

QML in the latent space of HEP events

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Introduction: The Challenge

Application: Searches at LHC

Finding Signal in a dataset dominated by Background

Look in mJJ resonance spectrum

2 Scenarios:

	Supervised	Unsupervised
Truth	known	unknown
Training Data	MC with signal model	Data
Search	model-dependent	model-agnostic

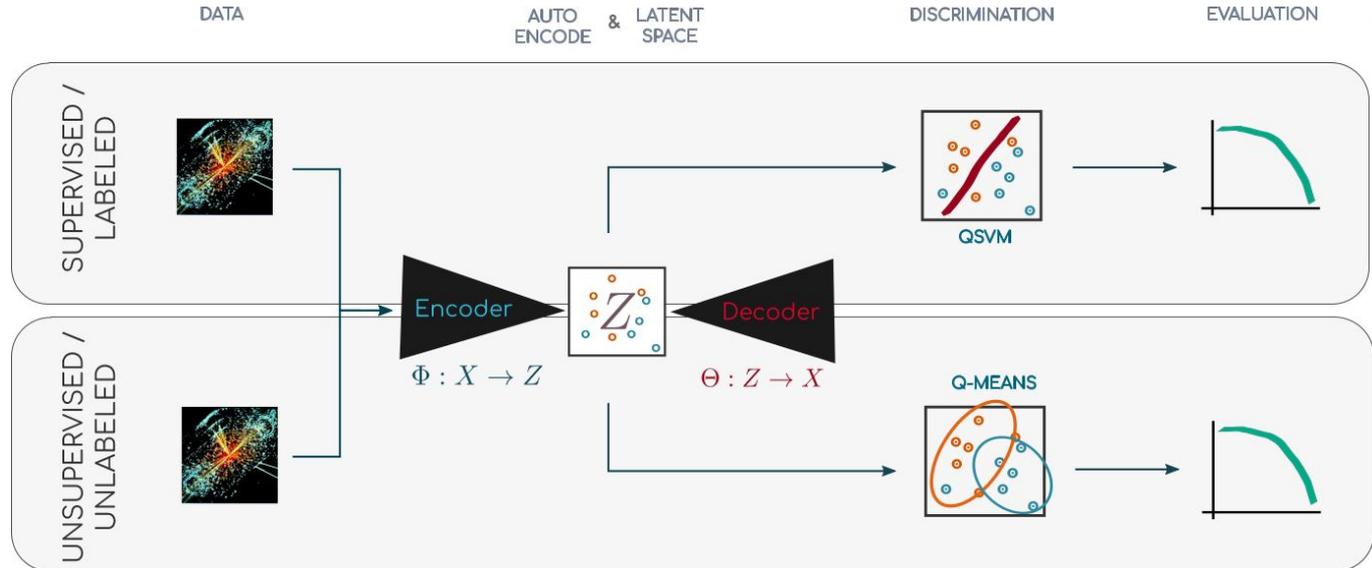
Goal: Compare classic to quantum algorithm performance

Rationale for Quantum:

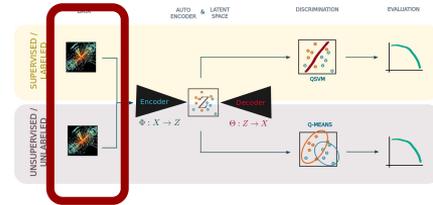
Improved accuracy (because data intrinsically quantum, quantum can find patterns that classic can't)

Introduction: Workflow

- **Data:** Reduce dimensionality of input to make treatable by noisy quantum computers through **Autoencoder**
- **Algorithms:**
 1. **SVM** Classification for supervised scenario
 2. **K-Means** for unsupervised scenario
- **Evaluation:** Signal- vs Background-**Accuracy**



Data & Quantum Embedding



Input:

Dijet Events

Particle list ($\Delta\eta$, $\Delta\phi$, p_T)

$\Delta\eta$	$\Delta\eta$	$\Delta\eta$	$\Delta\eta$...	$\Delta\eta$	$\Delta\eta$	$\Delta\eta$	$\Delta\eta$
$\Delta\phi$	$\Delta\phi$	$\Delta\phi$	$\Delta\phi$...	$\Delta\phi$	$\Delta\phi$	$\Delta\phi$	$\Delta\phi$
p_T	p_T	p_T	p_T	...	p_T	p_T	p_T	p_T

100 particles

Autoencoder Training:
Define **data sideband**
(dominated by BG)
as $|\Delta\eta| > 1.4$

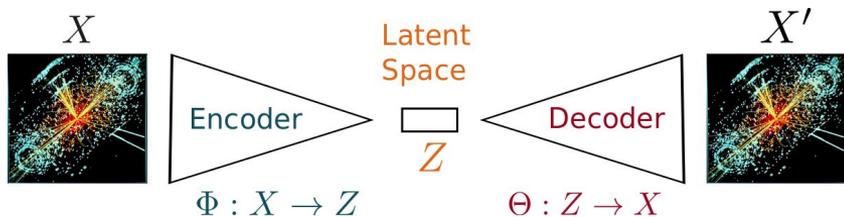
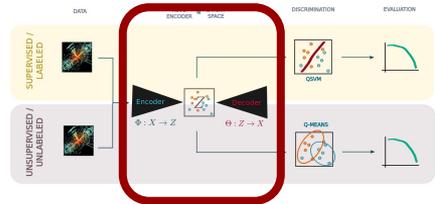
Encoding inputs into quantum state

- Amplitude encoding (QK-means)
- Dense angle encoding (QSVM)

Training and Testing

- AE train: QCD sideband (2M events)
- Clustering train: QCD signalregion (2M events QK-means, 600 events QSVM)
- Clustering test: QCD signalregion (1K events)

Autoencoding for Dimensionality Reduction



Originally designed to **compress** and **decompress** inputs, passing through **bottleneck** (latent space)

Idea

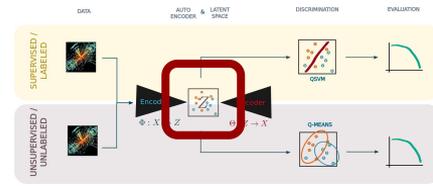
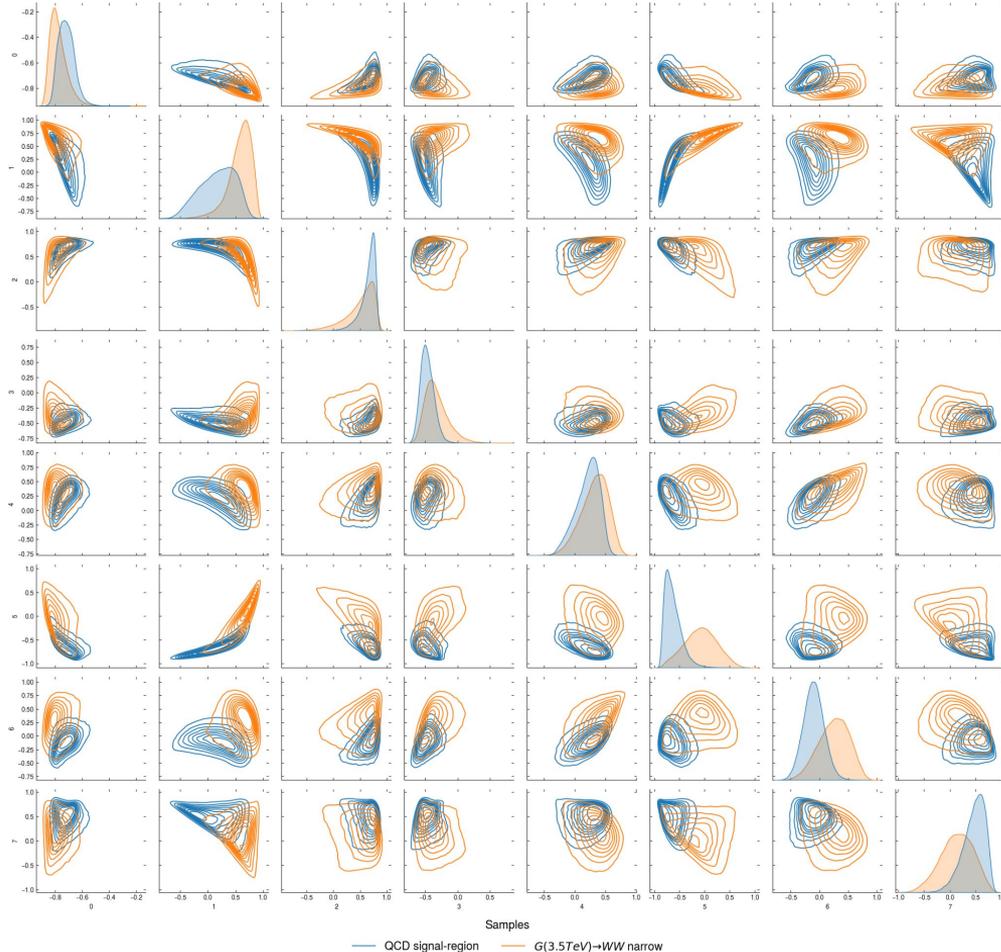
Make AE learn how to compress **BG**, it will fail when seeing **SIG** event (reconstruction error)

Architecture: Convolutions + Dense, Latent Space $Z \in \mathbb{R}^8$

Latent Activation: tanh

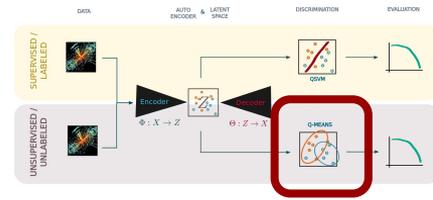
Loss Metric: Chamfer-Loss / Pairwise distance
$$L_R = \sum_{i \in input} \min_j ((x^{(i)} - x^{(j)})^2) + \sum_{j \in output} \min_i ((x^{(j)} - x^{(i)})^2)$$

Results: Latent Space Representation



- Encoder Output
- $\mathbb{R}^{300} \rightarrow \mathbb{R}^8$
- Separation of Background and Signal

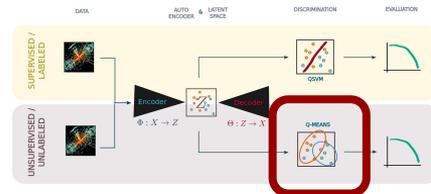
Unsupervised Clustering: Q-MEANS



Algorithm in 3 parts:

- 1) Quantum distance calculation: distance to cluster
- 2) Quantum minimization (Grover / Duerr & Hoyer): closest cluster assignment
- 3) New cluster center calculation (classic)

Unsupervised Clustering: Q-MEANS



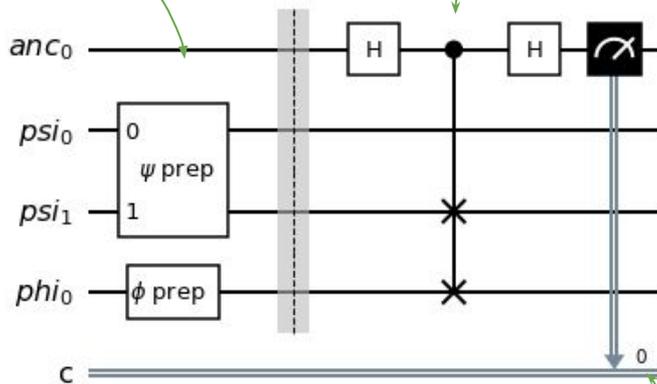
1) Quantum distance calculation: distance to cluster

Prepare 2 quantum states

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0, u\rangle + |1, v\rangle)$$

$$|\phi\rangle = \frac{1}{\sqrt{Z}}(|u| |0\rangle - |v| |1\rangle)$$

$$Z = |u|^2 + |v|^2$$



Measure ancilla in zero state

$$P_{anc}(|0\rangle) = \frac{1}{2} + \frac{1}{2} |\langle \phi | \psi_A \rangle|^2$$

Do Swap Test

$$|x_0\rangle = |0, a, b\rangle$$

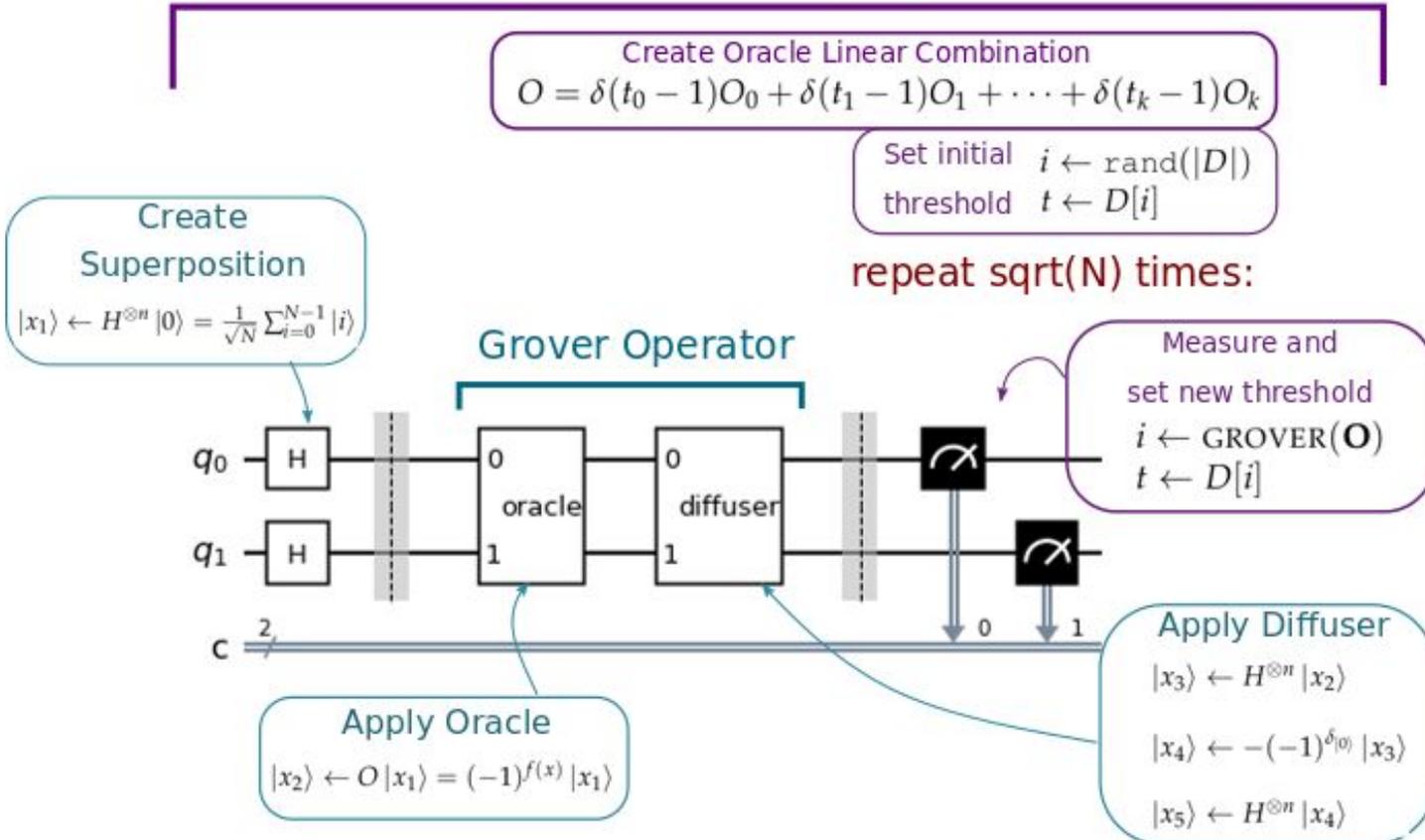
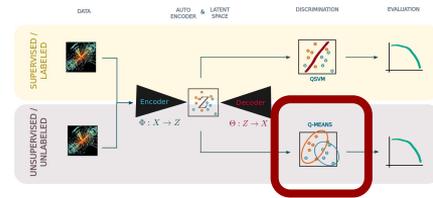
$$|x_1\rangle = \frac{1}{\sqrt{2}}(|0, a, b\rangle + |1, a, b\rangle)$$

$$|x_2\rangle = \frac{1}{\sqrt{2}}(|0, a, b\rangle + |1, b, a\rangle)$$

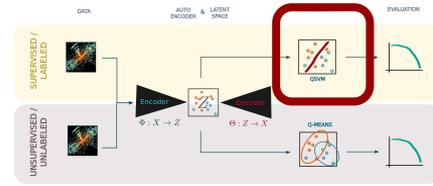
$$|x_3\rangle = \frac{1}{2} |0\rangle (|a, b\rangle + |b, a\rangle) + \frac{1}{2} |1\rangle (|a, b\rangle - |b, a\rangle)$$

Unsupervised Clustering: Q-MEANS

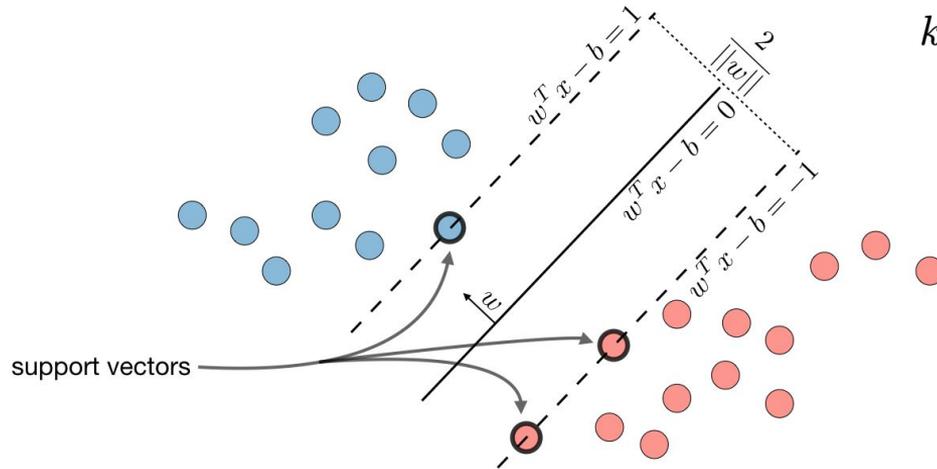
Duerr & Hoyer Minimization (input: distances D)



QSVM Classifier

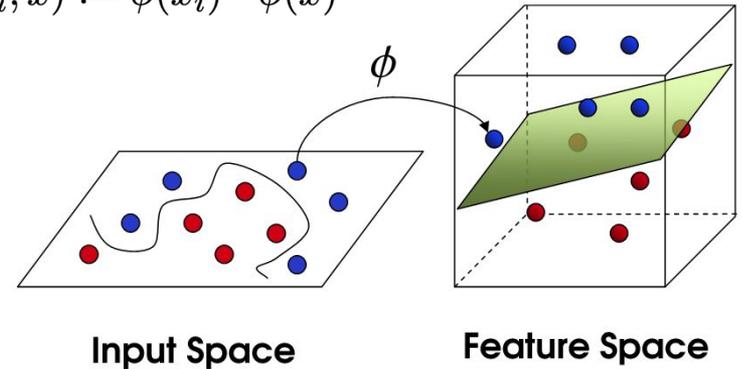


- Supervised training on 600 qcd (background) and 600 G_{RS} (signal) samples.
- Train to find the optimal separating hyperplane \rightarrow convex optimisation task.
- Feature maps enable SVM to construct non-linear decision boundaries.



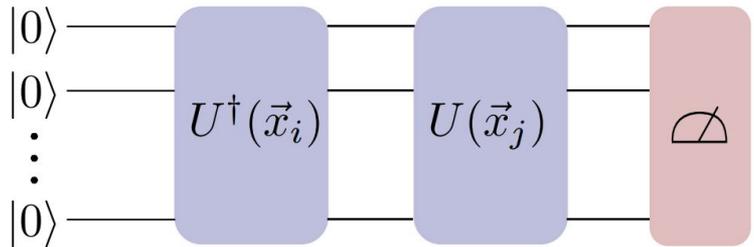
The kernel is defined via the feature map:

$$k(x_i, x) := \phi(x_i)^\dagger \cdot \phi(x)$$



Source: <https://towardsdatascience.com/the-kernel-trick-c98cdbcaeb3f>

QSVM Classifier

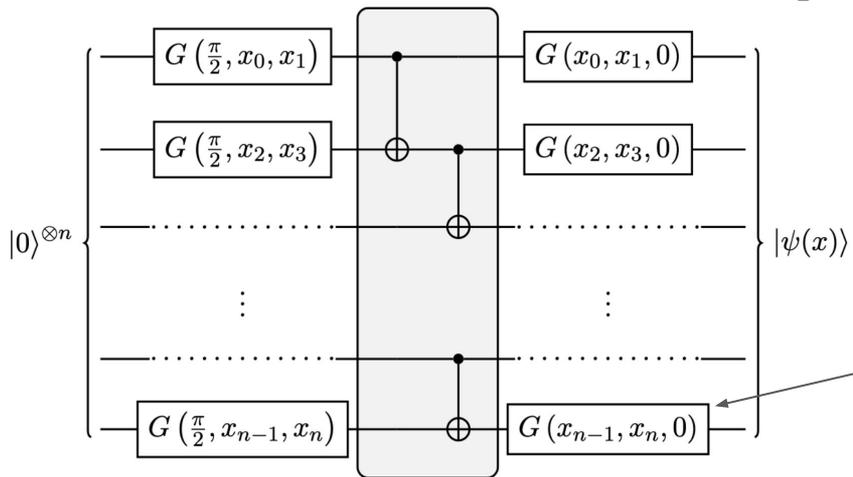


$$\Rightarrow K_{ij} = |\langle 0|U^\dagger(\vec{x}_i)U(\vec{x}_j)|0\rangle|^2$$

Quantum Kernel

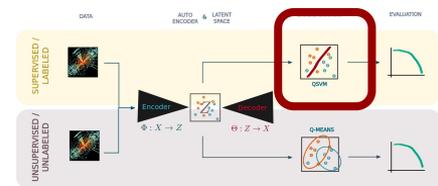
- Quantum kernel is sampled from a quantum device.
- The optimisation of the objective function remains on a classical computer.

Linear entanglement

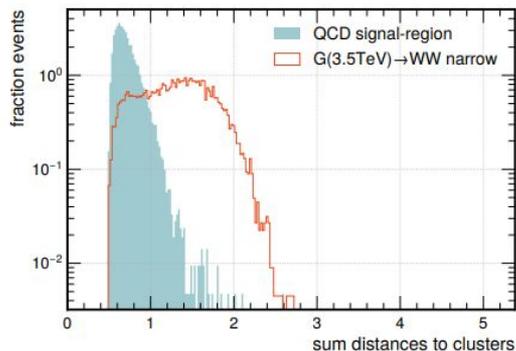
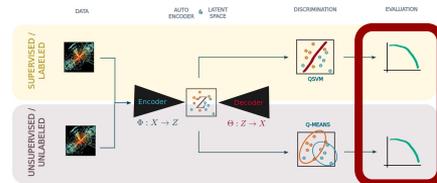


$G \in \text{SU}(2)$

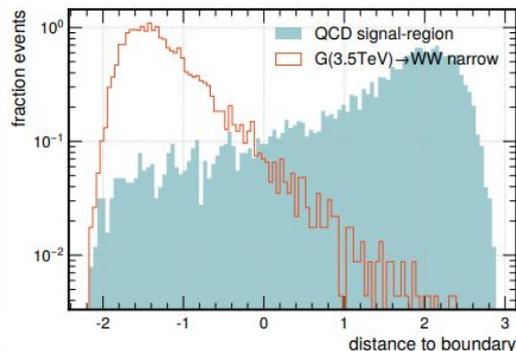
Feature map circuit $U(x)$, for latent dim = 16, and $n = 8$ qubits.



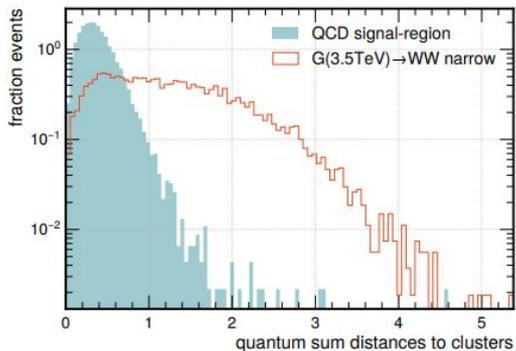
Discrimination Metric Distributions



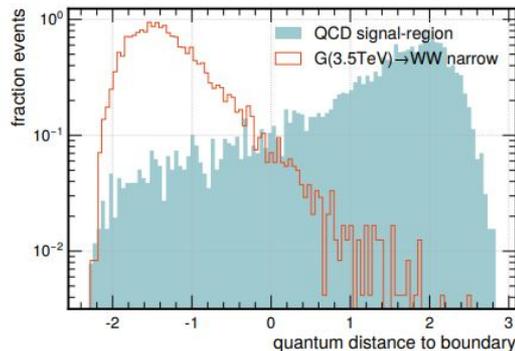
(a) K-Means classical



(b) SVM classical



(c) K-Means quantum



(d) SVM quantum

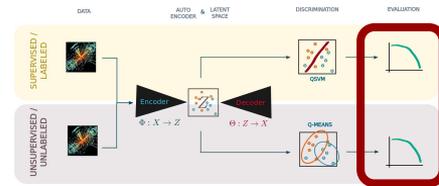
Metric

- QK-means: sum squared distance to cluster centers
- QSVM: Distance from decision boundary

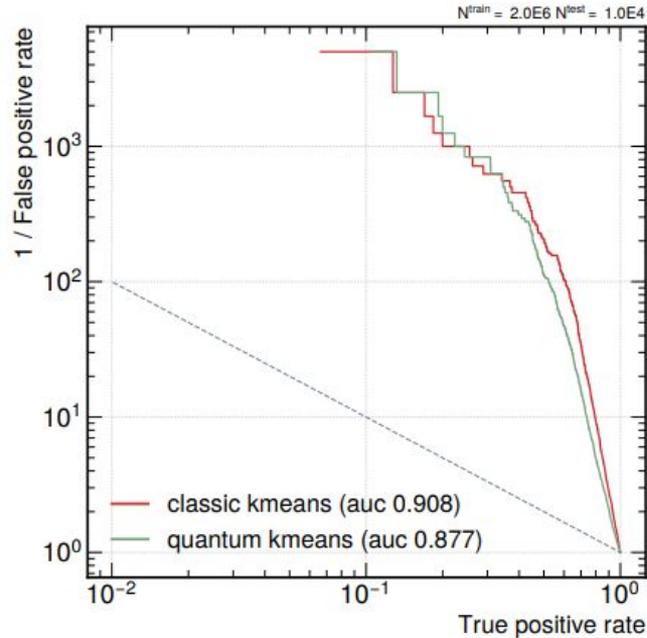
Results

- Good separation of background vs signal
- Set cut-threshold β for signal efficiency
- Cut on tail for QK-means (e.g. $\beta > 2$)
- Cut on left mode for QSVM (e.g. $\beta < -1$)

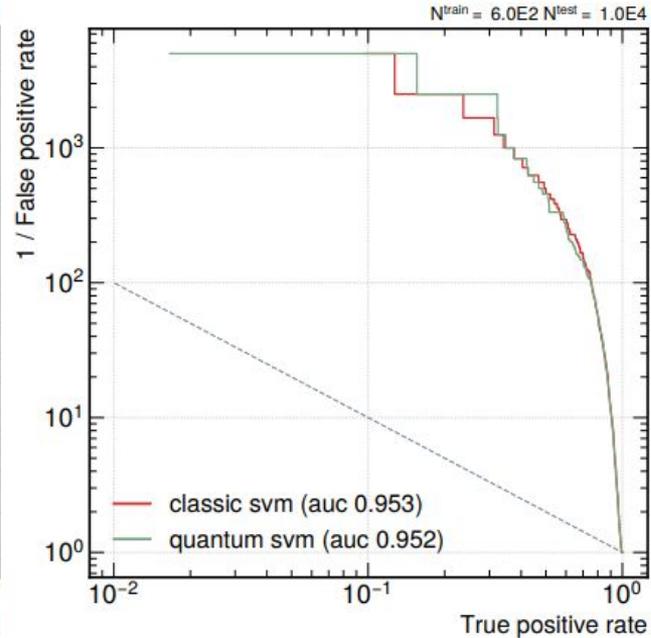
ROC



Unsupervised (Q)K-means



Supervised (Q)SVM



- very good overall performance with high AUC values around and beyond 0.9 for both QK-means and QSVM algorithms
- supervised approach outperforms unsupervised approach but QK-means viable approach for solving model-agnostic problems
- performance of quantum algorithms is competitive when compared to classical counterparts

Conclusion

- We studied a quantum anomaly detector and a quantum classifier operating in a latent space representation of HEP events
- Both, QK-means and QSVM, proved effective in discriminating background from signal data-sets
- Supervised QSVM method (e.g. model-dependent searches) shows superior results compared to the unsupervised q-K-means approach (e.g. model-independent searches)
- Performance of quantum algorithms is competitive when compared to their classical counterparts

Based on results, we conclude that quantum algorithms are applicable to both, a model-independent and model-dependent analysis and could contribute to extend the sensitivity of the LHC experiments.

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