Application of Quantum Machine Learning on PID at BESIII

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Outline

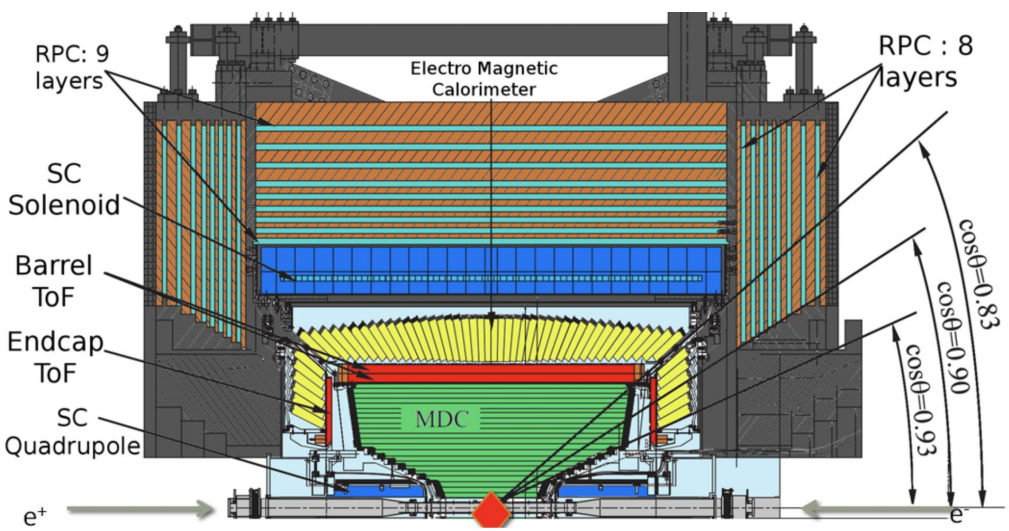
- Motivation
- Method I: Quantum Support Vector Machine
- Method II: Variational Quantum Classifier
- Summary

Motivation: Quantum Machine Learning

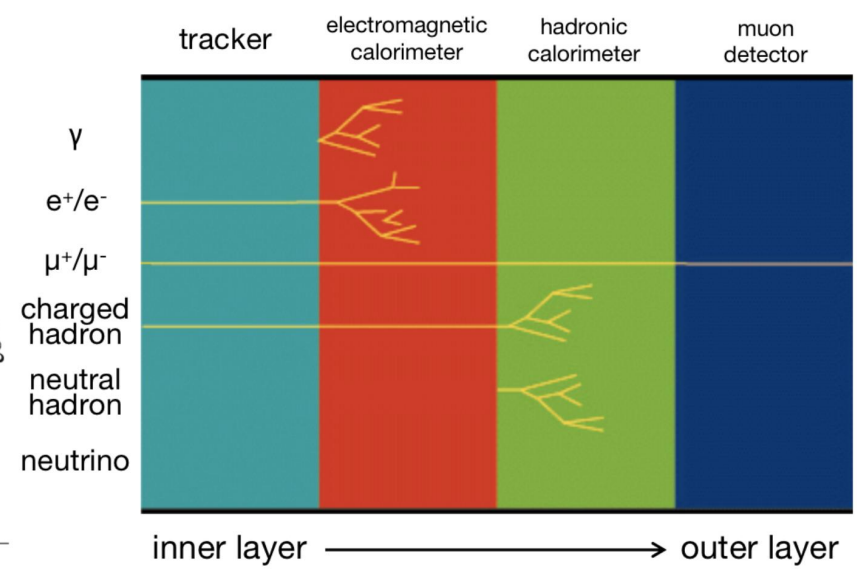
- Quantum computer provides a new set of tools for ML
  - Serve as a valuable alternative for classical ML models
- Potential quantum advantage for ML problems
  - Potential speed-up for training [1]
  - Data is processed in a high dimensional Hilbert spaces that is intractable on classical computers [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. analysis, tracking, ...)

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

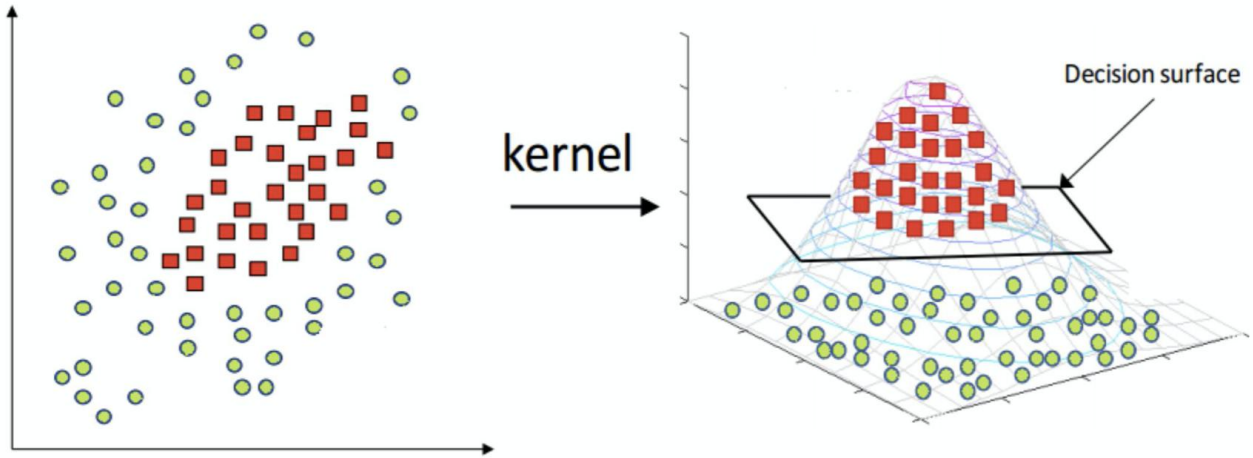
Training Sample and Baseline Models

- 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

Method I
Quantum Support Vector Machine

Classical Support Vector Machine

- Support Vector Machine (large margin classifier)



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

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

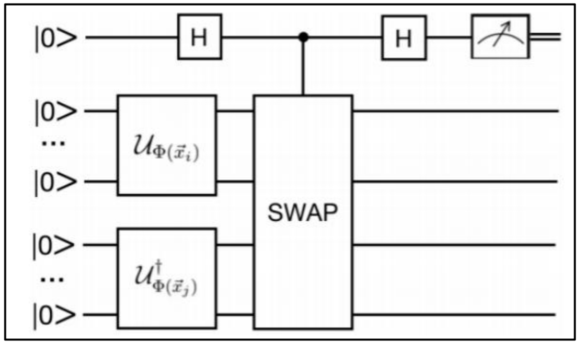
$$subject\ to \quad \sum_{i=1}^{N} \alpha_i y_i = 0 \ and \ \alpha_i \geq 0, \forall i = 1, 2, ..., N$$

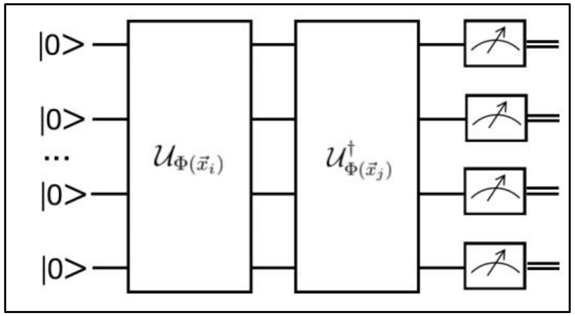
- Quantum device provides an extension of the kernel methods

Quantum Support Vector Machine

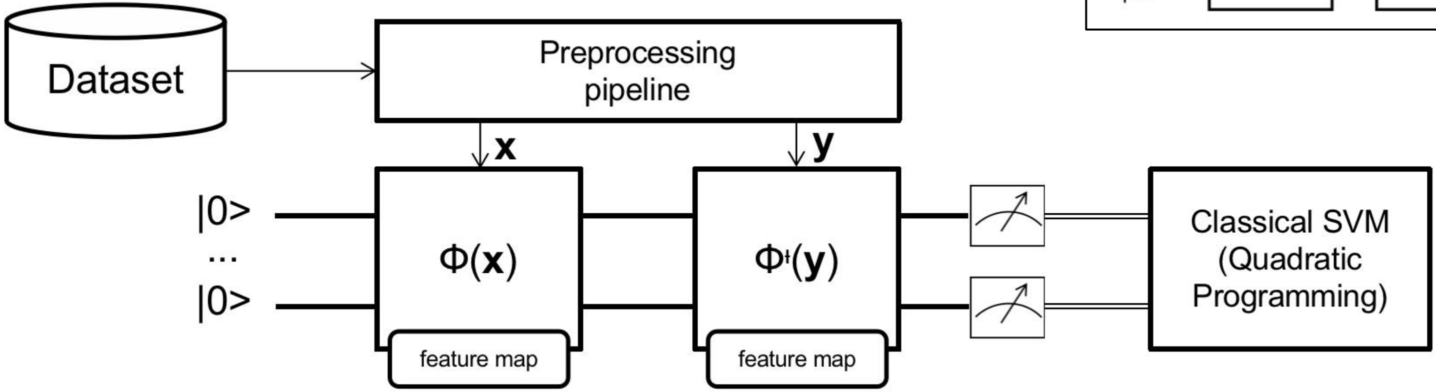
- The inner product of two quantum states representing two data points can be seen as the kernel [6]

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





- Overview of Quantum SVM:



Quantum Feature Map

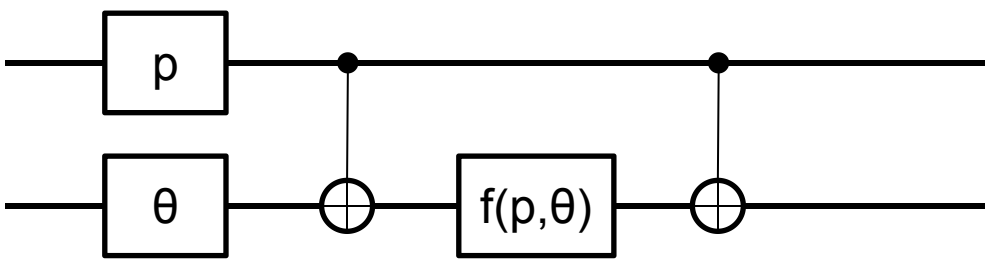
- The core part of QSVM is the encoding circuit (feature map) [7]

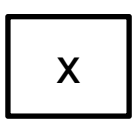
$$|\Phi(\vec{x}_i)\rangle = \mathcal{U}_{\Phi(\vec{x}_i)} \left| 0^{\otimes n} \right\rangle = H^{\otimes n} U_{\Phi(\vec{x}_i)} H^{\otimes n} U_{\Phi(\vec{x}_i)} \left| 0^{\otimes n} \right\rangle$$

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

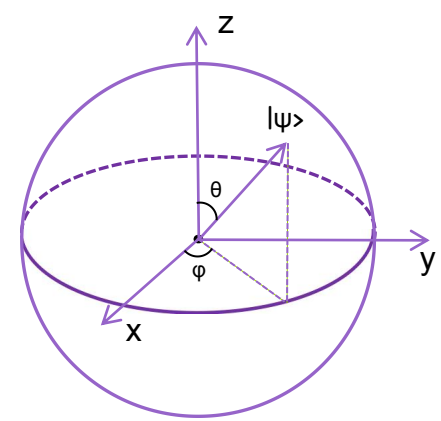
$$U_{\Phi(\vec{x})} = exp(i \sum_{S \in [n]} \Phi_s(\vec{x}) \prod_{i \in S} P_i) \qquad \Phi_s(\vec{x}) = \begin{cases} x_i & \text{for the i-th qubit} \\ (\pi - x_i)(\pi - x_j) & \text{for the i-th and the j-th qubits} \end{cases}$$

Z,ZZ





: rotate x angle around z axis



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

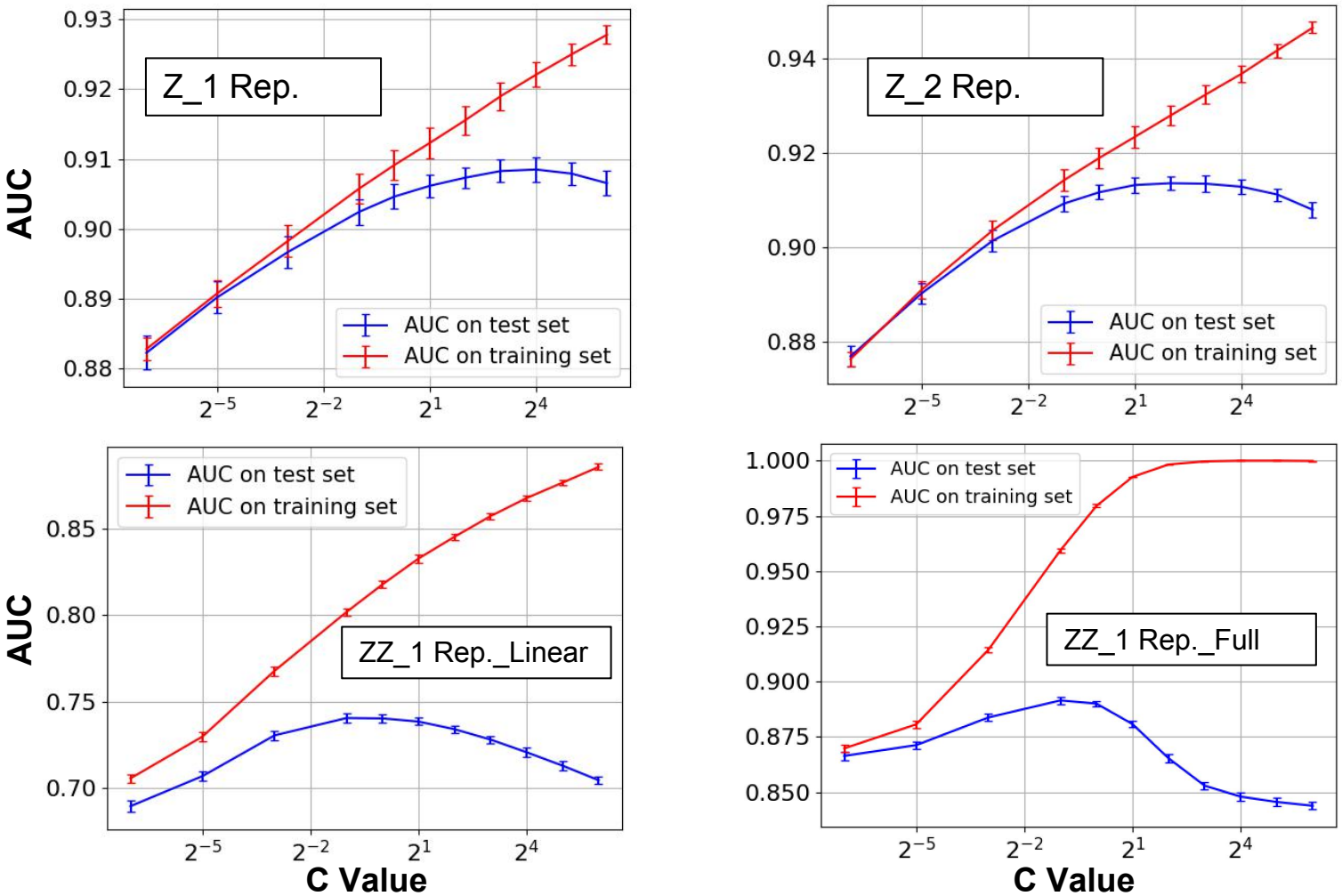
Circuit	Rep.	Entanglement	Test set AUC	Training set AUC
X	2	none	0.90834±0.0030	0.91658±0.0021
	3		0.91238±0.0036	0.93055±0.0027
Z	1	none	0.90834±0.0030	0.91658±0.0020
	2		0.91238±0.0036	0.93055±0.0027
	3		0.89240±0.0036	0.90949±0.0009
XX	2	linear	0.73146±0.0037	0.84744±0.0017
		full	0.86332±0.0052	0.99887±0.0001
	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

Classical Model	AUC
SVM	0.91234±0.0030
BDT	0.91292±0.0024

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

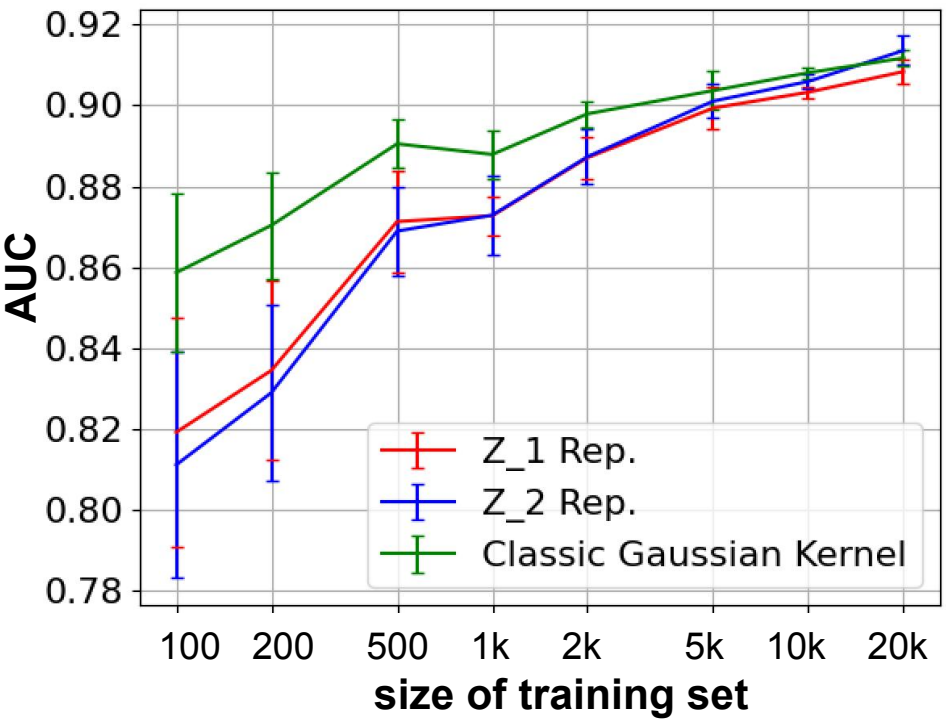
Influence of the Regularization Parameter

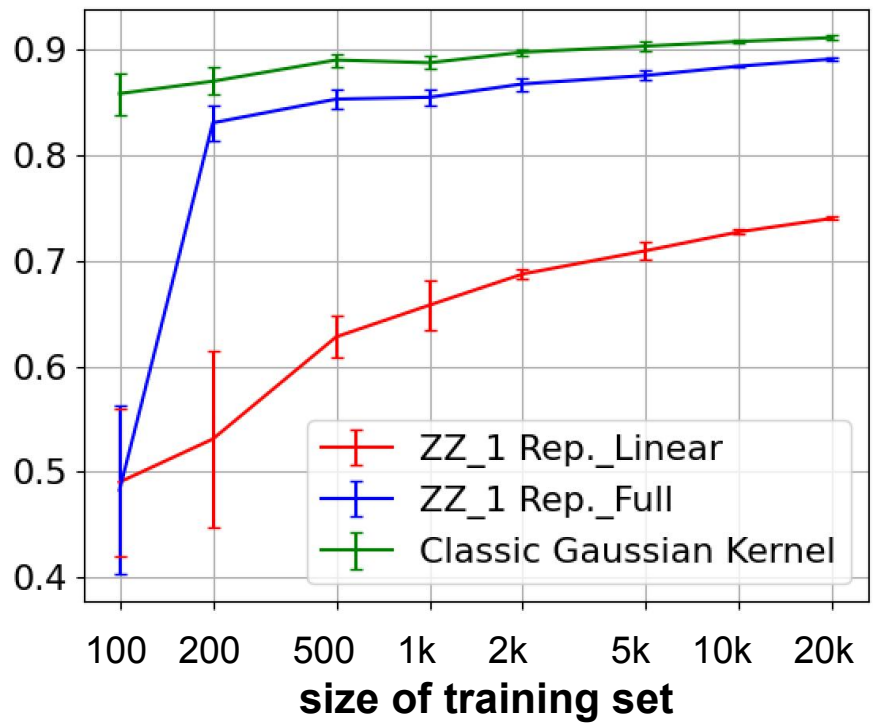
- The influence of the SVM regularization parameter can be carefully tuned to handle the overfitting/underfitting trade-off



Influence of the training size

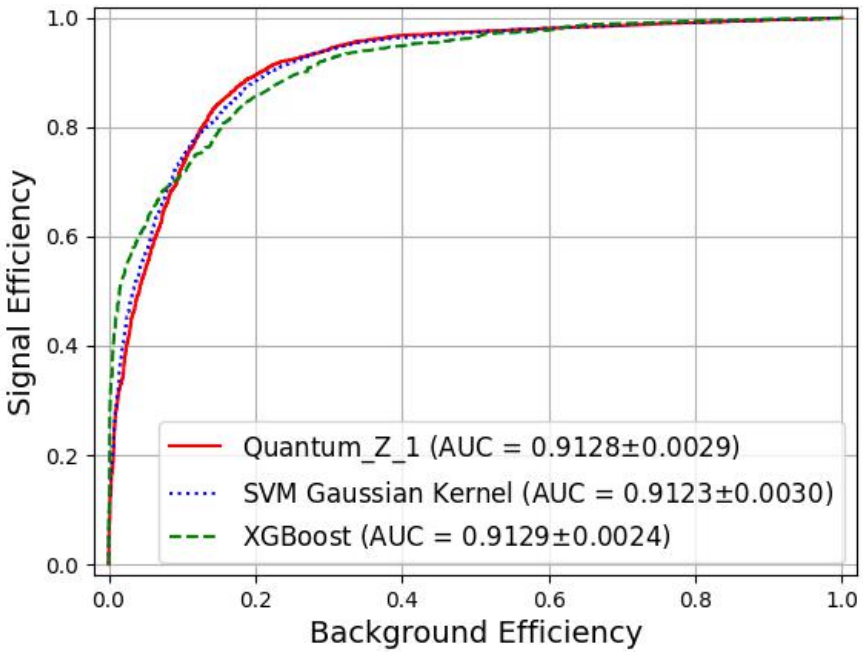
- Different size of the training set are tested
  - The quantum SVM usually shows unstable performance when the training size is small
  - Some circuits start to overtake Gaussian kernel with larger training sets

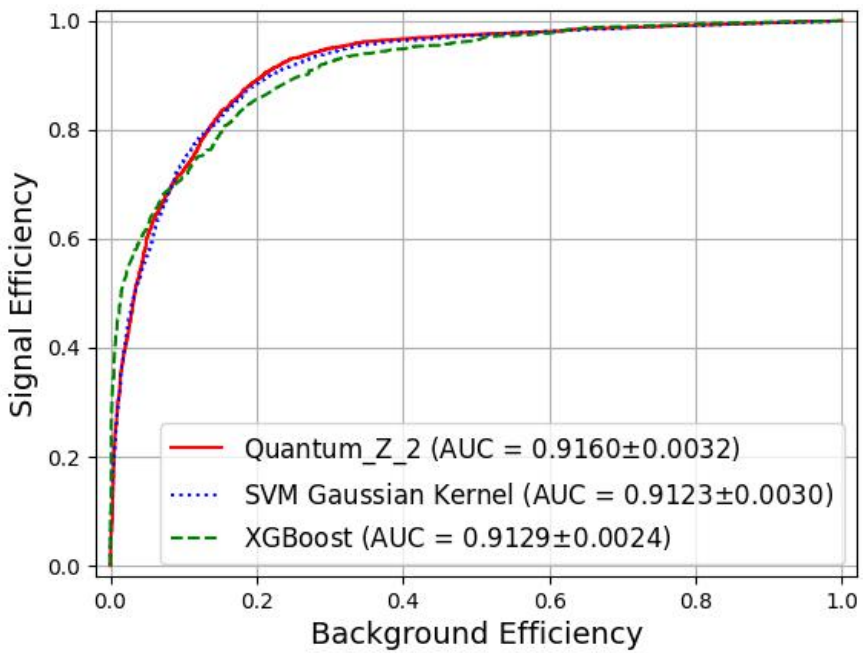




Comparison with Traditional Models

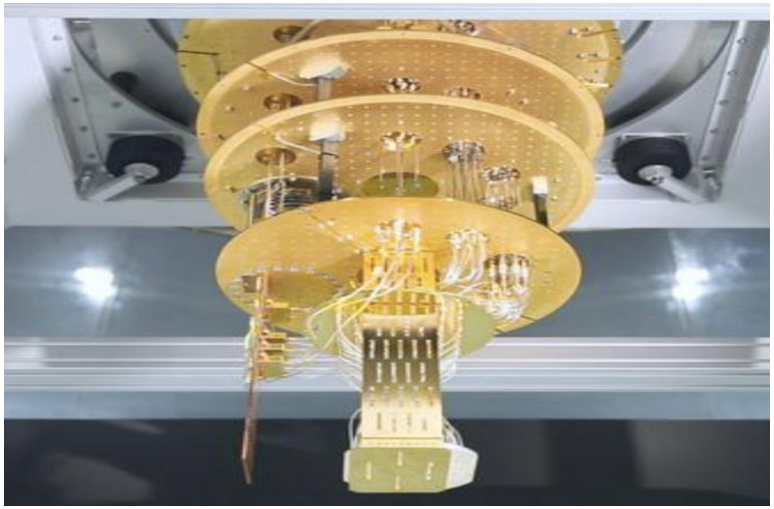
- The discrimination power is compared with the baseline models
  - After the fine tuning of hyper-parameters
  - Similar discrimination power can be achieved





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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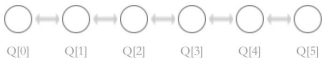
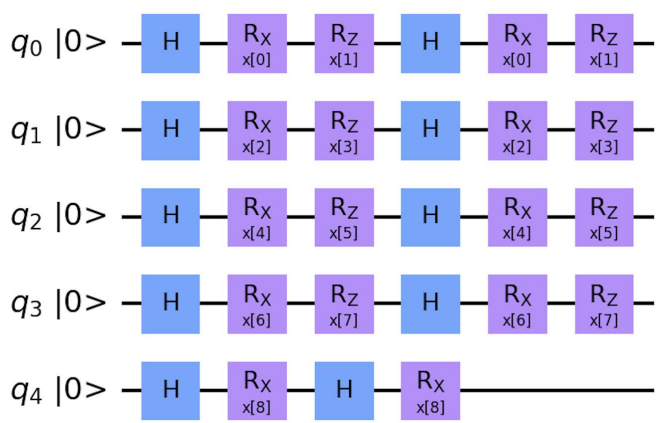


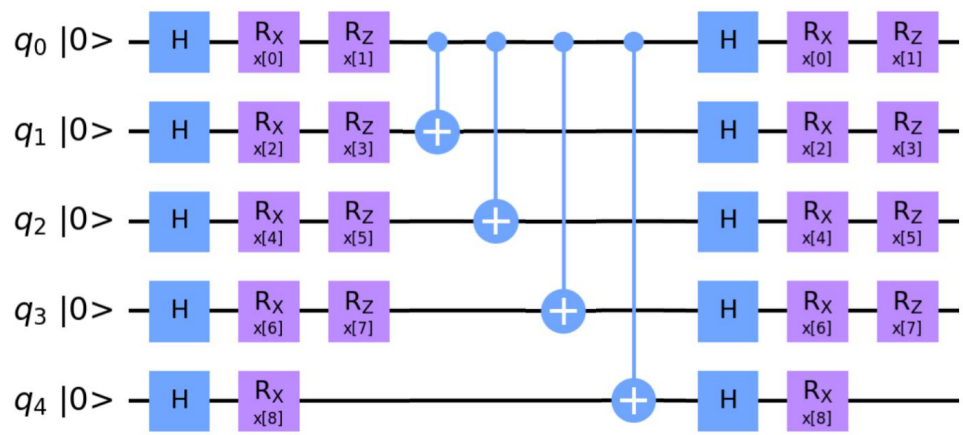
芯片详细参数

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

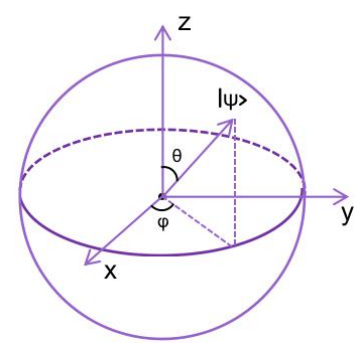
Compressed Feature Map on Quantum Hardware

- 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



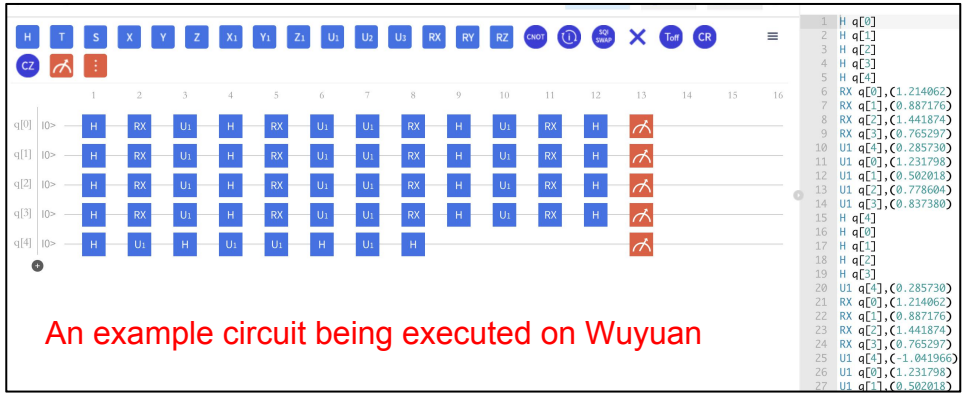


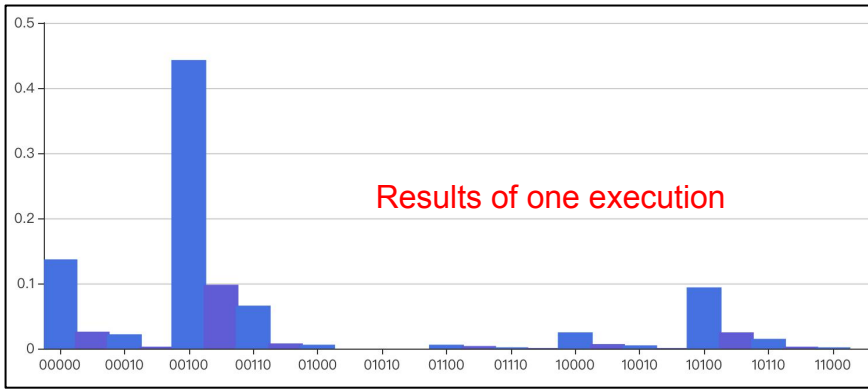
  - The feature map structure is carefully tuned for the best simulation results
    - AUC (1): 0.90373±0.0024
    - AUC (2): 0.91029±0.0023



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 optimized against the Wuyuan system

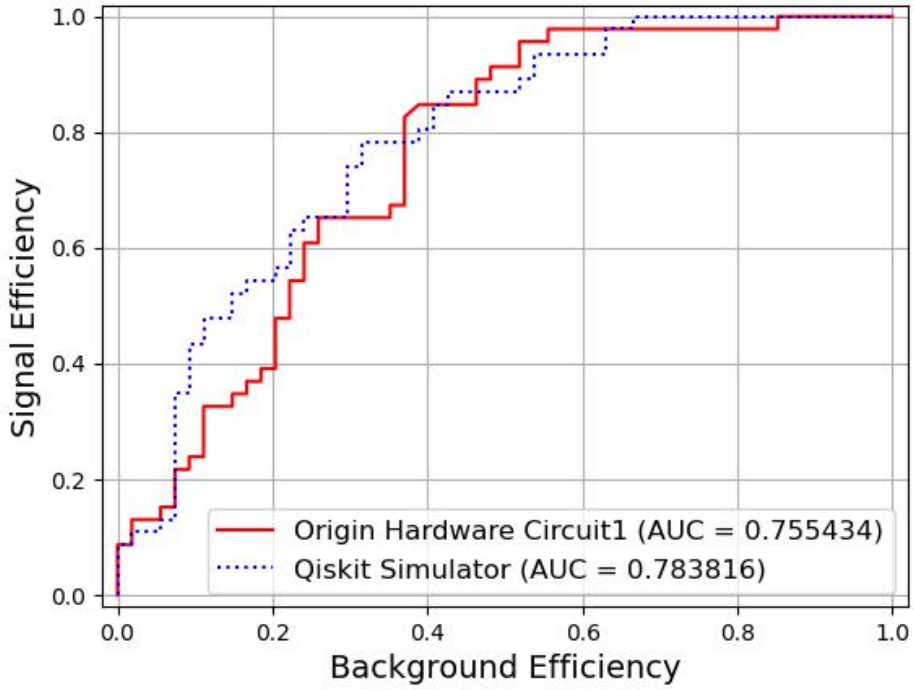


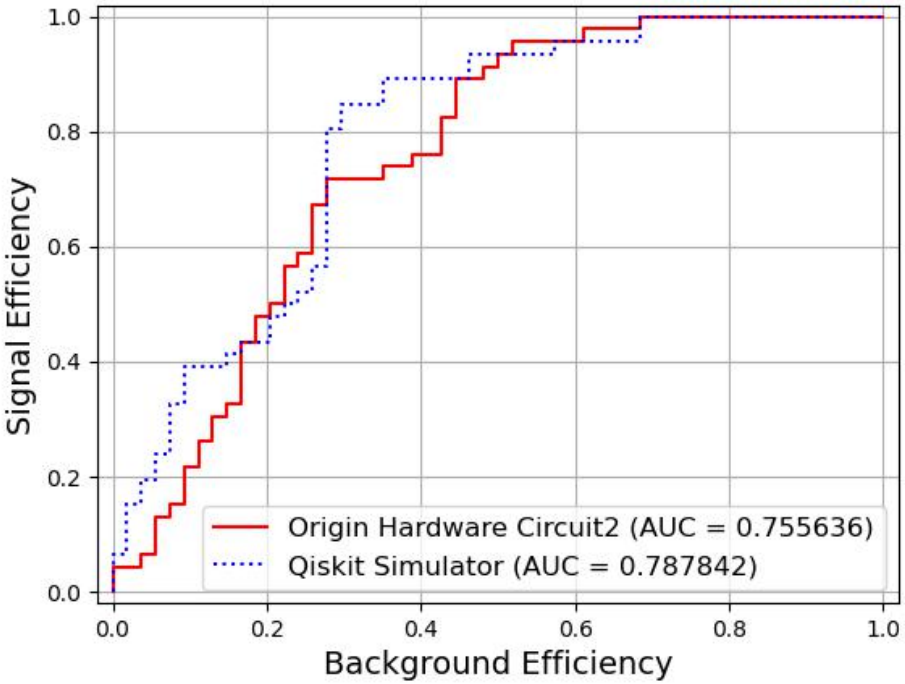


  - Results are transferred back to the classical computer for downstream computations

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

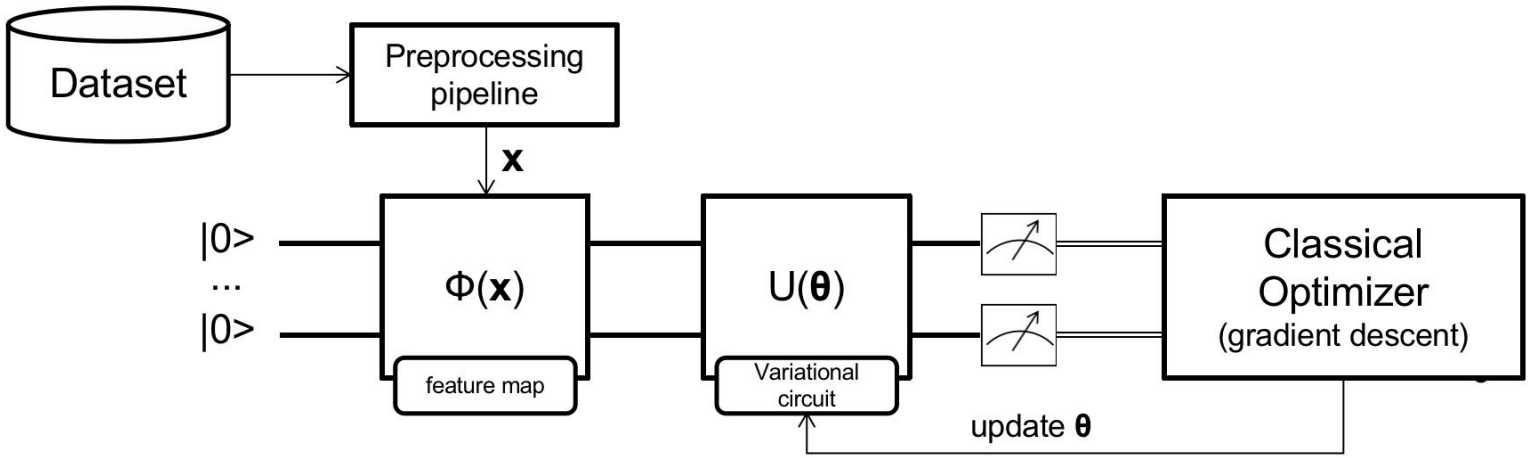




Method II
Variational Quantum Classifier

Variational Quantum Classifier: Introduction

- Variational Quantum Classifier as a hybrid model



- A subsequent variational (train-able) circuit performs a linear transformation on the prepared state
- The parameters of the variational circuit can be trained based on the gradients calculated classically
- Data is classified by measuring the output qubit(s). (estimating the probabilities of each state)

Optimization of VQC

- As a 'quantum neural network', the key issue is to optimize the free parameters of the variational circuits
  - Traditional backward propagation is impossible due to the limits of quantum theory
  - The numerical differentiation method was usually used previously to calculate the gradients

$$\frac{\mathrm{d}f(\theta)}{\mathrm{d}\theta} \approx \frac{f(\theta+h)-f(\theta-h)}{2h} + \boxed{O\left(h^2\right)} \longrightarrow \text{the } \textit{error} \text{ term}$$

  - Currently, the gradient is more popularly computed based on the **parameter shift rule** [9]

$$\frac{d}{d\theta} f(\theta) = r(f(\mu+s) - f(\mu-s))$$

Search of Optimal Encoding Circuits

- A wide range of encoding circuits is simulated as well
  - Relatively simpler (X_3, Z_2) circuits provide better discrimination power. This is simillar with results from qSVM
  - Overfitting is less obvious comparing to qSVM

Circuit	Repetitions[1]	Entanglement[2]	Training set AUC[3]	Test set AUC[3]
X	2	none	0.85733±0.0158	0.83719±0.0334
	3		0.86581±0.0242	0.84354±0.0309
XX	2	linear	0.70366±0.2394	0.62051±0.0511
		full	0.74656±0.1962	0.61870±0.0456
	3	linear	0.69882±0.0331	0.56579±0.0850
		full	0.73998±0.0367	0.53483±0.0422
Z	1	none	0.84914±0.0416	0.81800±0.0607
	2		0.87338±0.0134	0.84729±0.0282
	3		0.75637±0.0349	0.70577±0.0965
ZZ	1	linear	0.69493±0.0274	0.59169±0.0770
		full	0.76208±0.2652	0.61317±0.0334
	2	linear	0.71653±0.0280	0.61720±0.0519
		full	0.72435±0.0267	0.55957±0.0497
	3	linear	0.71762±0.0274	0.59083±0.0377
		full	0.75620±0.0242	0.50290±0.0308
X,XX	2	linear	0.68095±0.0195	0.48709±0.0310
		full	0.74749±0.0258	0.52300±0.0423
	3	linear	0.68118±0.0165	0.51419±0.0288
		full	0.75874±0.0262	0.52024±0.0295
Z,ZZ	1	linear	0.65018±0.0100	0.49202±0.0327
		full	0.75312±0.0161	0.50179±0.0274
	2	linear	0.67567±0.0243	0.50894±0.0372
		full	0.75500±0.0259	0.50336±0.0324
	3	linear	0.65160±0.0179	0.50692±0.0387
		full	0.75223±0.0195	0.50762±0.0359
X,ZZ	1	linear	0.66164±0.0242	0.49825±0.0429
		full	0.74262±0.0202	0.50841±0.0288
	2	linear	0.66667±0.0248	0.50124±0.0381
		full	0.75893±0.0163	0.49098±0.0483
	3	linear	0.68708±0.0228	0.50050±0.0531
		full	0.75371±0.0240	0.48624±0.5777

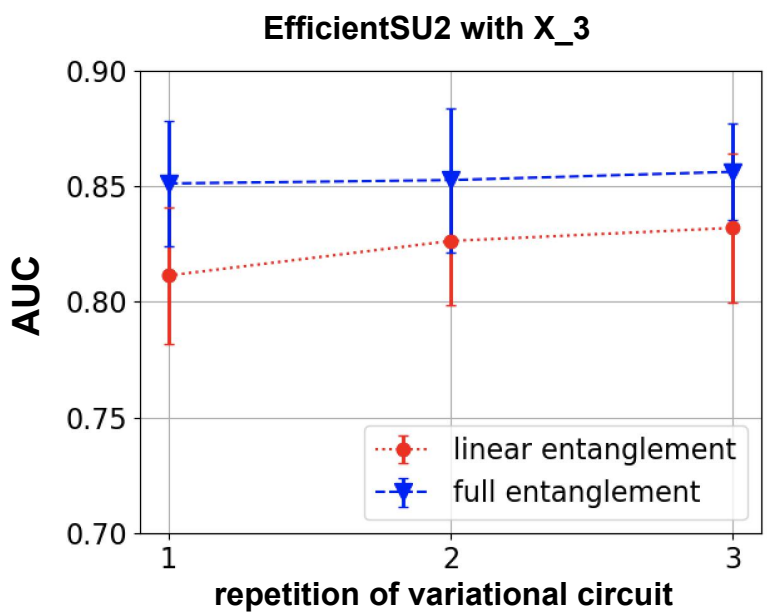
Search of Optimal Variational Circuits

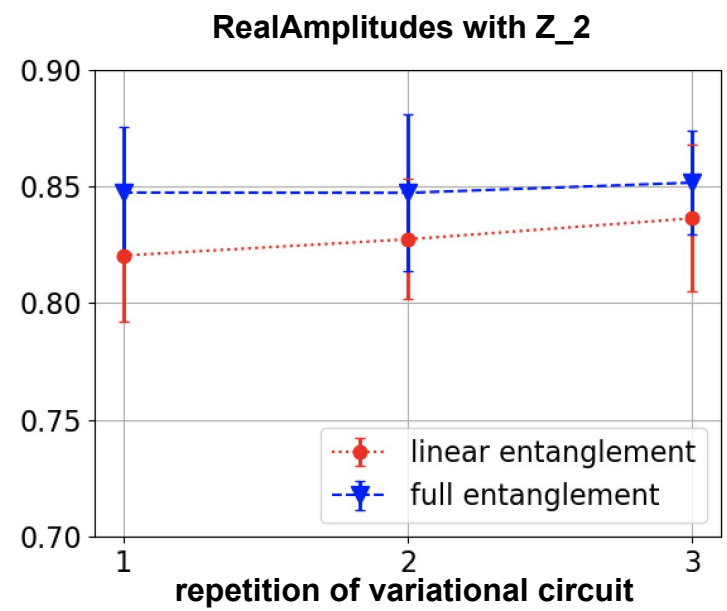
- A set of pre-studied N-Local ansatz are scanned based on the optimal encoding circuits
  - EfficientSU2: ansatz with single qubit spanned by SU(2) and CX
  - PauliTwoDesign: ansatz with single qubit Pauli rotations and pairwise CZ entanglements
  - RealAmplitudes: ansatz with single qubit Y rotations and pairwise CX entanglements
  - TwoLocal: ansatz with flexible rotation layers and entanglement layers
  - ExcitationPreserving: heuristic excitation-preserving wave function ansatz
- For X_3 and Z_2, the best variational circuits are EfficientSU2 and RealAmplitudes, respectively

variational circuit	Test set AUC with X_3	Test set AUC with Z_2
EfficientSU2	0.84983±0.0292	0.84514±0.0365
ExcitationPreserving	0.42660±0.0327	0.52333±0.0280
PauliTwoDesign	0.74614±0.0277	0.76688±0.0425
RealAmplitudes	0.84656±0.0303	0.84711±0.0277
TwoLocal	0.84102±0.0330	0.84707±0.0272

Search of Optimal Variational Cirtcuits

- Performance of different ansatz structures
  - Different entanglement methods and ansatz depth are simulated to study the impact on the performance
  - In general, the full entanglement method, and deeper ansatz (with more trainable parameters) always gives better discrimination power, but also consumes much more computing resource

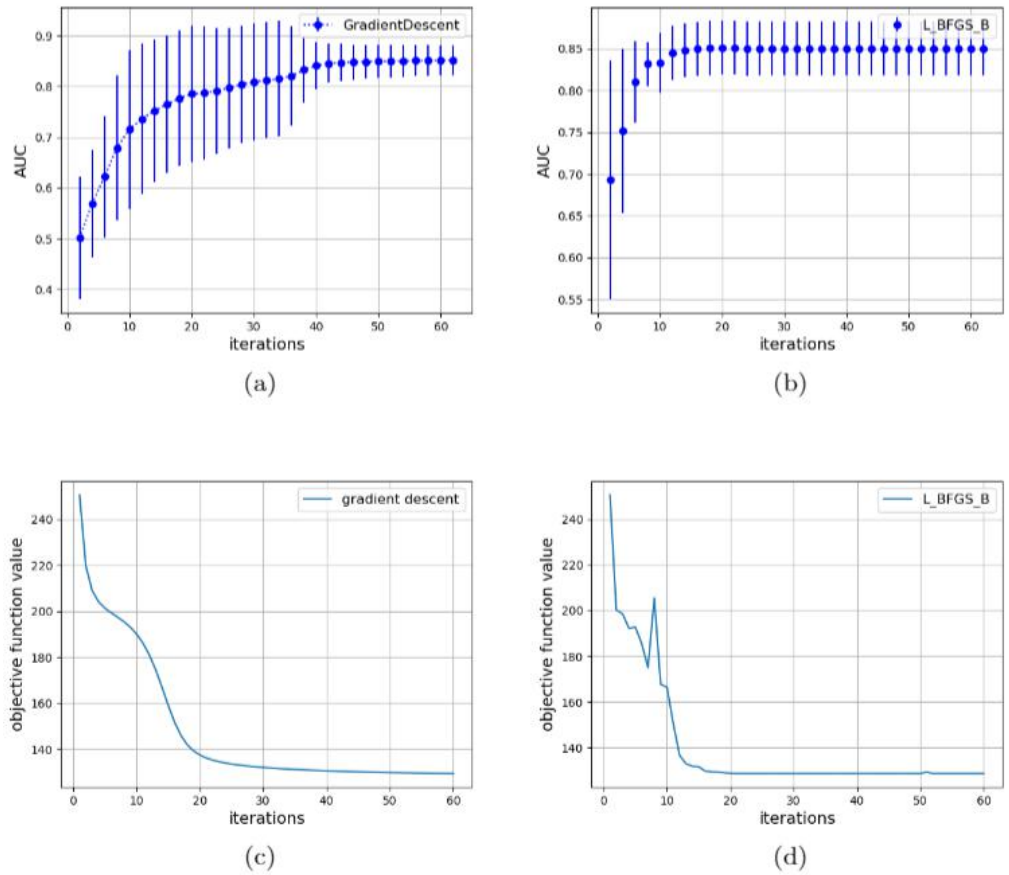




Optimization of VQC

- Common gradient descent method and Quasi-Newton method are compared

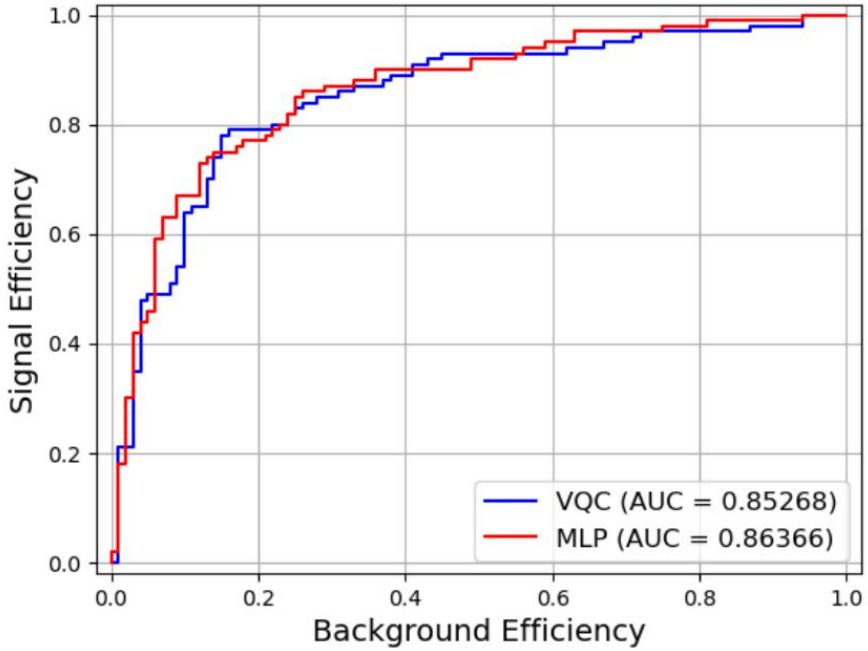
- Since L_BFGS_B (Quasi-Newton method) invokes the second derivative of the loss function, the convergence can be achieved much faster



(a)(c) Variation of AUC with the number of iterations
(b)(d) Variation in the objective function during the iteration.

Comparison with Classic MLP

- The optimal VQC is compared with the classical MLP neural network
  - VQC config: EfficientSU2 with X_3 and L_BFGS_B optimizer
  - MLP config: 400x200x100x50x15 (relu, adam)
- On small samples, VQC performs similarly to the classical MLP neural network



Summary

- Targeting at the BESIII μ/π identification problem, we studied the qSVM and VQC algorithms as a proof of concept
  - 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 are made to run the qSVM model on the Wuyuan system
  - Different optimization method and variation ansatzs are studied for the VQC
    - The design of ansatzs heavily depends on the specific problem
    - Automated way to find optimal ansatzs is desired
- The QML models show quite comparable performance comparing to their classical counterparts, showing potential to apply QML on HEP experiments

Thanks for your attention!

References

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