs
  - The noise compromises the performance, but at a controllable level





Summary and Work in Progress

- **Summary**
  - A μ/π classifier based on quantum SVM is developed and studied
  - A wide range of encoding methods are evaluated
    - A few ones show comparable performance with classical models
    - Others show potential to classify much more complicated data
  - Efforts have been made to run the model on real quantum hardware
- **Work in progress**
  - A quantum neural network model is also being evaluated

References

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