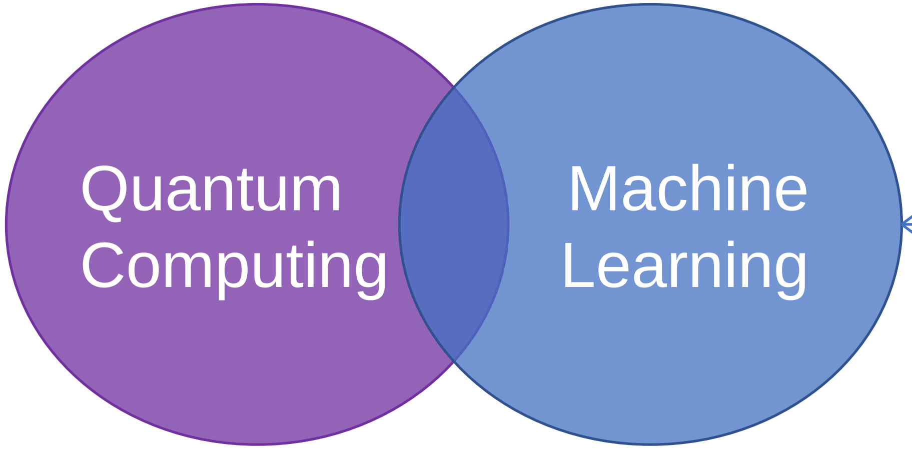
Quantum Kernels Studies:
Metrics for Quantum Advantage and Quantum Projection to Approximate Classical Representation.



- Supervised Learning → Classification
- Unsupervised Learning
- Reinforcement Learning

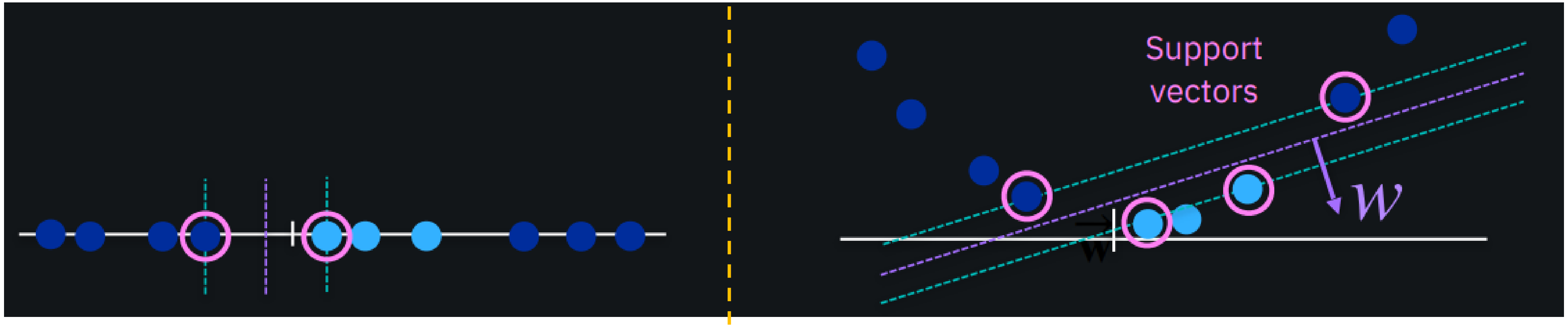
2022 CERN openlab Technical Workshop
Sofia Vallecorsa
Michele Grossi

QUANTUM TECHNOLOGY INITIATIVE

Kernel Methods for Support Vector Machine (SVM)

- **Non-linearly** separable datasets may become linearly separable by including new features.

- This transformation is called a **feature map**

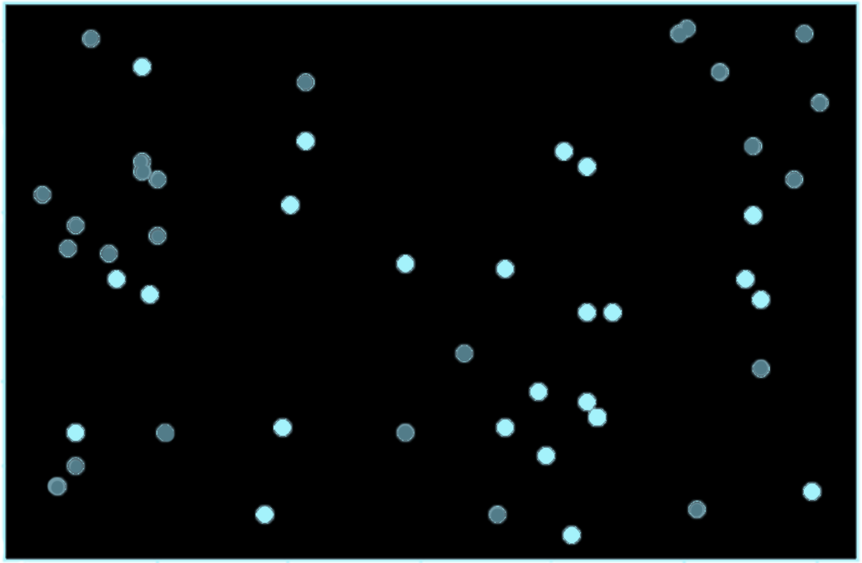


Hyperplane: $w^T x + b = 0$

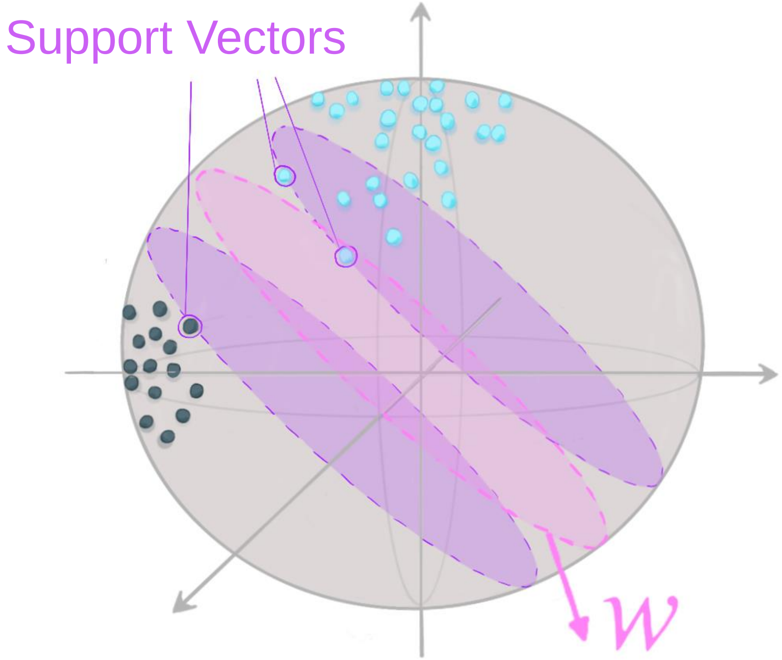
Hyperplane: $w^T \varphi(x) + b = 0$

Quantum Encoding

- **Non-linearly** separable datasets may become linearly separable by including new features.



- This transformation is called a **quantum feature map**



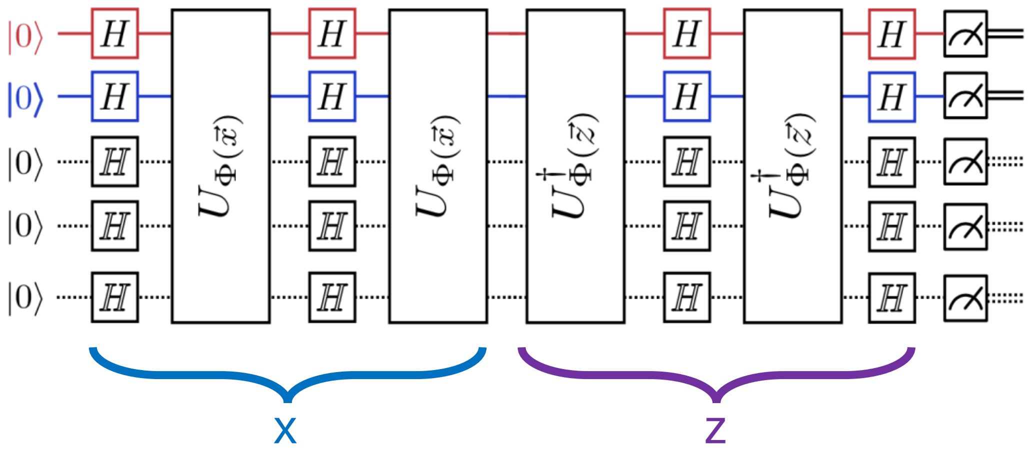
Quantum Kernel Estimation for SVM (QSVM)

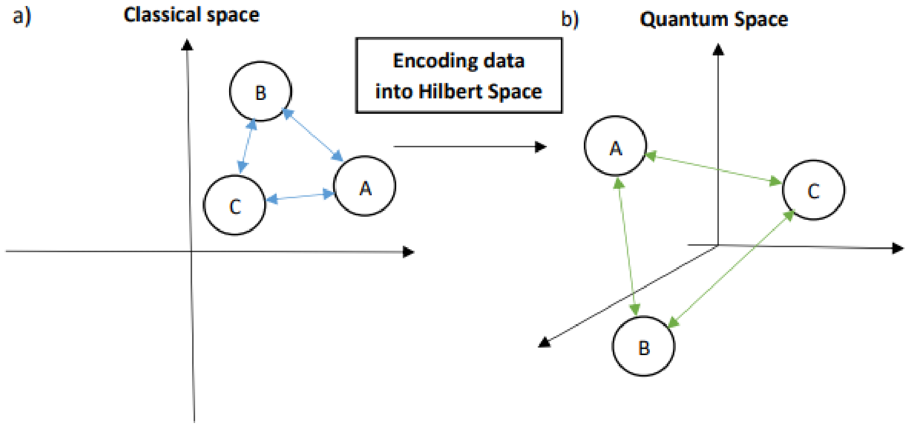
We use quantum computer to:

- encode the data
- estimate the kernel estimating the ***fidelity*** between pairs of feature vectors
- Classical computer implementing the quantum kernel $K_{i,j}$ is then used to do the SVM according to:

$$label(z) = sign\Big(\sum_{i \in T} \alpha_i y_i \boldsymbol{K}(x_i, z) + b \Big)$$

$$|\langle \Phi(\vec{x}) | \Phi(\vec{z}) \rangle|^2 = |\langle 0^n | \mathcal{U}^{\dagger}_{\Phi(\vec{x})} \mathcal{U}_{\Phi(\vec{z})} | 0^n \rangle|^2$$





V. Havlicek et al, Nature 567, 209 (2019)

S. Moradi et al, Scientific Reports 12, 1851 (2022)

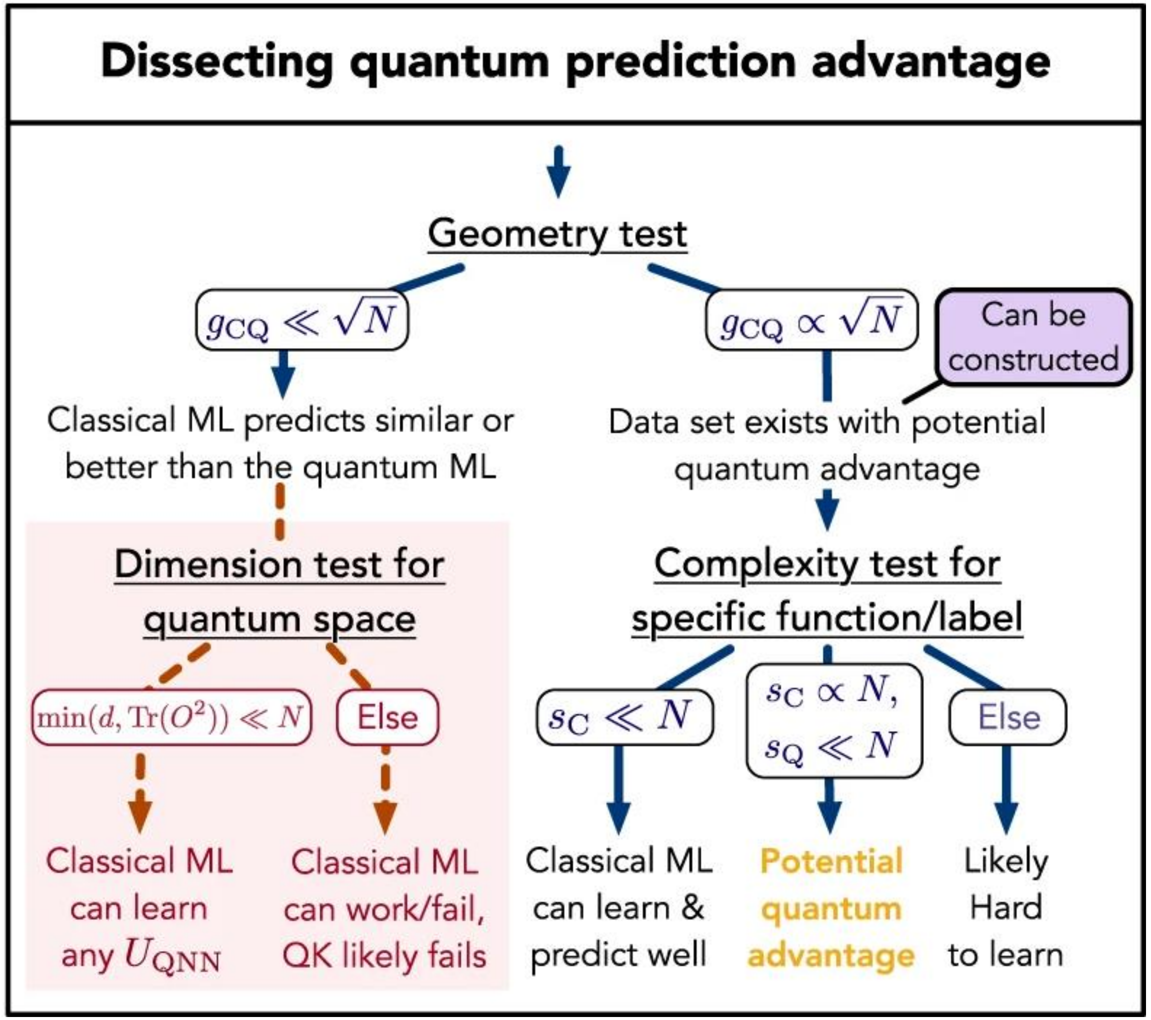
Metrics for Potential Quantum Advantage

- Computations exponentially hard classically ✓
- Expressivity of QML hinder generalization ✗

So far, results found with trial and error but we need a reliable theoretical framework.

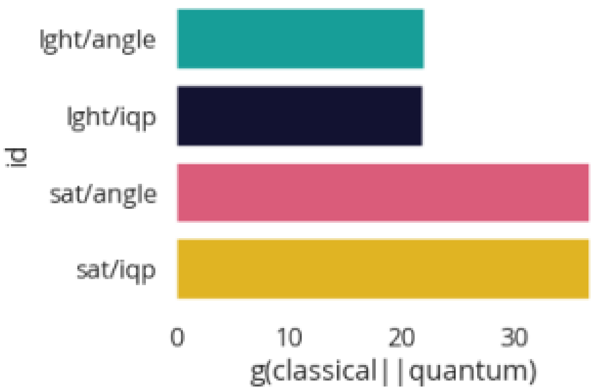
↓

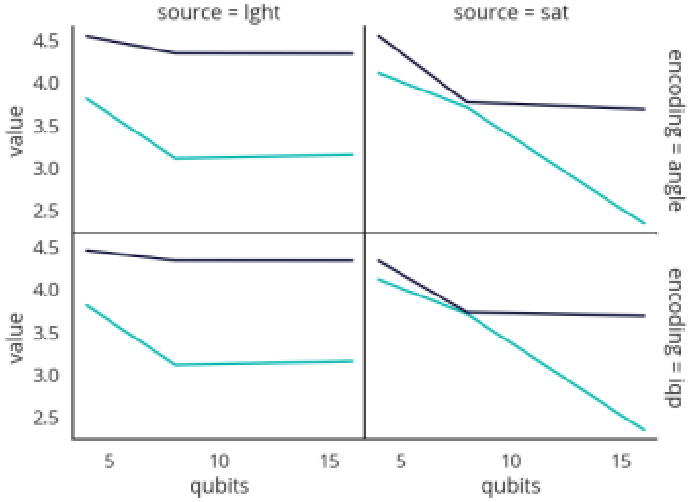
A priori methodology to assess quantum advantage according to data and kernels considered.



HY. Huang et al, Nature Communication 12, 2631 (2021)

Real world datasets & Huang metrics





Synthetic weather radar using hybrid quantum-classical machine learning

G. R. Enos et al, Arxiv 12, 1851 (2022)

Clinical data classification with noisy intermediate scale quantum computers

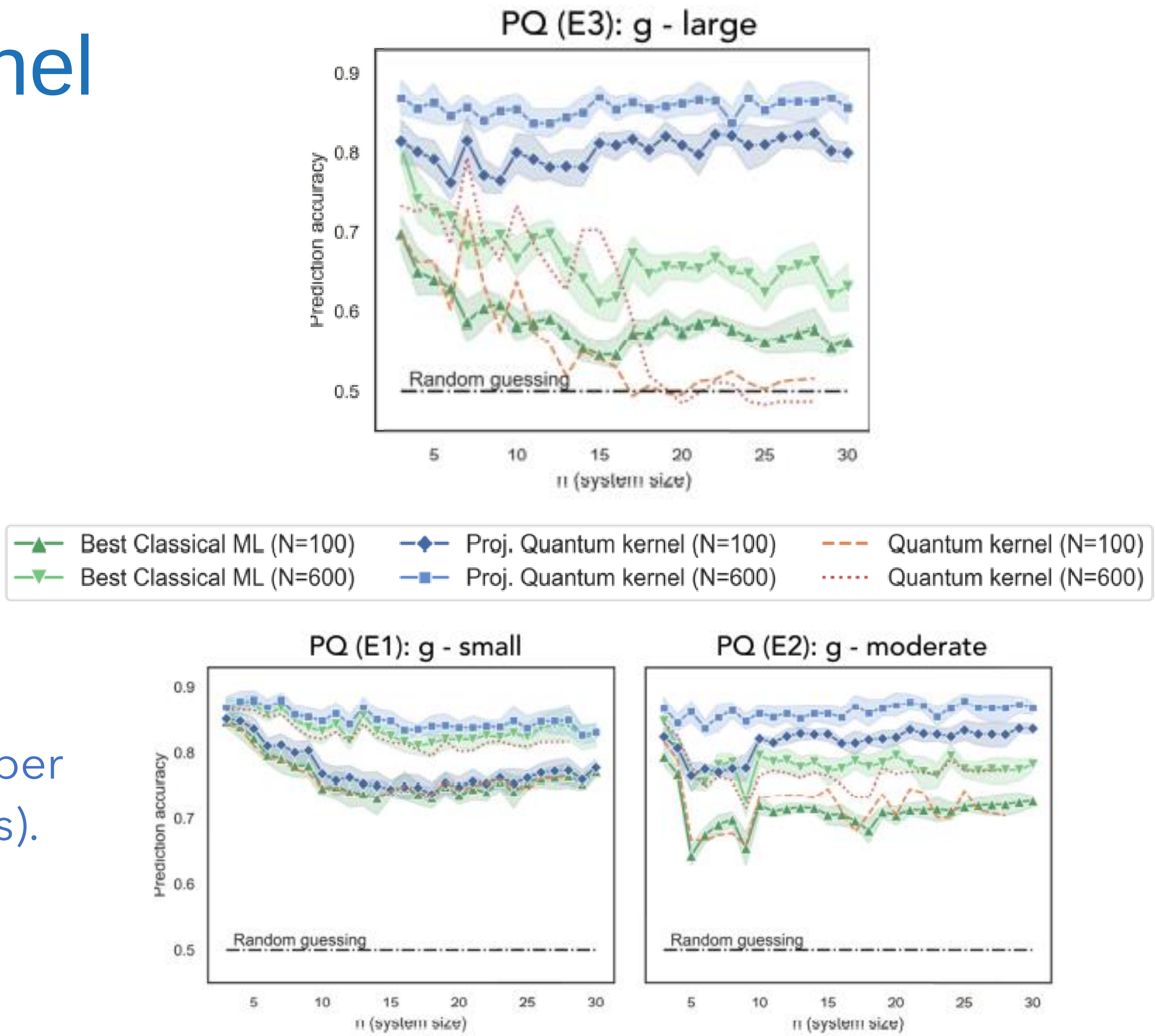
S. Moradi et al, Scientific Reports 12, 1851 (2022)

Dataset	#Samples	Imbalance Ratio	#Features	g_{CQ}	Reference
Pediatric Bone Marrow Transplant 2-year survival	134	0.33	8	0.40	27
			16	0.60	
Wisconsin Breast Cancer Malign-vs-benign	569	0.37	8	1.30	28
			16	3.50	
Heart Failure Mortality	300	0.5	8	0.42	29

Projected Quantum Kernel

- Reduce the dimensionality of Feature Space by projection of QK:
  - ➢ To better generalize
  - ➢ To keep features into states classically hard

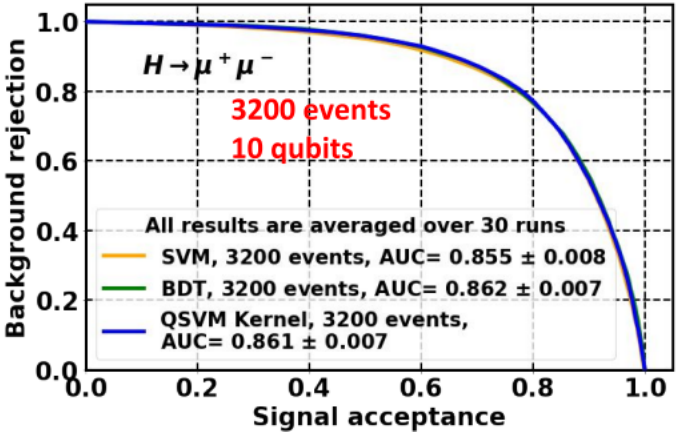
This projected kernel defines a feature map in a subspace of the large Hilbert Space. It can still express an high number of arbitrary functions (and their powers).

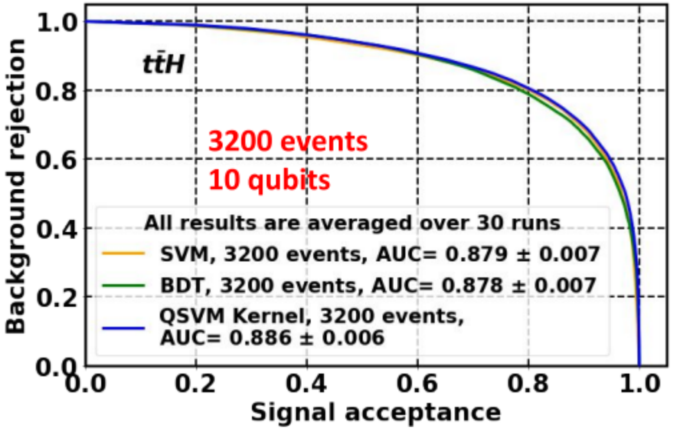


HY. Huang et al, Nature Communication 12, 2631 (2021)

QML for HEP: Past and Future

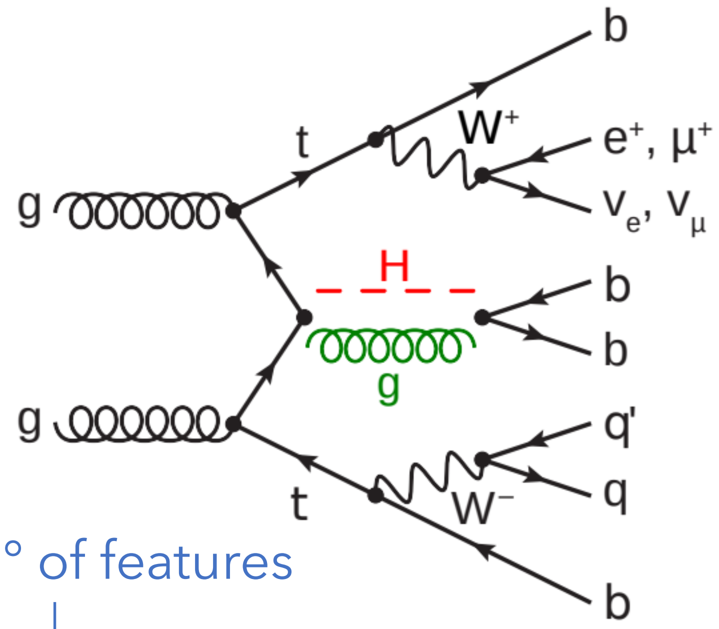
Employing Quantum SVM Kernel method with IBM statevector simulator for Higgs decays analysis.





S.L. Wu, QuantHEP Seminar, 11/2020

$t\bar{t}H(b\bar{b})$



high n° of features

high n° of qubits → high computational cost for QK

openlab qti machines

V. Belis, EPJ Web of Conferences 251, 03070 (2021)

Conclusions

- Geometry and Complexity tests to assess for potential Quantum Advantage.
- Quantum Kernels can have too expressive power hindering generalization and learnability.
- Only restricted embeddings allow to learn from data, these are called Projected Quantum Kernels and are hard to reproduce by classical models.

Can QML bring a speed-up in data analysis for HEP?

Thanks!

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KTH VETENSKAP OCH KONST