Identifying the Higgs boson production with Quantum Classifiers

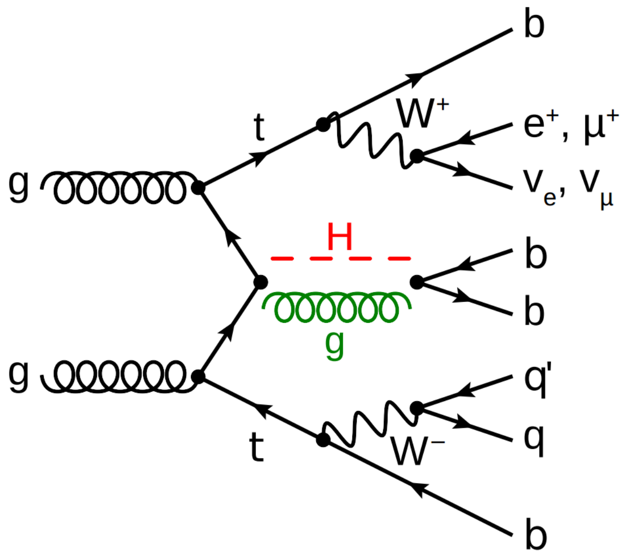
CERN openlab Technical Workshop 2021

Vasilis Belis (ETH Zurich,CERN)

Samuel G. Castillo(U. Oviedo), Christina Reissel(ETH Zurich), Sofia Vallecorsa (CERN), Elias F. Combarro (U. Oviedo,CERN)

Higgs boson production process

Consider a specific production and decay process of H :



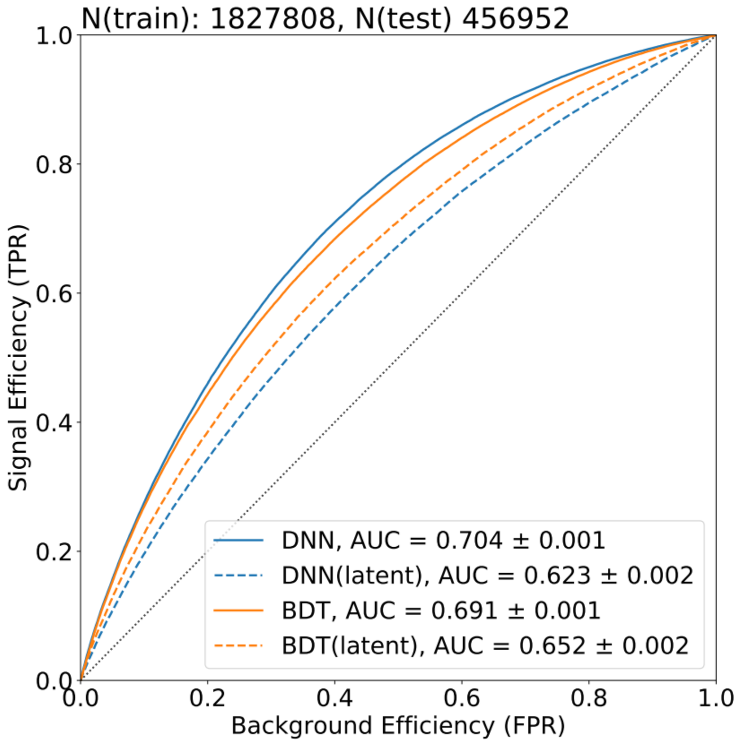
Features of each event :

→ 67 physical observables (p_T, E, ϕ etc.)

Typical approaches in HEP :

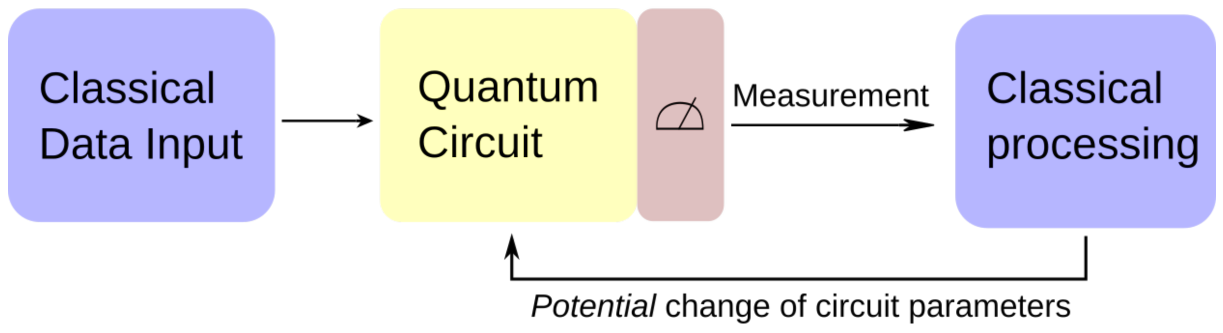
→ Deep Neural Networks (DNN)

→ Boosted Decision Trees (BDT)



Hybrid Quantum-Classical machine learning models

Implementing quantum algorithms on *Noisy Intermediate Scale Quantum* (NISQ) devices :



→ Limited number of qubits

→ Compact circuits (circuit depth and qubit connectivity)

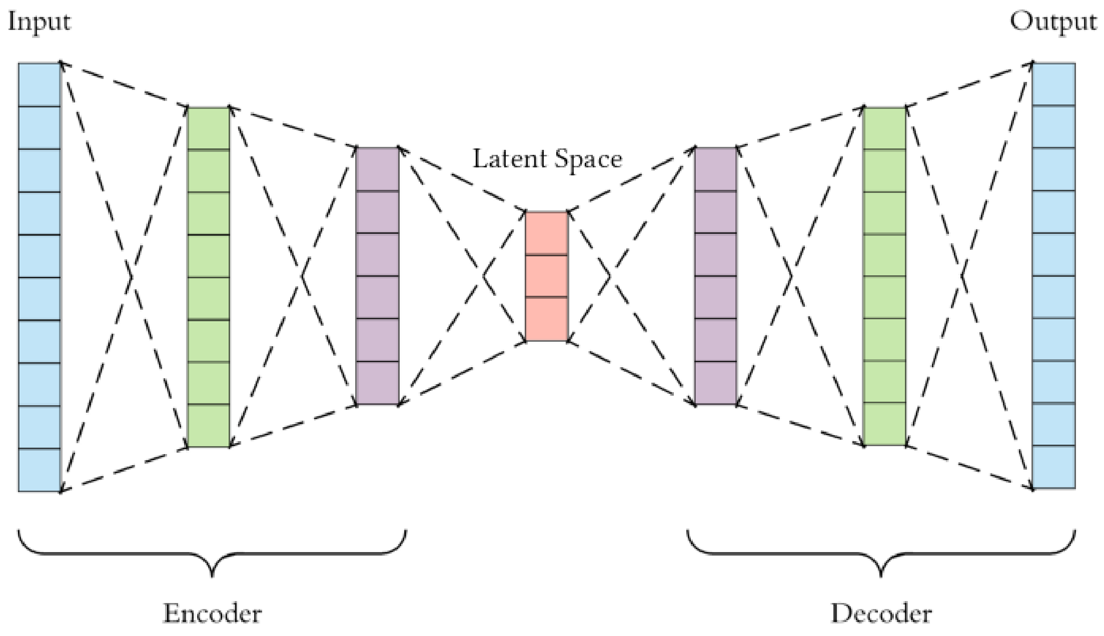
Quantum Machine Learning models for classification :

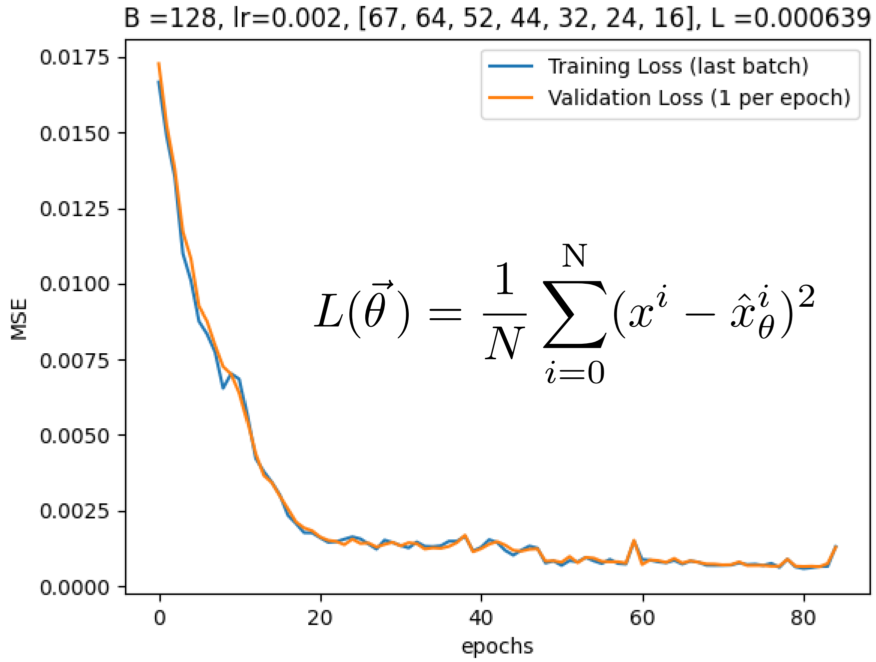
- Kernel methods → convex optimization (*Quantum Support Vector Machines*)
- Quantum Neural Network → non-convex optimization (*Variational Quantum Circuits*)

Input Feature dimensionality reduction

Autoencoder for feature reduction : 67 → 16 latent space features :

- Preserve non-linear correlations between input features in the latent representation





$$L(\vec{\theta}) = \frac{1}{N}\sum_{i=0}^{N}(x^i - \hat{x}^i_\theta)^2$$

Quantum Support Vector Machine

SVM quadratic optimization problem :

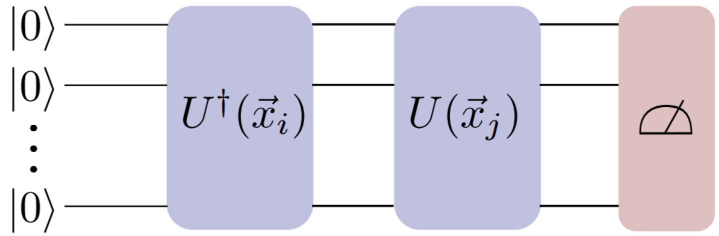
$$\text{maximize } L(c_1 \dots c_n) = \sum_{i=1}^{n} c_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i c_i (\vec{x}_i \cdot \vec{x}_j) y_j c_j,$$

$$\text{subject to } \sum_{i=1}^{n} c_i y_i = 0, \text{ and } 0 \leq c_i \leq \frac{1}{2n\lambda} \equiv C \text{ for all } i.$$

→ Kernel substitution trick :

$$(\vec{x}_i \cdot \vec{x}_j) \to k(\vec{x}_i, \vec{x}_j) \equiv \phi(\vec{x}_i) \cdot \phi(\vec{x}_j)$$

Substitute Kernel with a *quantum* one !



$$\Rightarrow K_{ij} = |\langle 0 | U^\dagger(\vec{x}_i) U(\vec{x}_j) | 0 \rangle|^2$$

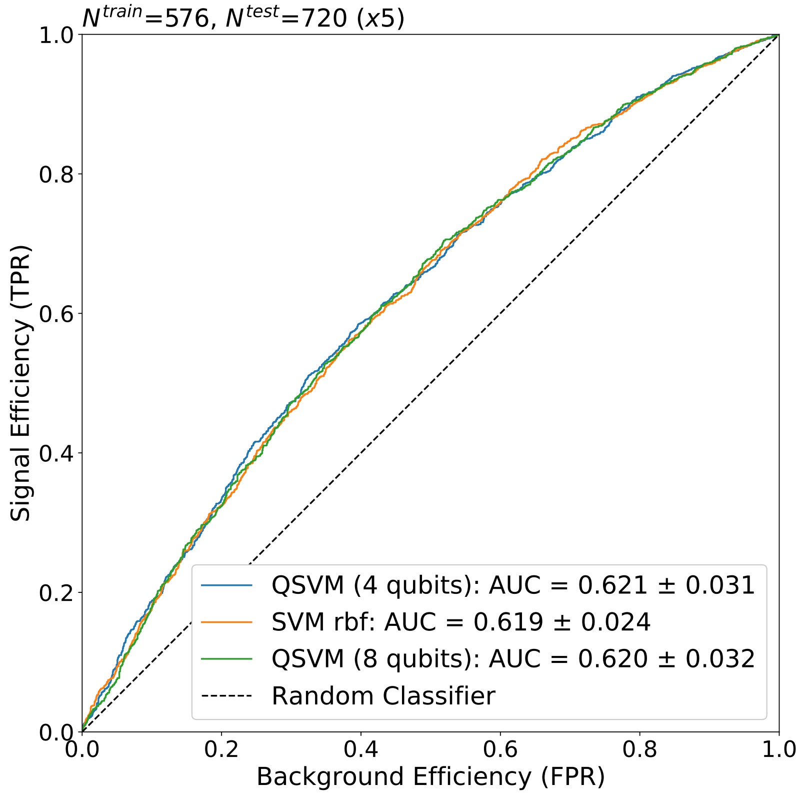
→ Sample kernel matrix with a quantum device

→ Maximize objective function of SVM on a classical computer

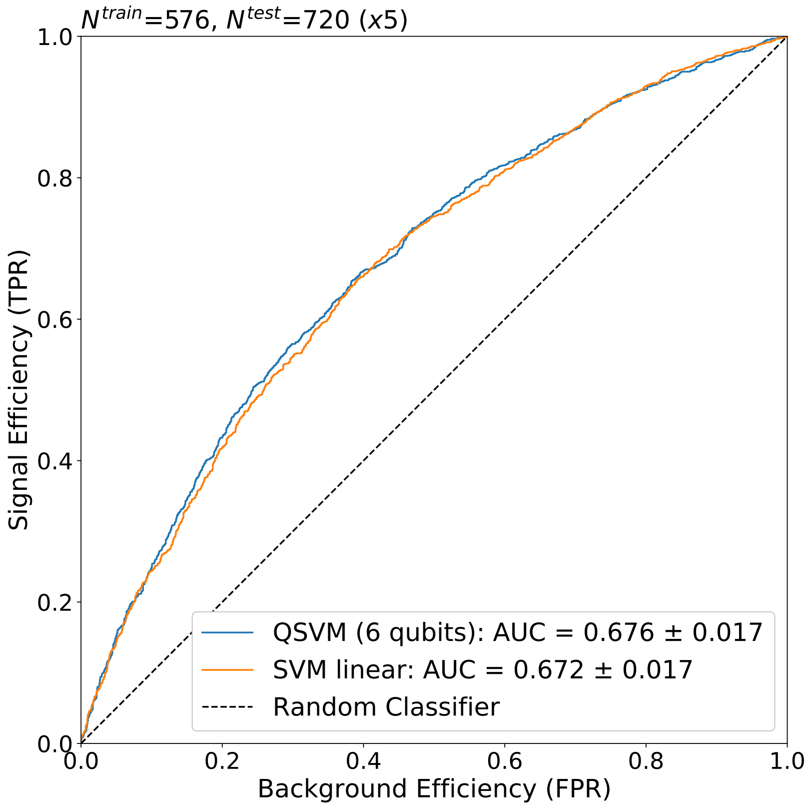
Results and classical benchmarks

QSVM models vs best performing classical models

Autoencoder latent features (16) :



Input features (64 out of 67) :



Reminder : extremely challenging physical process

→ Similar performance between best quantum and classical models

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Future studies and outlook

1. Systematic study of data embedding circuits (feature maps)

   → Optimization for their discrimination power in the quantum Hilbert space

2. Investigation of other input feature reduction methods

   → Aim for less information loss (classification power) in the reduced space

3. Implementation of developed algorithms on NISQ devices :

   → Design algorithms with limited number of qubits, limited number of operation and robust against hardware noise

Thank you !

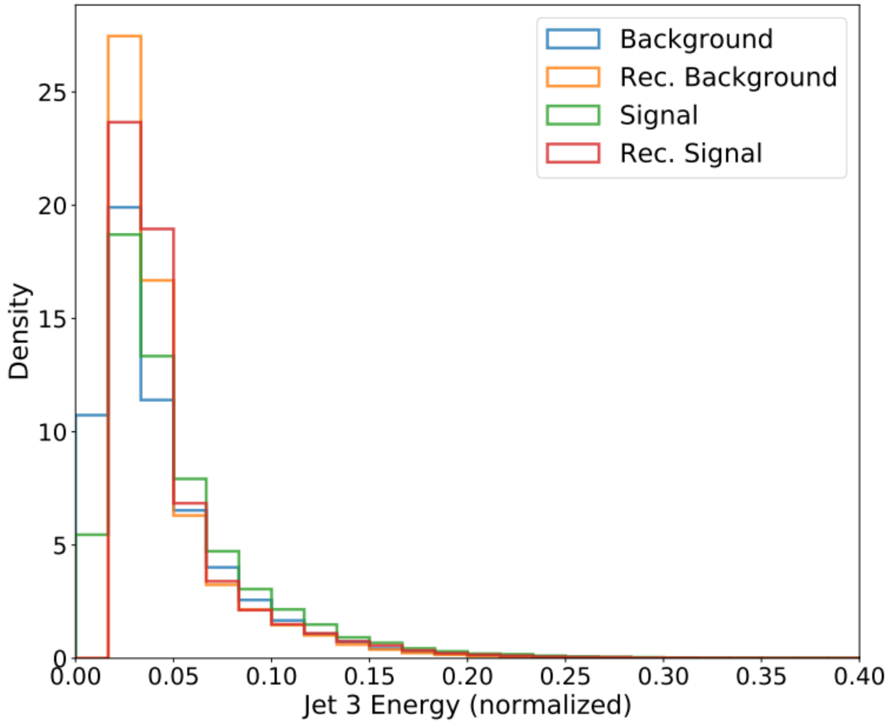
Questions ?

Back up

Autoencoder

Autoencoder for feature reduction : 67 → 16 latent space features :

- Input physical obs. normalized to [0,1]
- Latent space dim. = 16 (Sigmoid activation in latent and output space)
- ELU activation functions



Feature reduction and classical models results

Feature selection + Model	AUC
AUC + QSVM	0.66 ± 0.01
PyTorch AE + QSVM	0.62 ± 0.03
AUC + SVM rbf	0.65 ± 0.01
PyTorch AE + SVM rbf	0.62 ± 0.02
KMeans + SVM rbf	0.61 ± 0.02

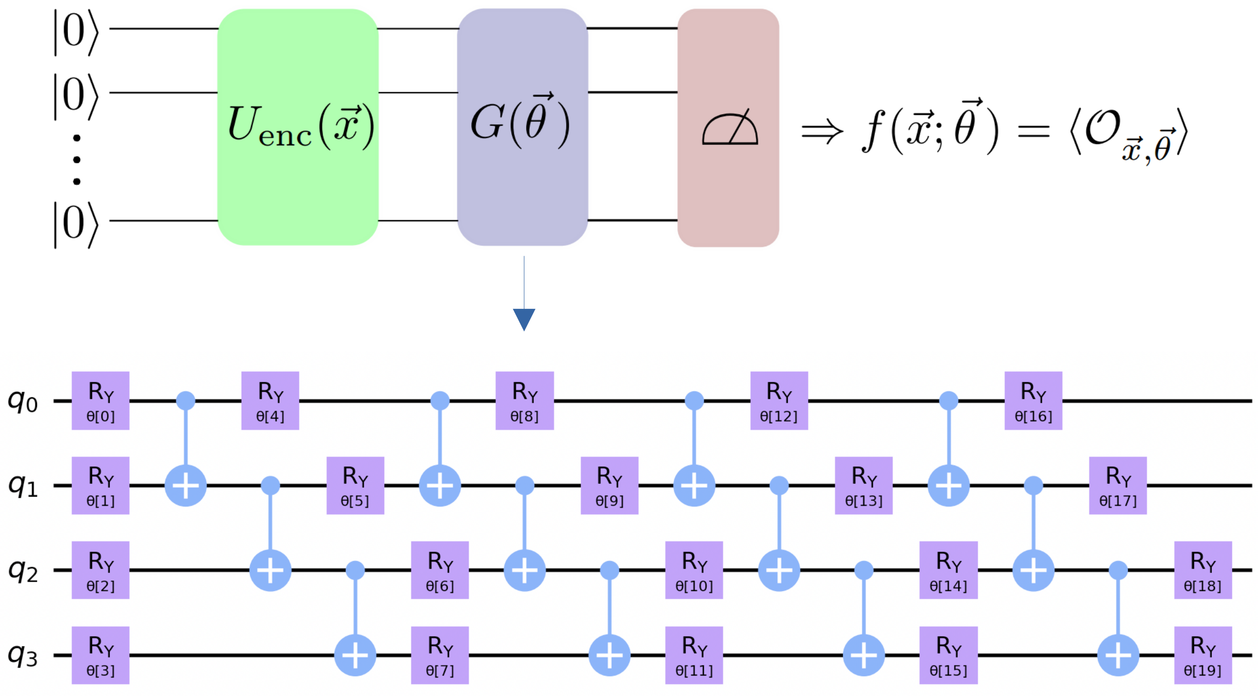
(a) 16 input variables

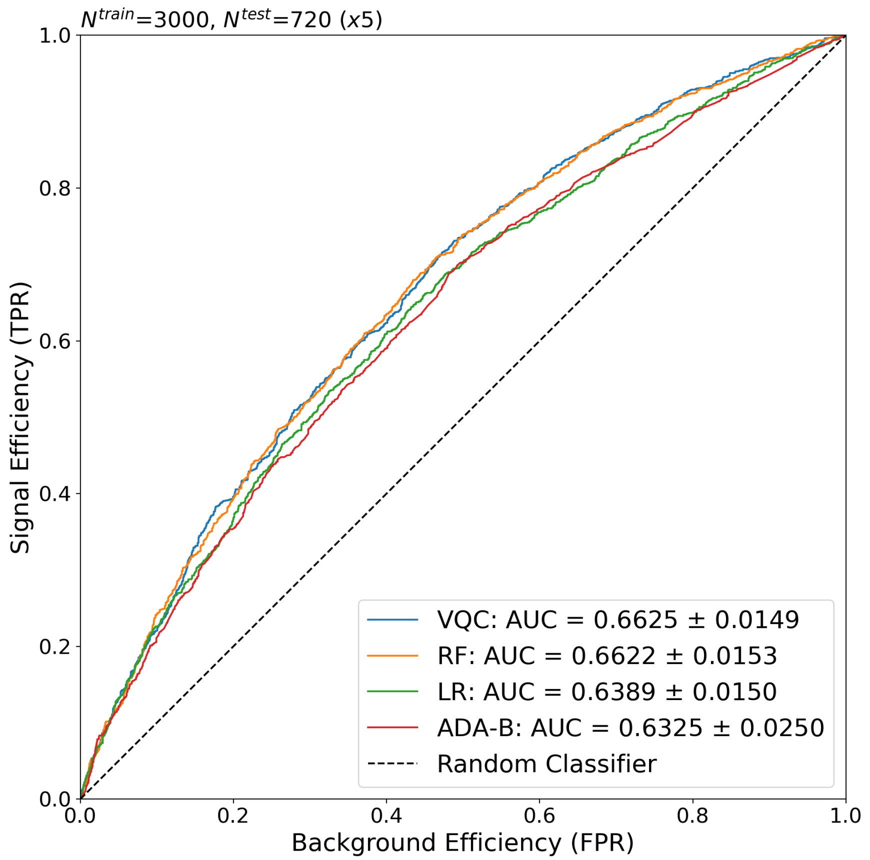
Feature selection + Model	AUC
AUC + QSVM	0.68 ± 0.02
AUC + Linear SVM	0.67 ± 0.02
Logistic Regression	0.68 ± 0.02

(b) 64 (QSVM, LSVM) and 67 (LR) input variables

Feature selection + Model	AUC
AUC + VQC	0.66 ± 0.01
AUC + Random Forest	0.66 ± 0.02
KMeans + Log. Regr.	0.64 ± 0.01
TensorFlow AE + AdaBoost	0.63 ± 0.03

VQC





To-do: Explore different architectures for the VQC and potential interplays with classical NN → Comparison of model power with respect to quantum kernel methods

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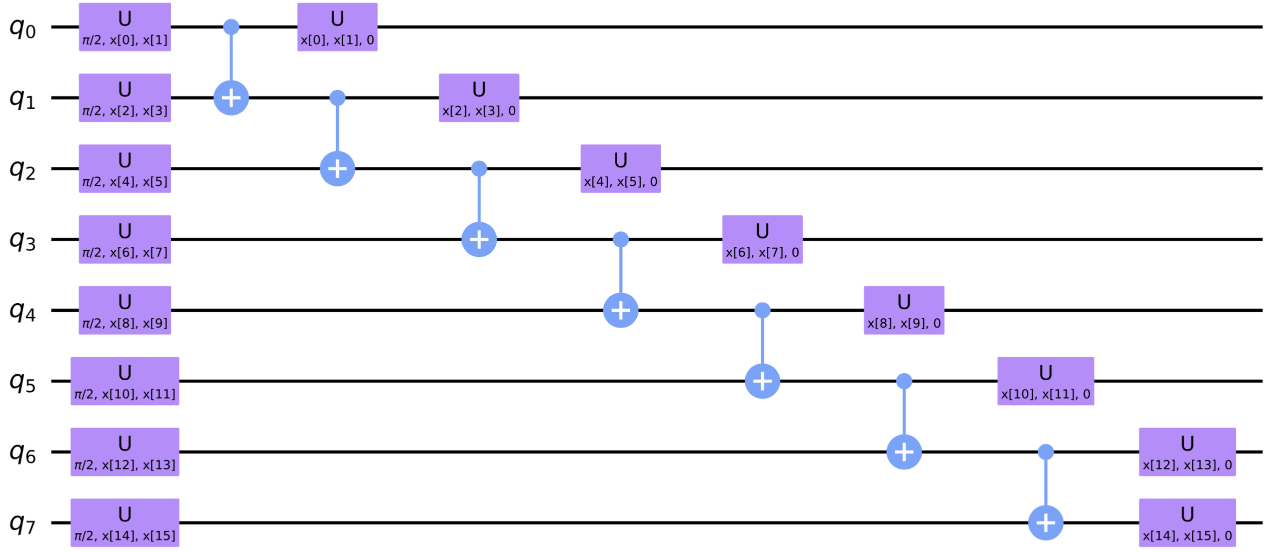
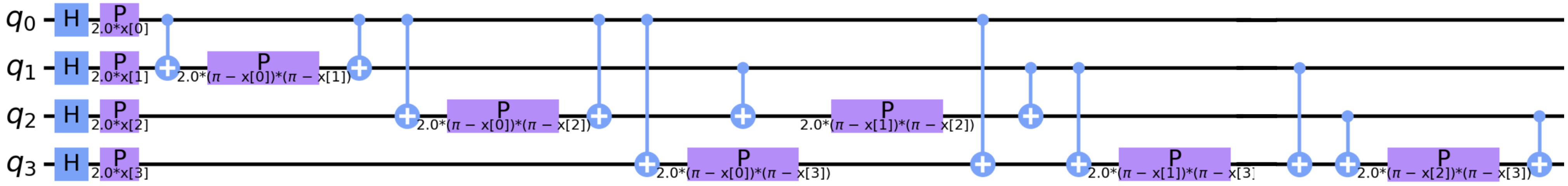
Feature maps circuits





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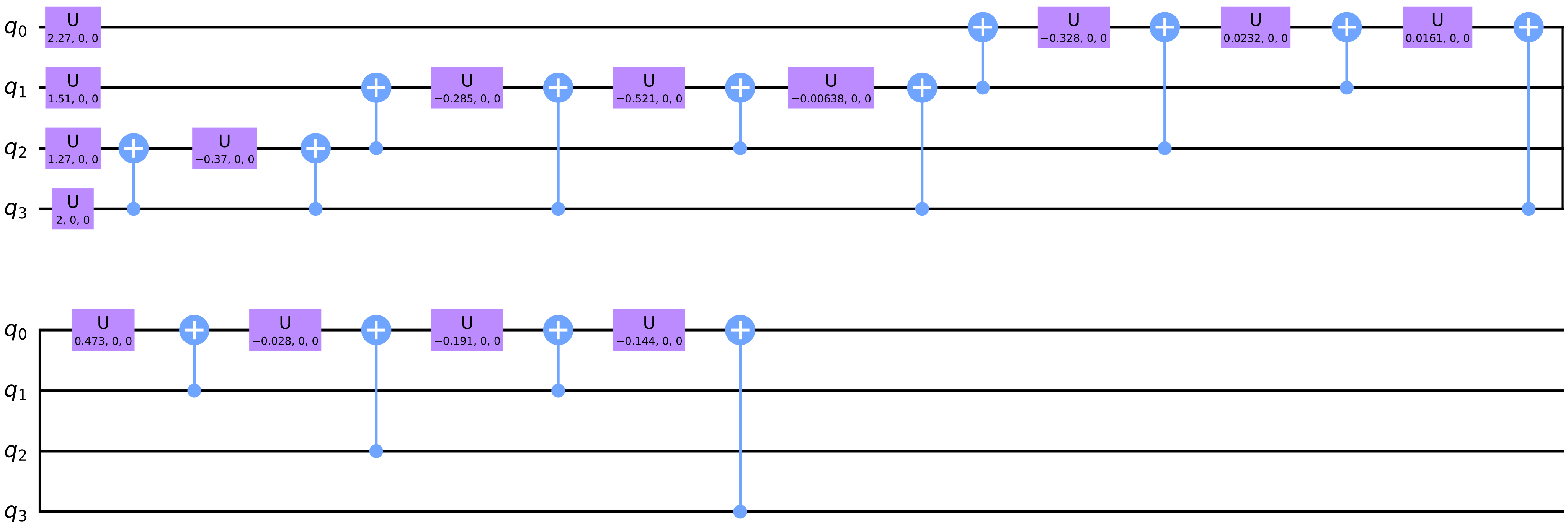
Feature maps circuits (Cont.)



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QSVM with 16 individual AUC-based feature selection