Quantum machine learning for anomaly detection at the LHC

Vasilis Belis (ETH Zurich)

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Outline

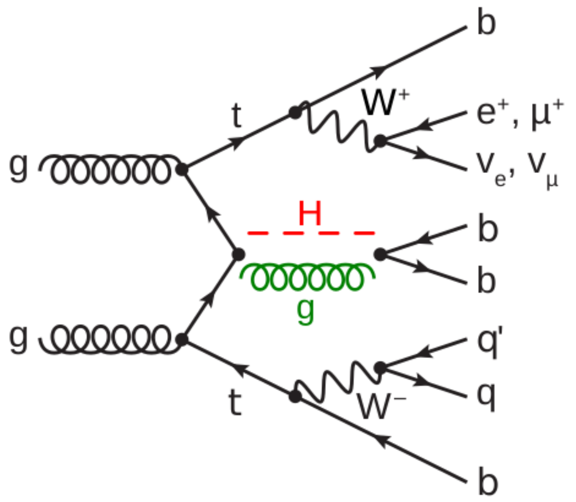
1. Model-independent searches and anomaly detection at the LHC.
   - Motivation
   - Unsupervised learning and anomaly detection

2. Quantum computing and machine learning.
   - Motivation

3. Quantum anomaly detection results
   - Detection of Gravitons and new Scalar bosons
   - Benchmark against classical counterpart.
   - Hardware Run.

Conventional searches at the LHC

Define *signal* and *background*.



e.g.: $t\bar{t}H(b\bar{b})$ process at leading order in the semi-leptonic channel.

VB, et al., **Higgs analysis with quantum classifiers**
EPJ Web Conf., 251 (2021) 03070

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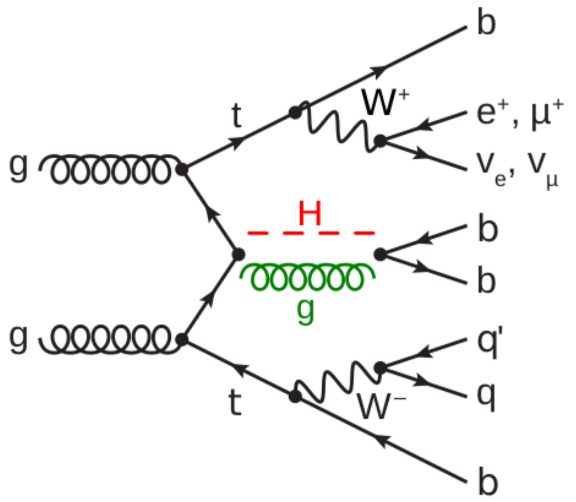

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Model-dependent searches of Beyond Standard Model (BSM) physics

Define....

...analysis objects

Jets, Leptons, MET, ...

...signal region

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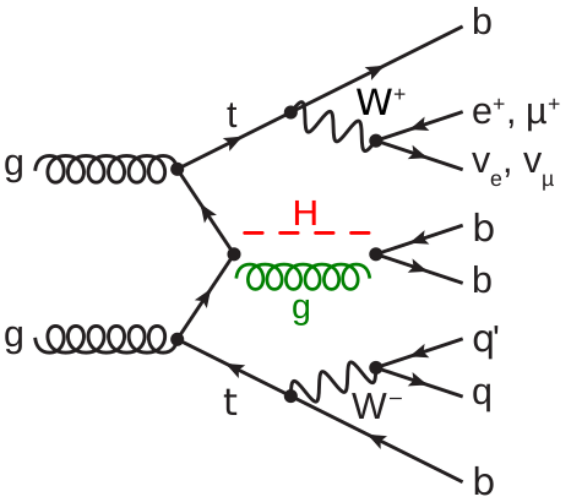

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[10.1007/JHEP05(2022)005]

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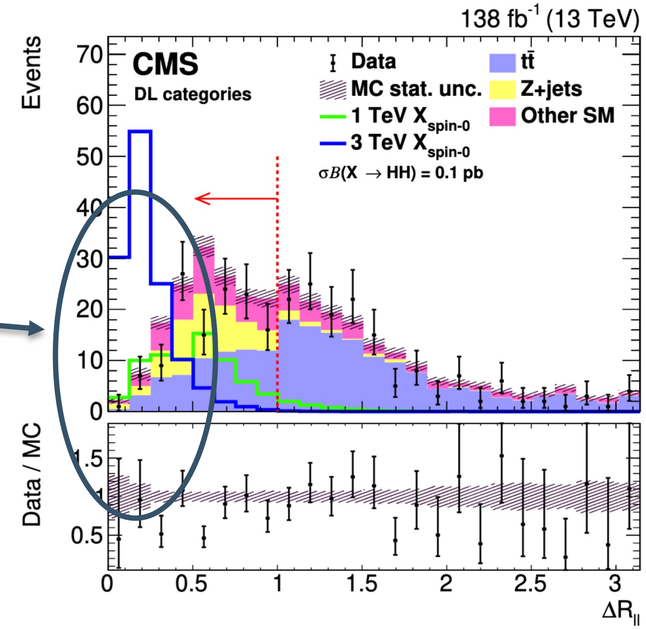
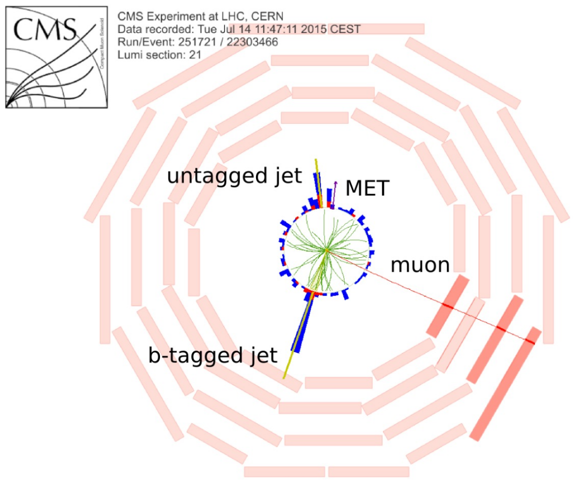


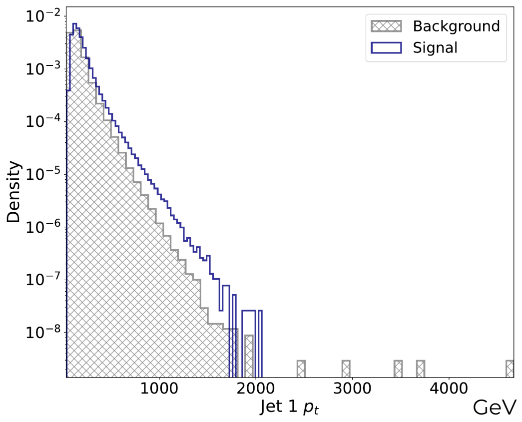
...discriminative variables of interest
For cuts or MVA classification.

Typical workflow: Model-dependent searches



MC Simulation

compute prob. distributions →



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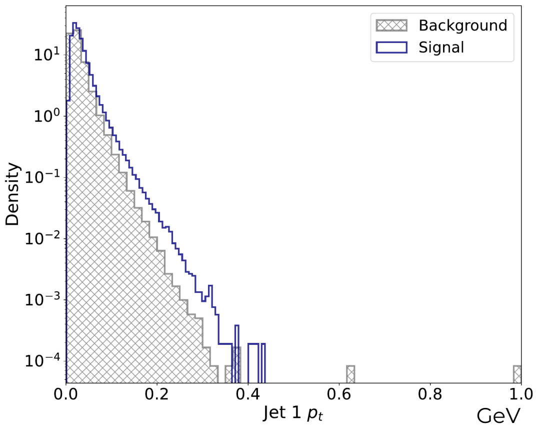
apply cuts and normalise →



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Input for classifiers models

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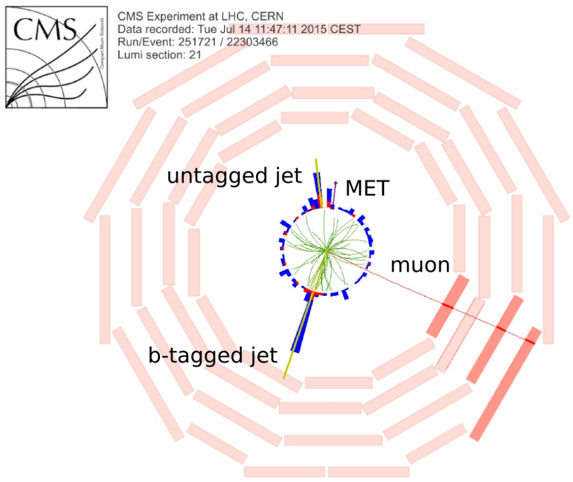

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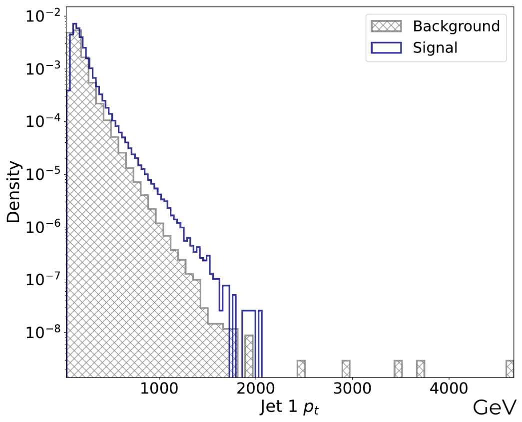

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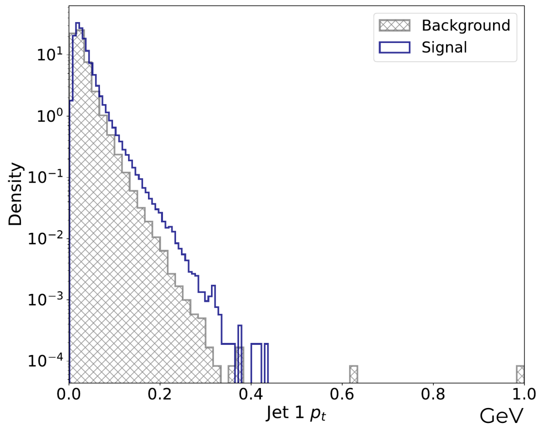

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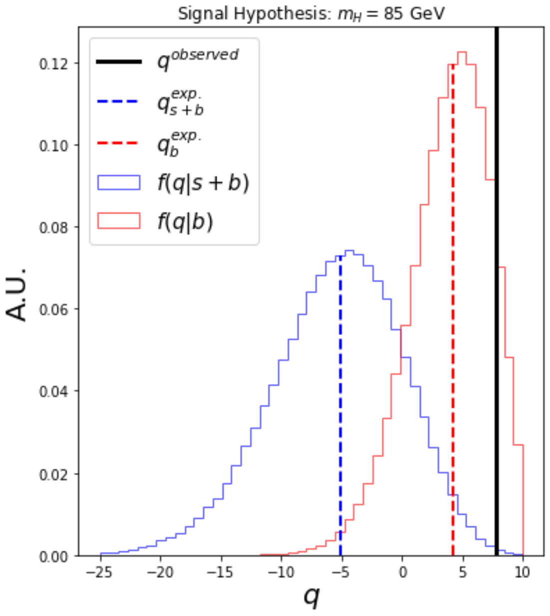
Classifier models:

cut-based or Machine Learning (BDT, NN, graph-net, etc.)

produce the *test statistic*



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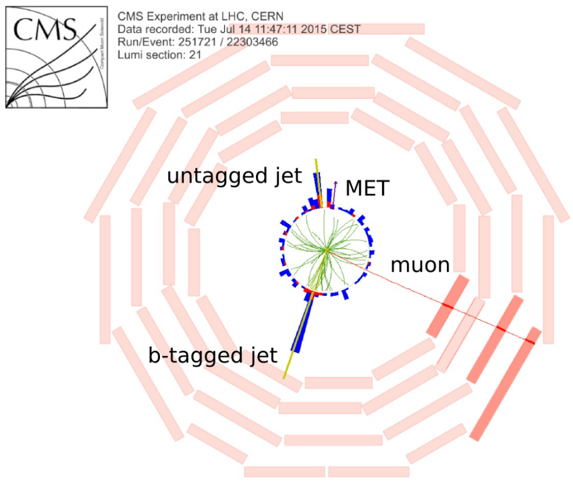

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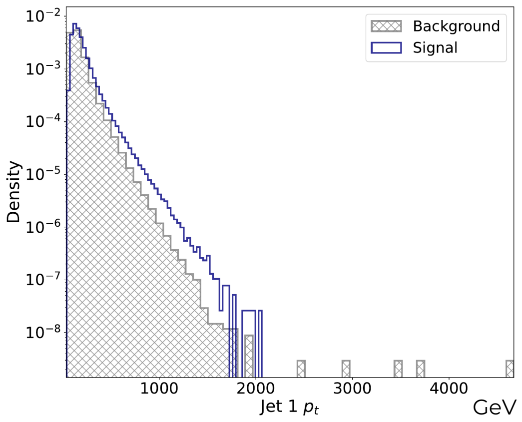

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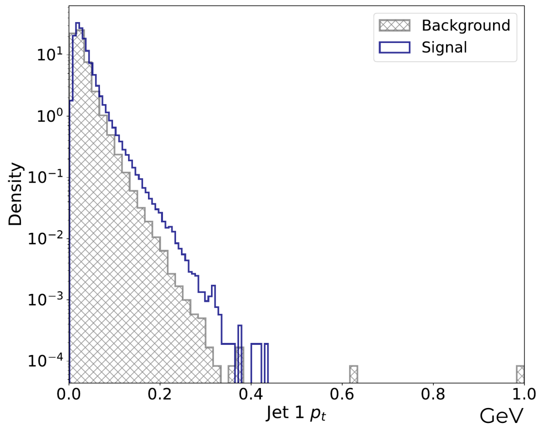

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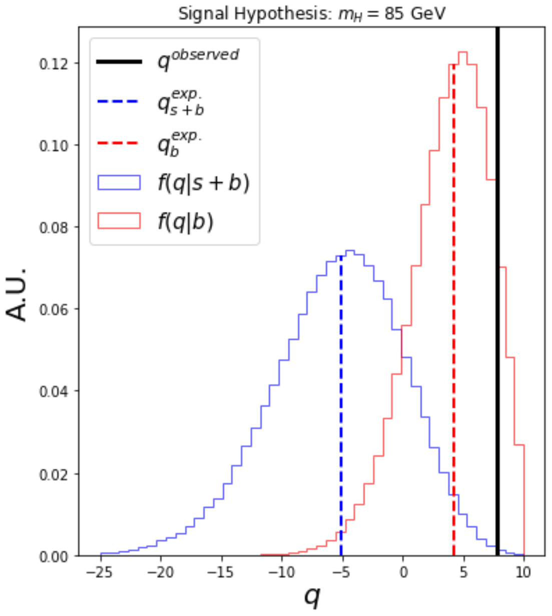


What if you do not know the signal?

Motivating model-independent searches

Bias is **not necessarily bad**. It can be **great!**

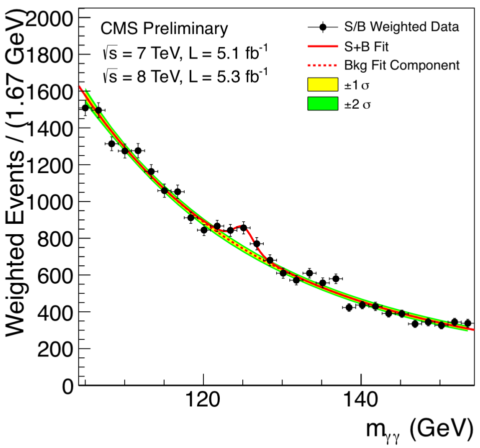
Higher bias $\longrightarrow$ lower variance of the statistical model

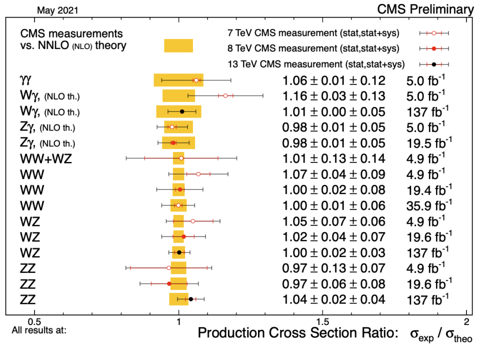
[Cramér–Rao bound]

So far, new-physics searches at the LHC:

assume SM + signal hypothesis….

[10.1016/j.physletb.2012.08.02]





Summary SM measurements @ CMS [link]

Motivating model-independent searches

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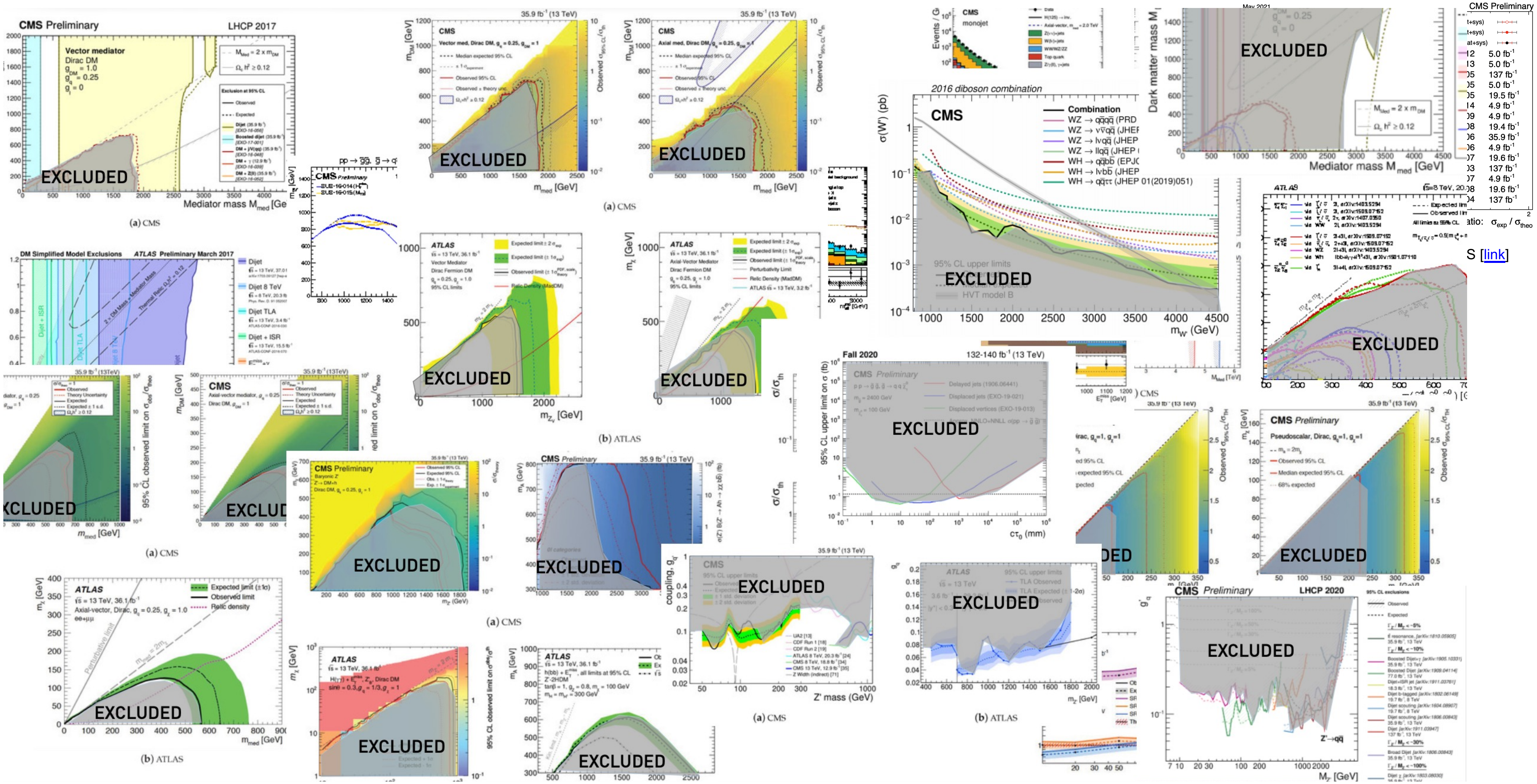

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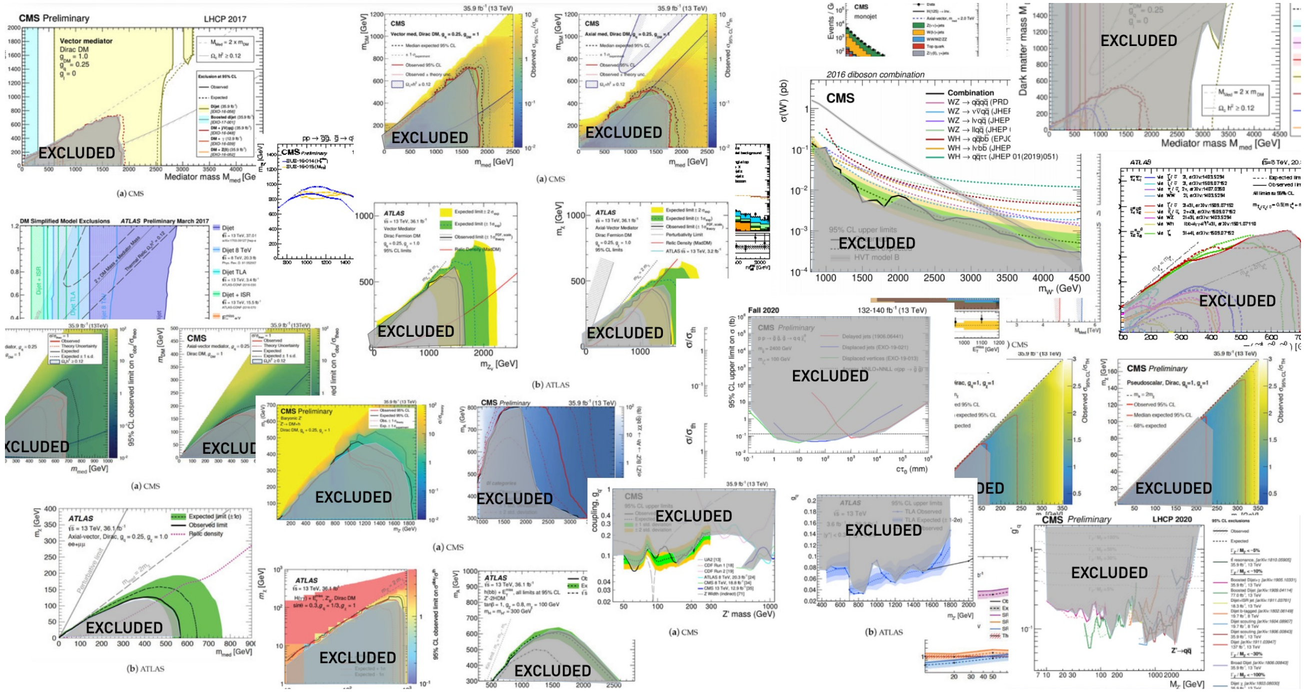

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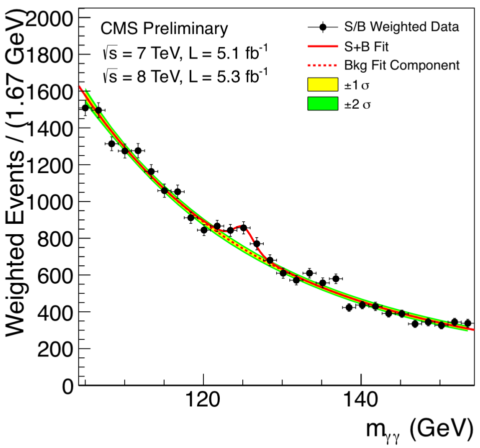

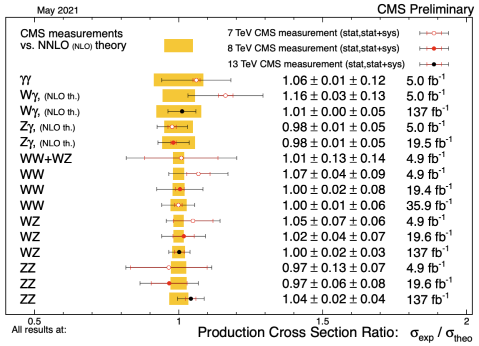

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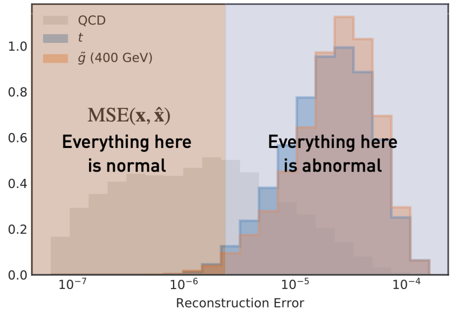
What if you don't know where to look for new-physics?

Look at nature with minimal bias.

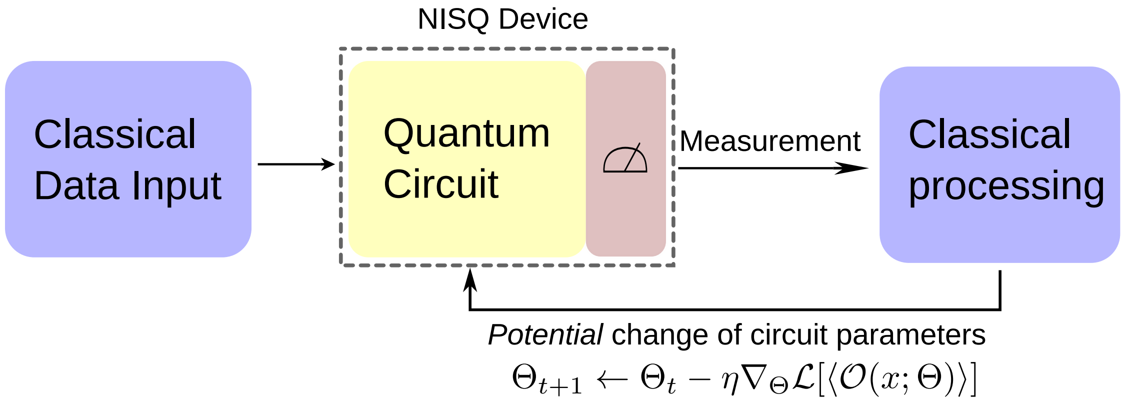
One possible solution:
Anomaly detection (ML/DL)



[Credit: Thea Årrestad; IPA Colloquium]

Quantum Machine Learning

Hybrid quantum-classical algorithms



Noisy intermediate scale quantum devices

- Circuit width: limited number of qubits.
- Circuit depth: limited number of operations per qubit (small decoherence times).
- Hardware noise.

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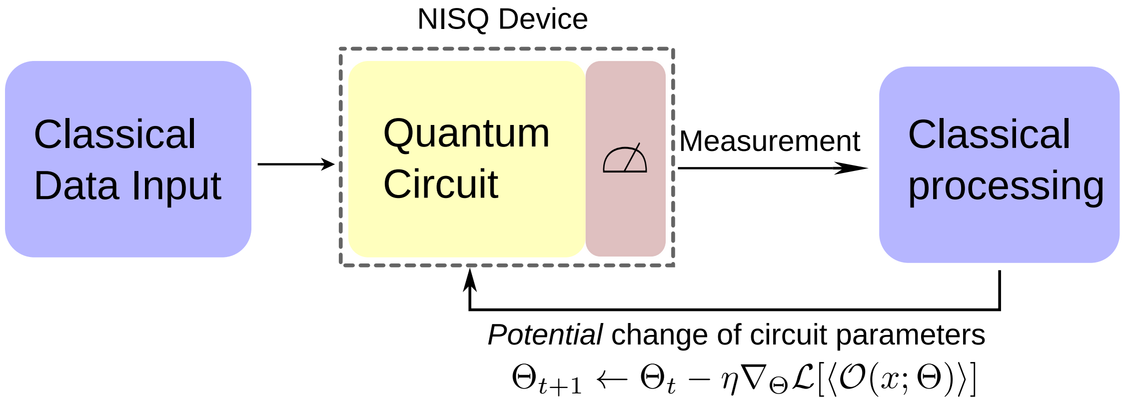

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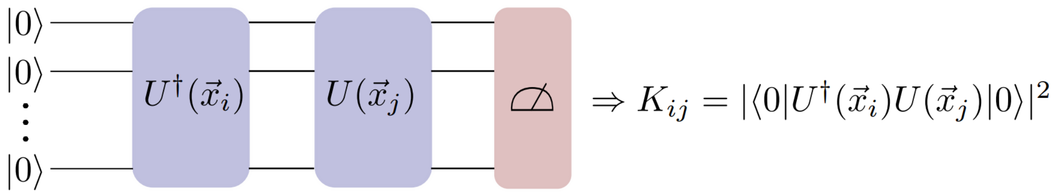
Quantum Machine Learning (QML) models for classification

<u>Kernel methods</u>
Quantum Support Vector Machines



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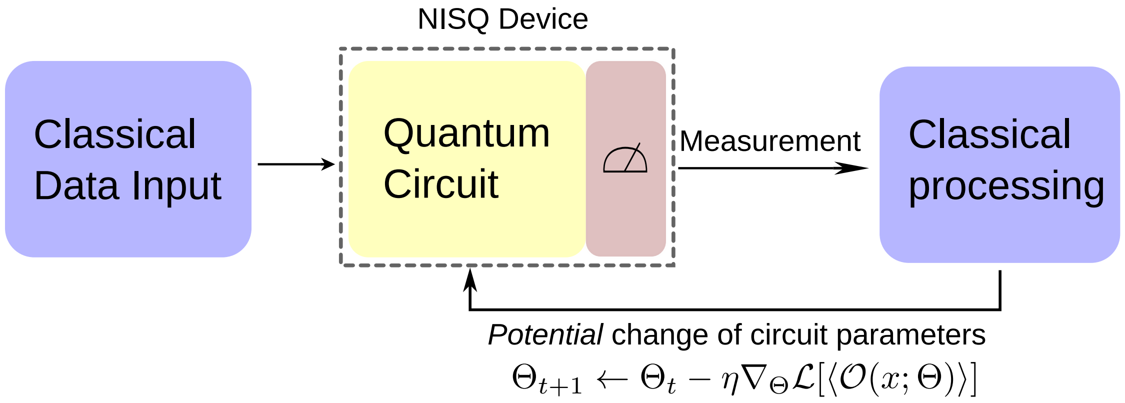

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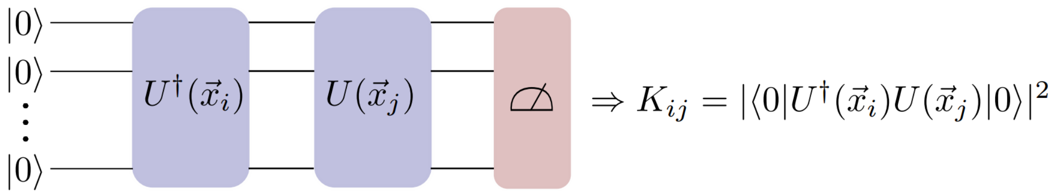
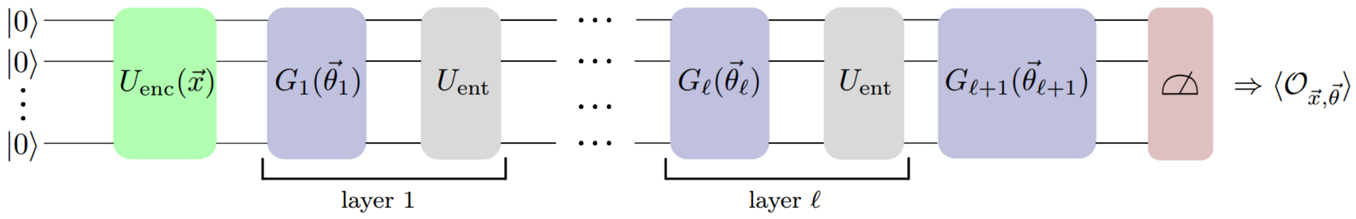


<u>Variational/Parametrised Quantum Circuits</u>
Quantum Neural Networks



Current hardware limitations: feature reduction presently needed for realistic datasets.

Motivation

Why quantum machine learning? Why for HEP?

Practical and exploratory answer

Investigate a new set of ML techniques to assess for advantages. Why not?

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Potentially, utilise the information and correlations (quantum remnants) inherent in HEP data? performance advantages?

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Theoretical results

Generalisation with few data, computational speed-ups, uncover correlations unrecognisable to classical methods

[M. Caro et al., Nature Communications 13, 4919 (2022)]
[A. Abbas et al., Nature Computational Science 1, 403 (2021)]
[Y. Liu et al., Nature Physics 17, 1013 (2021)]
[H. Huang et al., Nature Communications 12, 2631 (2021)]
[H . Huang et al.,, Science 376, 1182 (2022)]
[N. Pirnay et al., arXiv: 2212.08678 (2022)]
Among others...

Results

Finding new-physics in dijet events with QML

Identifying new-physics with quantum models

Anomaly detection with quantum machine learning

Background: QCD multi-jet events. $n^{\text{features}} = 300$ per jet $\longrightarrow$ Too many for current hardware

$G \to W^- W^+$ $\quad$ $A \to HZ \to ZZZ$

Tested BSM anomalies: Graviton **&** New Scalar Boson $\longrightarrow$ Multi-jet final state

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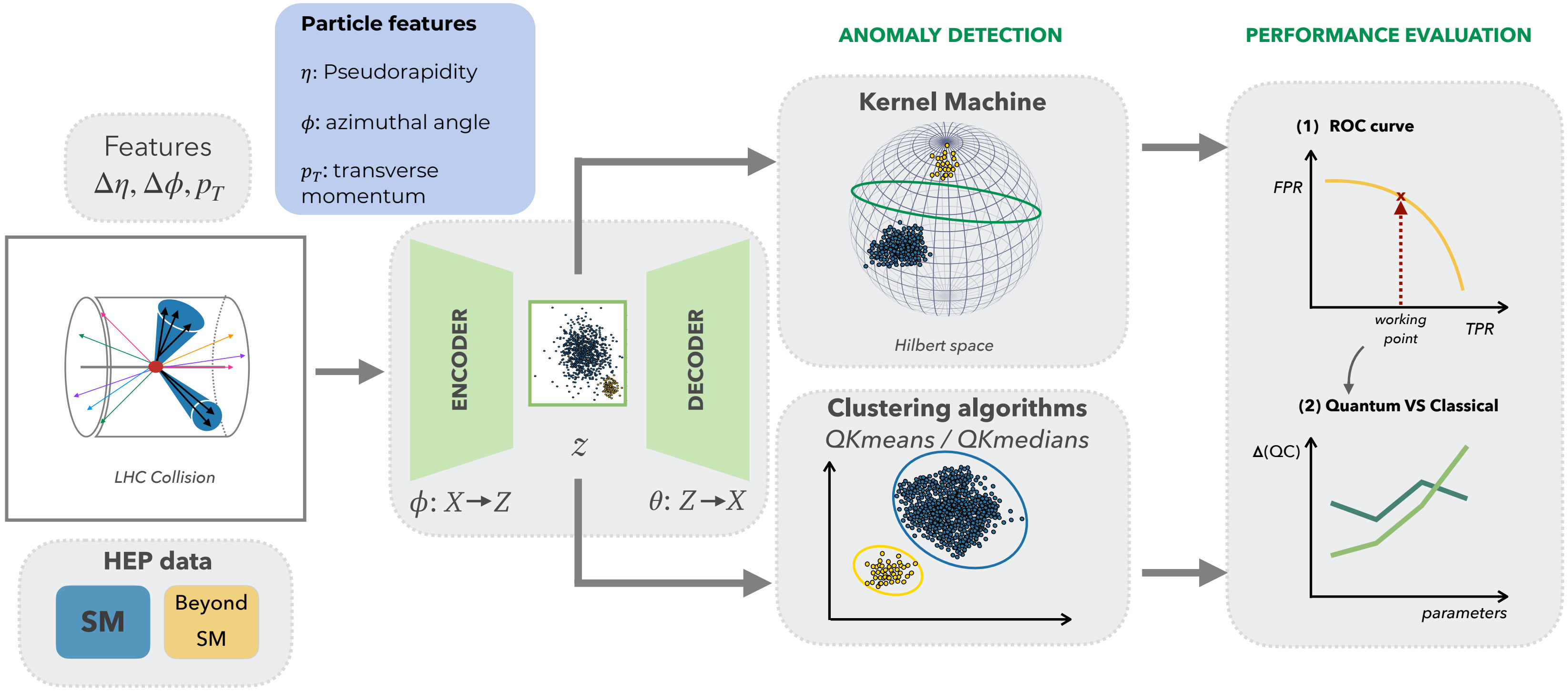
Tested BSM anomalies: Graviton ($G \to W^- W^+$) & New Scalar Boson ($A \to HZ \to ZZZ$) ⟶ Multi-jet final state



Suitable metric for anomaly detection

Background rejection @ working point

$$\varepsilon_{\mathrm{b}}^{-1}(\varepsilon_s; \mathcal{M})$$

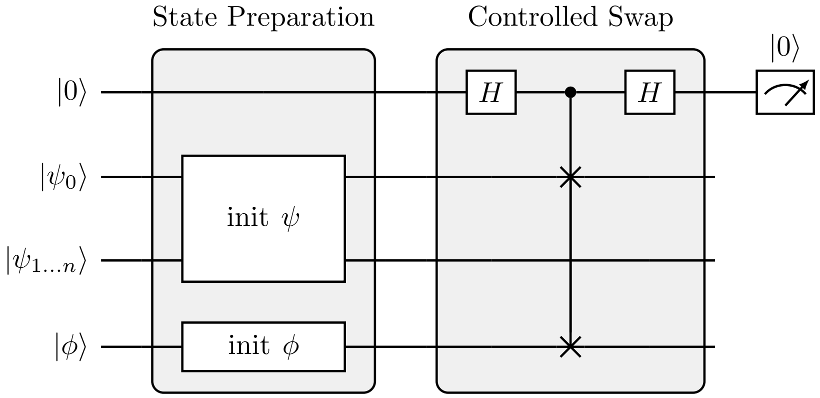
Compare models

$$\Delta_{\mathrm{QC}}(\varepsilon_s) = \frac{\varepsilon_{\mathrm{b}}^{-1}(\varepsilon_s; Q)}{\varepsilon_{\mathrm{b}}^{-1}(\varepsilon_s; C)}$$

Quantum clustering for anomaly detection

Construct clusters in the Hilbert space

Quantum distance calculation from clusters



Minimise the distance with **quantum** (QK-means) or hybrid/**classical** (QK-medians) optimisation algorithms

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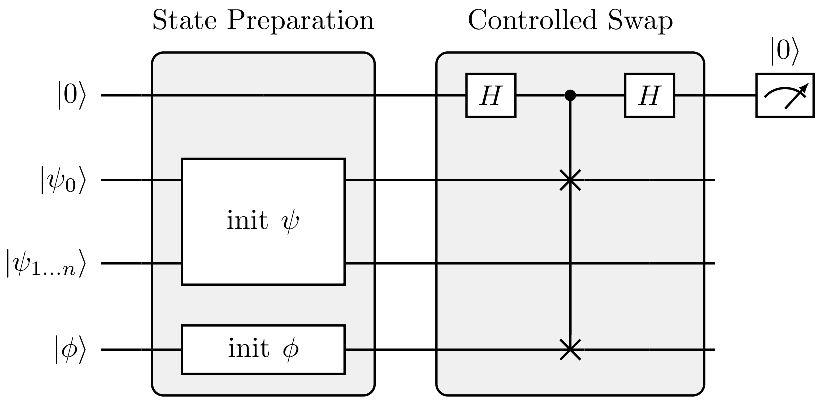

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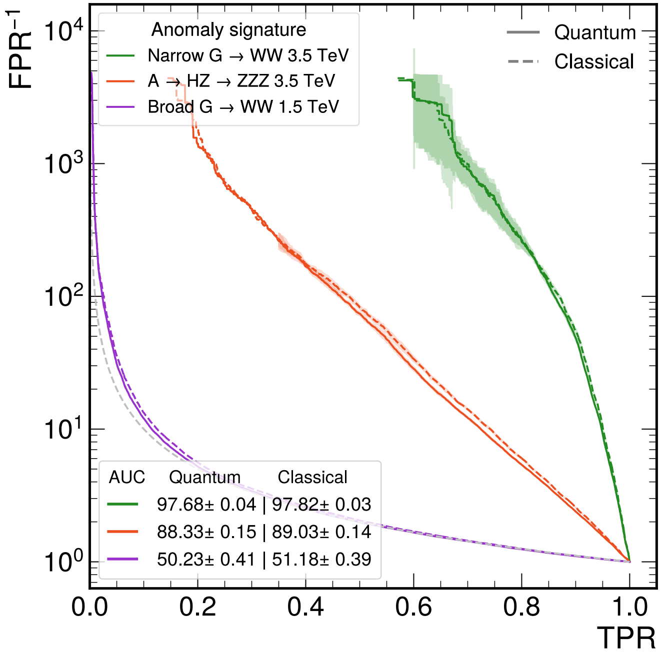
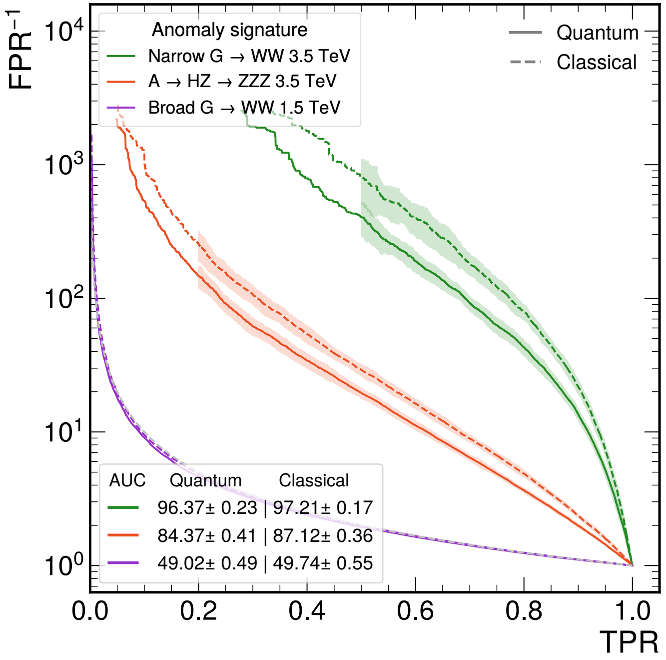
Quantum K-medians



Quantum K-means



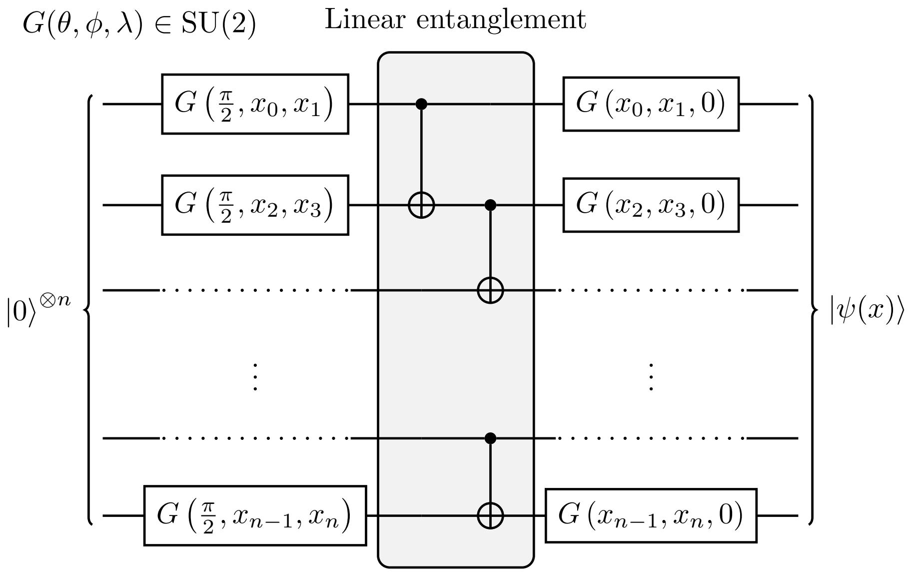
[K.A. Wozniak*, VB*, E. Puljak*, et al., arXiv: 2301.10780]

Quantum and classical anomaly detection has similar performance.

Kernel-based quantum anomaly detection

Unsupervised quantum kernel machine $\mathrm{K}_{ij} = |\langle 0|U^\dagger(\vec{x}_i)U(\vec{x}_j)|0\rangle|^2$

Designed data encoding circuit



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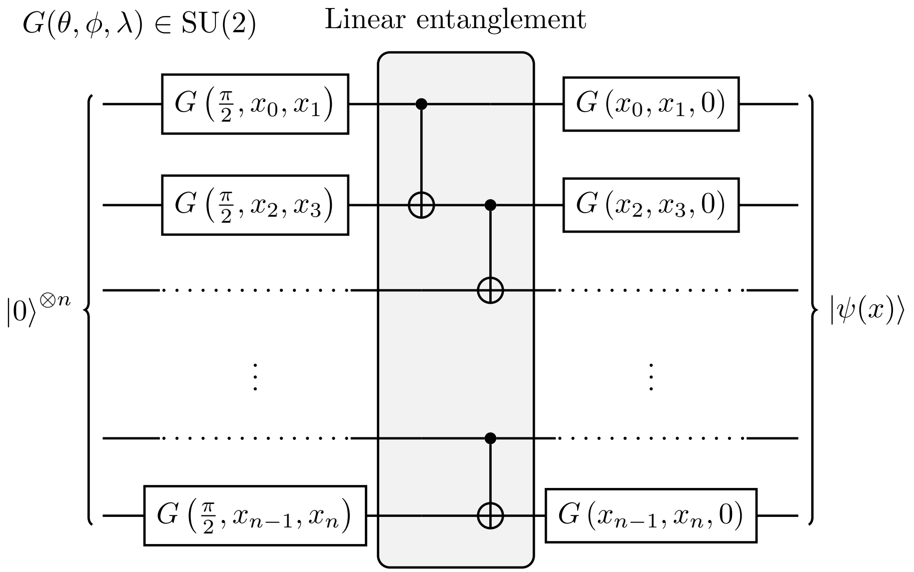
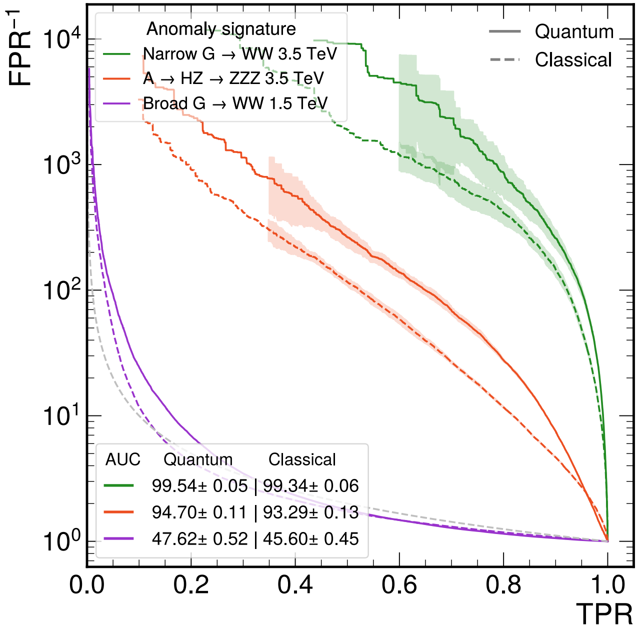
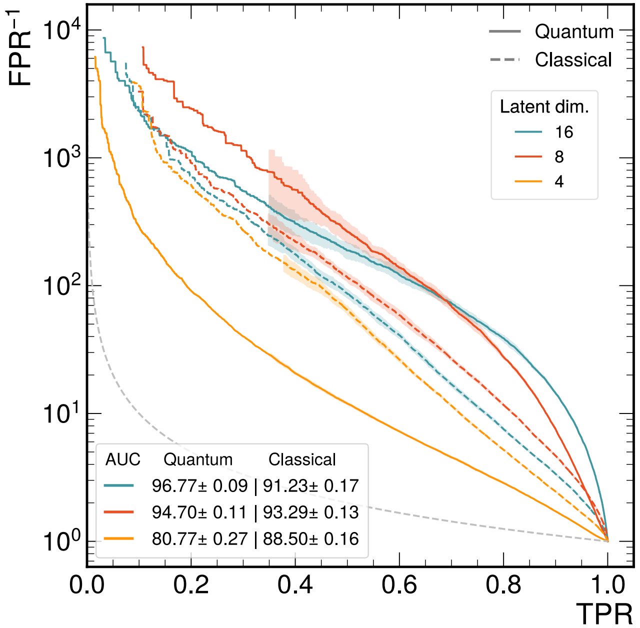


Different BSM scenarios



Different qubit number



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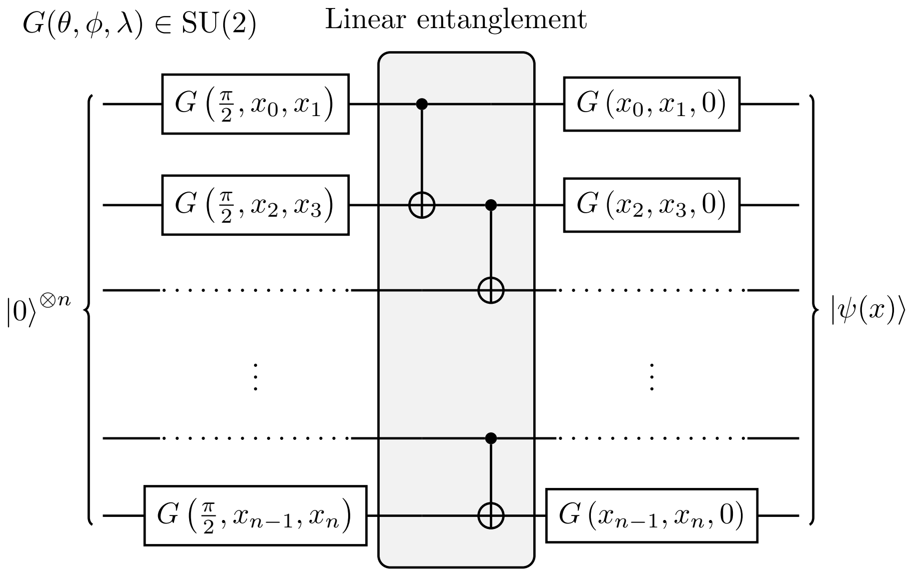

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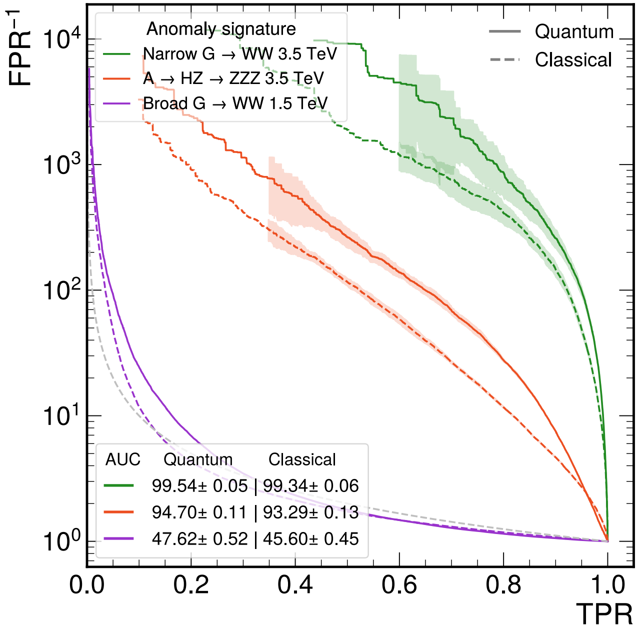

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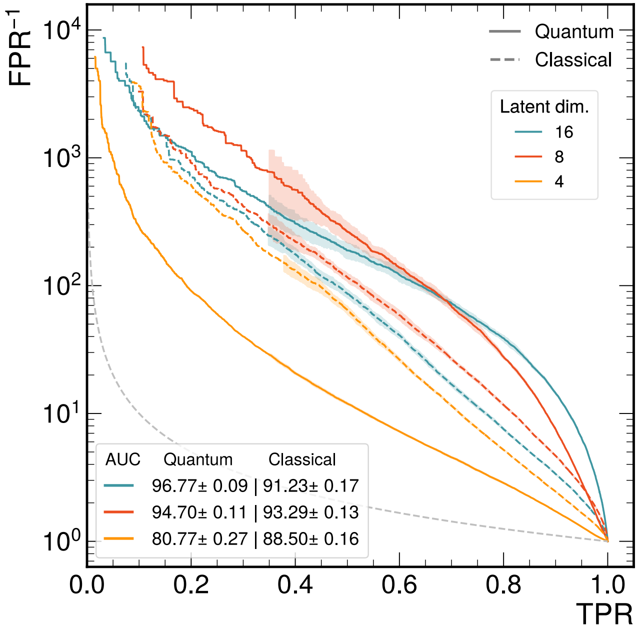

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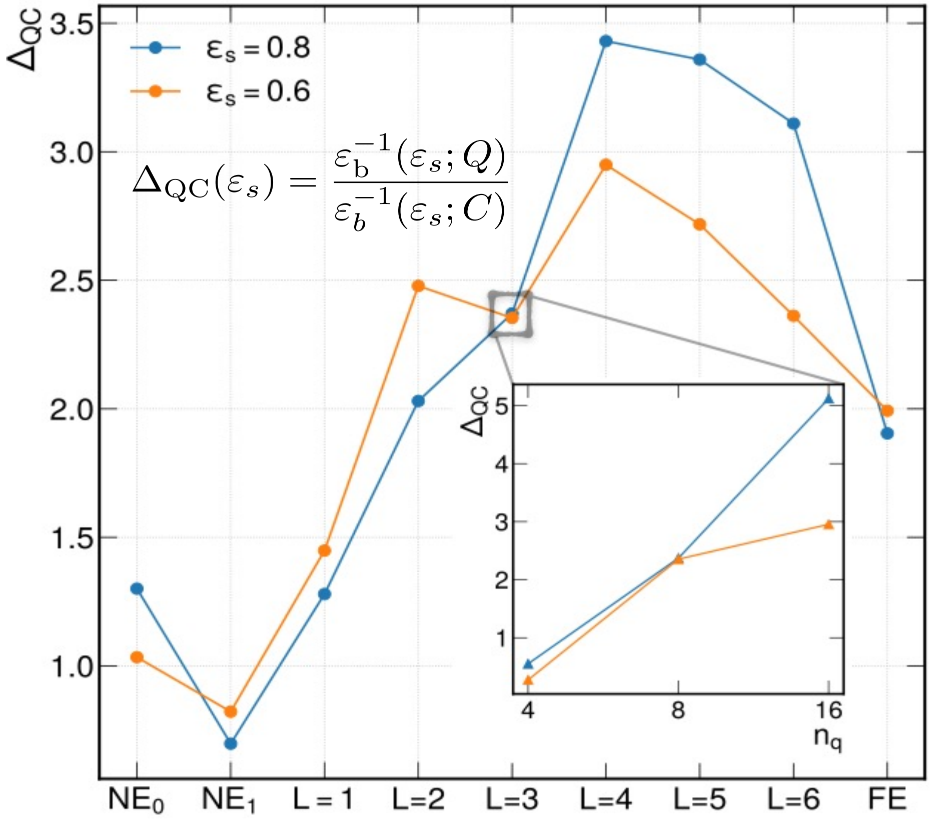
Instance of significant and consistent quantum performance advantage!

Very exciting and first of its kind result (HEP + Anomaly detection)!

Quantum circuit properties vs. performance

[K.A. Wozniak*, VB*, E. Puljak*, et al., arXiv: arXiv:2301.10780]

Performance vs. circuit architectures
Analysing circuit depth (expressibility) and amount entanglement

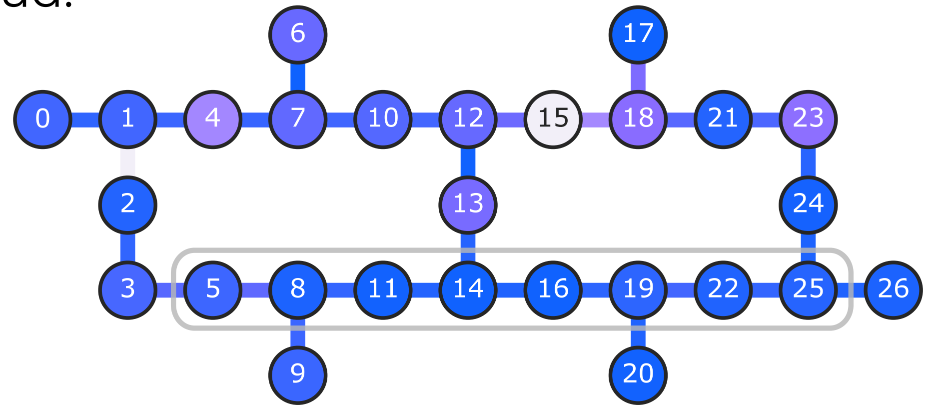


Importance of intrinsically quantum properties of the feature map.

Up to **five times** the performance of the classical model for 16 qubits!

Quantum hardware runs

Submit jobs to a real machine (ibm_toronto) using IBMQ cloud.
(CERN quantum-hub)



Map algorithm to hardware qubits.

Minimal instance 100 + 100 (train + test) datapoints.

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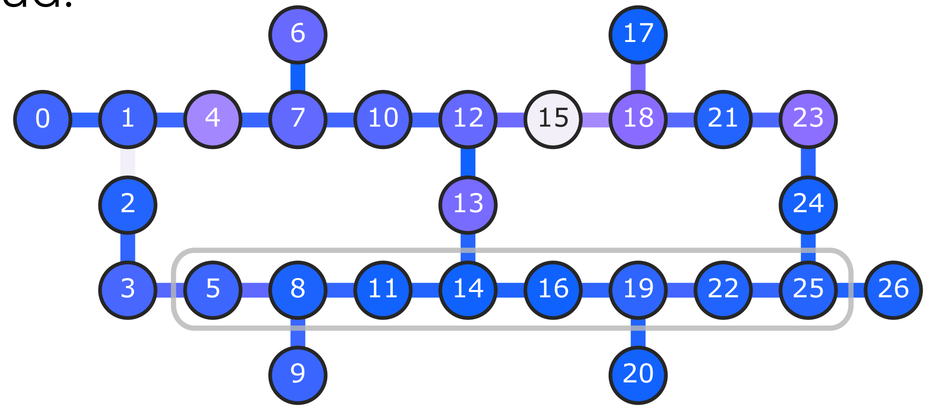

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Kernel Machine Run	AUC	$\langle \mathrm{tr}\rho^2 \rangle$
Hardware $L = 1$	0.844	0.271(6)
Ideal $L = 1$	0.999	1
Hardware $L = 3$	0.997	0.15(2)
Ideal $L = 3$	1.0	1
Classical	0.998	-

Purity of fully mixed state: $1/2^{n_q} \approx 0.39 \times 10^{-2}$
(decoherence = loss of “quantumness”)

$$\langle \mathrm{tr}\rho^2 \rangle = \langle K(x_i, x_i) \rangle$$

$$\rho(x_i) = U(x_i)|0\rangle\langle 0|U^\dagger(x_i)$$

Proposed data encoding circuit realistic and suitable for current devices

Conclusions

Quantum anomaly detection for HEP

Fundamentally different way of data representation and processing.

Model-independent (unsupervised learning) approach for minimally biased searches of new-physics.

Promising results identifying a **significant and consistent advantage** in anomaly detection!

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For more details checkout:

- K.A. Wozniak*, VB*, E. Puljak*, et al., **Quantum anomaly detection in the latent space of proton collision events at the LHC,** arXiv:2301.10780

- J. Shuhmacher, L. Bogia, VB, et al. **Unravelling physics beyond the standard model with classical and quantum anomaly detection,** arXiv: 2301.10787

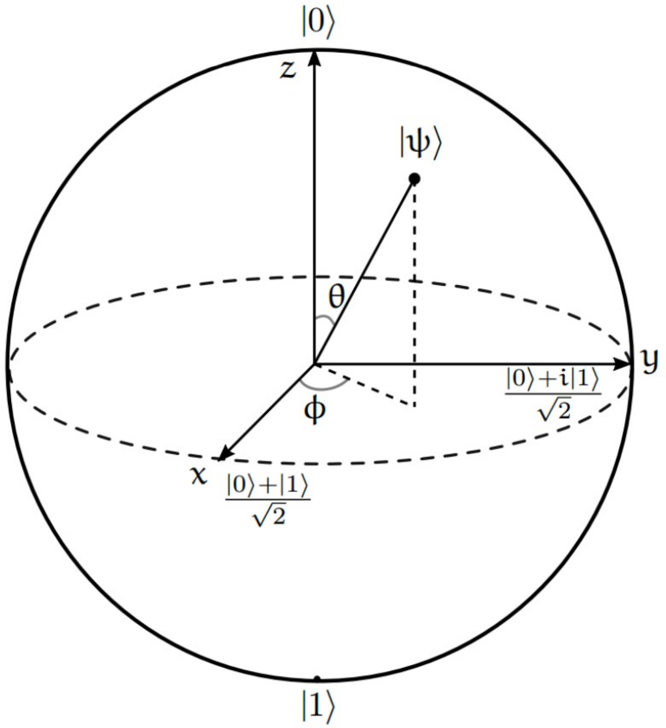
Questions?

Backup slides

Basics of quantum information processing

The qubit:

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \;\equiv \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$

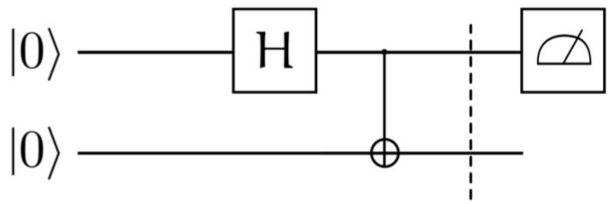


Generic qubit operations (quantum gates) $U = e^{-i\vec{\theta}\cdot\frac{\vec{\sigma}}{2}} \in \mathrm{SU}(2)$:

$$U(\theta,\phi,\lambda) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -e^{i\lambda}\sin\left(\frac{\theta}{2}\right) \\ e^{i\phi}\sin\left(\frac{\theta}{2}\right) & e^{i(\phi+\lambda)}\cos\left(\frac{\theta}{2}\right) \end{pmatrix}$$

Construct all possible gates from $U(\theta,\phi,\lambda)$

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \equiv U\left(\frac{\pi}{2}, 0, \pi\right)$$



$$|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Quantum Gate Universality [DiV95]: The above “building blocks” can construct any quantum circuit acting on n qubits, i.e. $\mathrm{SU}(2^n)$, operating on at most *two-qubits* at a time.

Quantum gates and universality

Single qubit gates:

- A generic quantum gate can be decomposed in a series of R_y and R_z [BBC+95]

$$U(\theta,\phi,\lambda) = R_z(\lambda)R_y(\theta)R_z(\phi)$$

Multi-qubit gates:

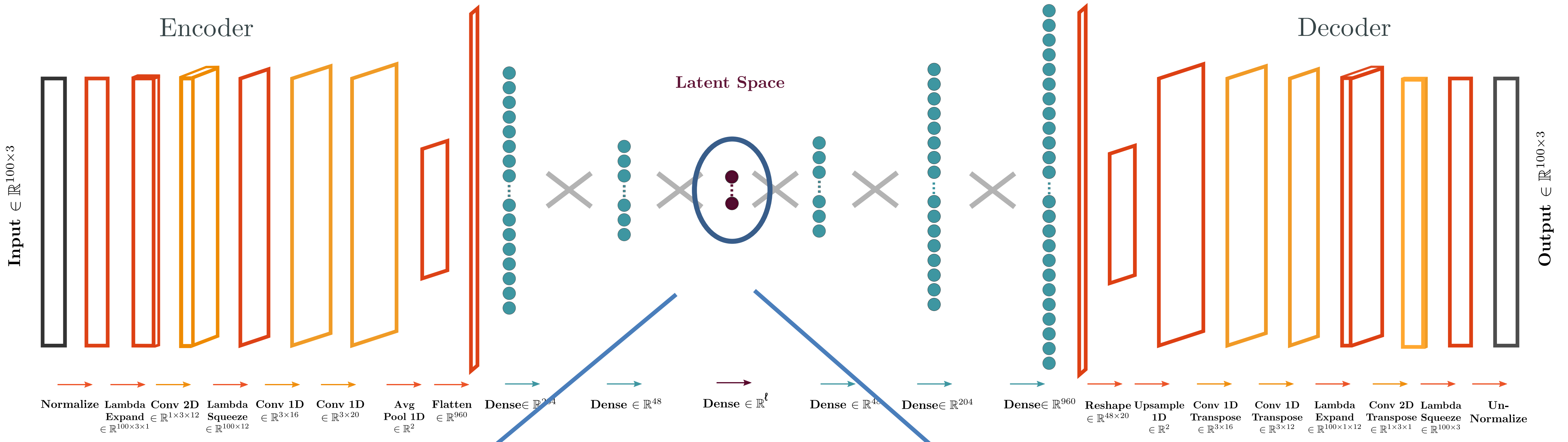
- 2-qubit SWAP and CNOT (Control-X) gates and the 3-qubit Toffolli gate

$$CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

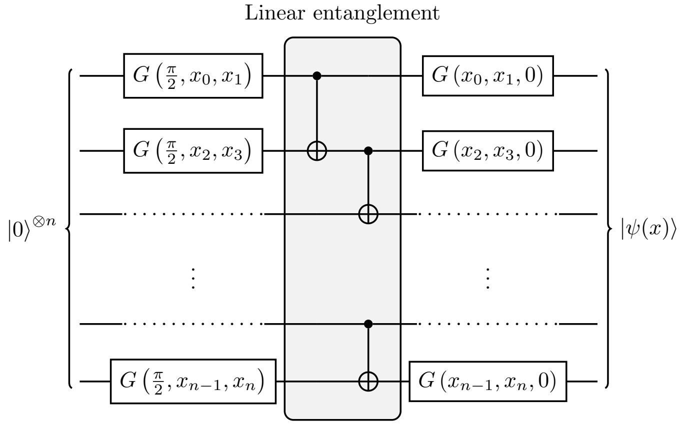
- Any control-U gate can be written as a combination of CX, R_y and R_z gates.

Quantum Gate Universality [DiV95]: The above "building blocks" can construct any quantum circuit acting on n qubits, i.e. SU(2^n), operating on at most *two-qubits* at a time.

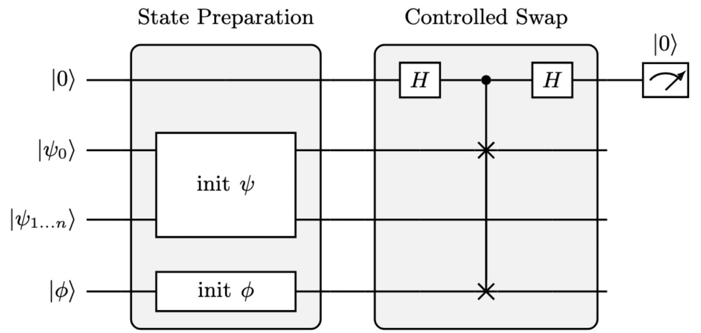
Convolutional autoencoder architecture



Unsupervised kernel machine

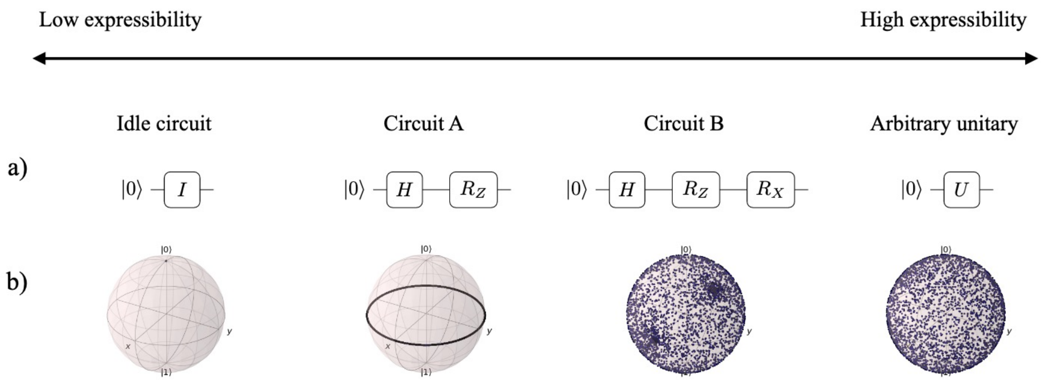


Quantum clustering algorithms

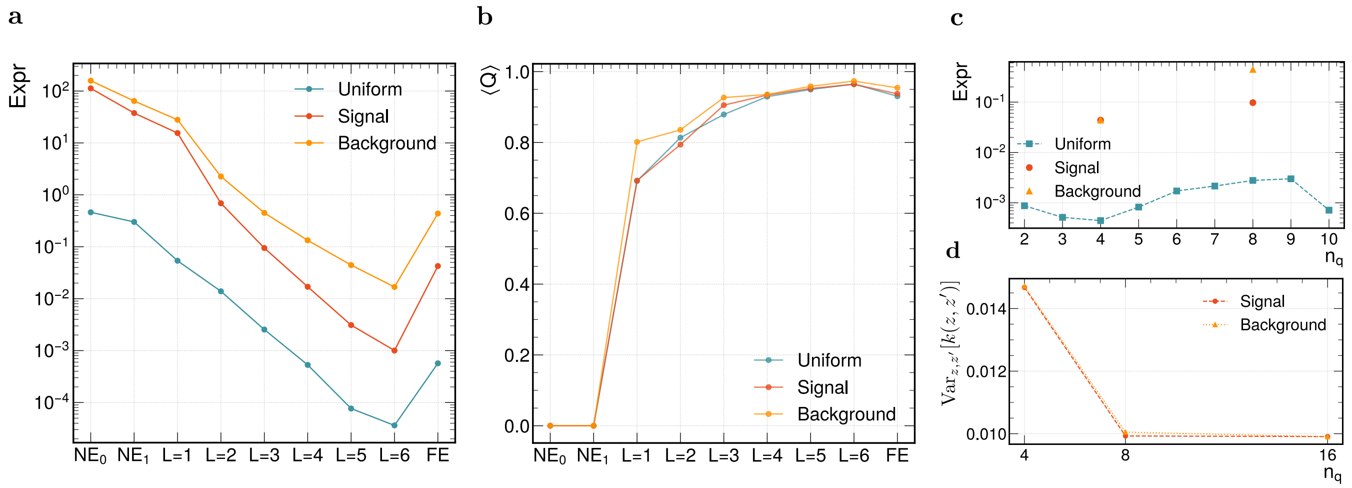


Expressibility and entanglement capability

Expressibility [S. Sim, et al., Adv. Quantum Technol. 2 (2019) 1900070]



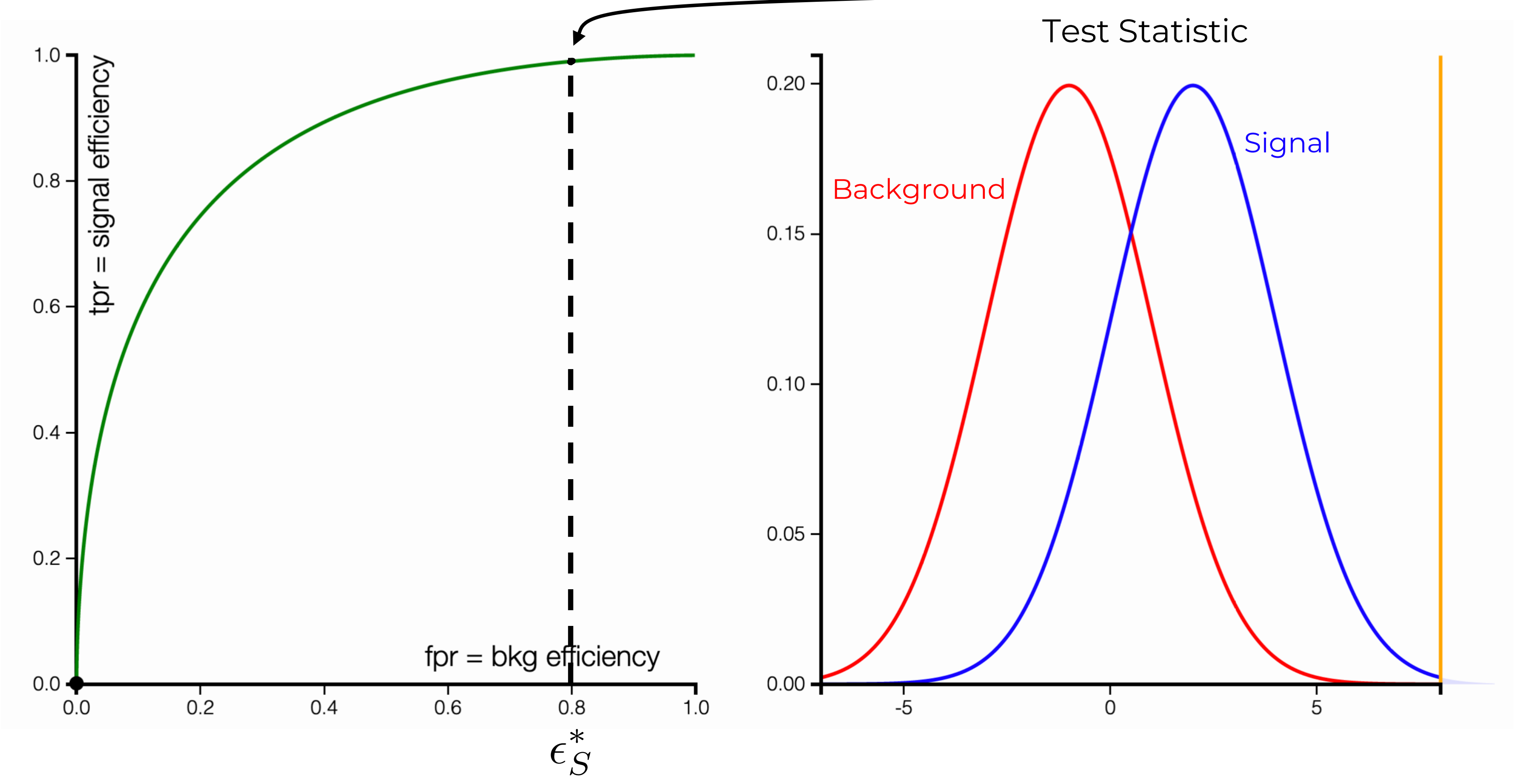
Expressibility & Entanglement capability of our data encoding circuit



[K.A. Wozniak*, **VB***, E. Puljak*, et al., arXiv:2301.10780]

Performance Metric

- The normalised data samples are split into training, validation, and testing data sets.
- Classification power metric: Receiver Operating Characteristic (ROC) curve.
- More compact metric: Area Under Curve (AUC) of the ROC curve.
- More practical metric: working point of an analysis $\epsilon_B(\epsilon_S^*)$



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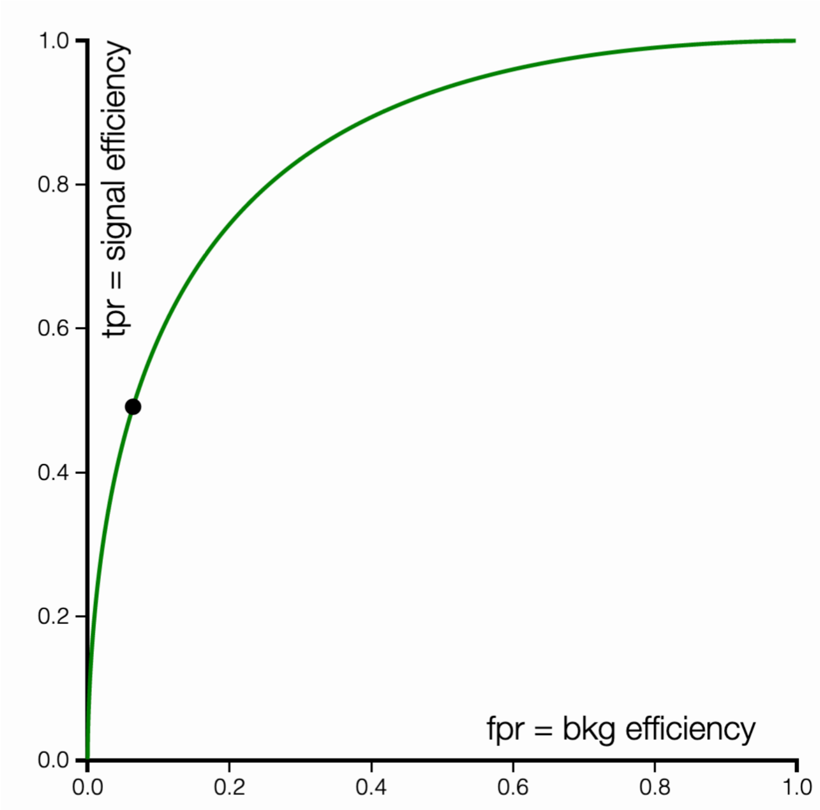

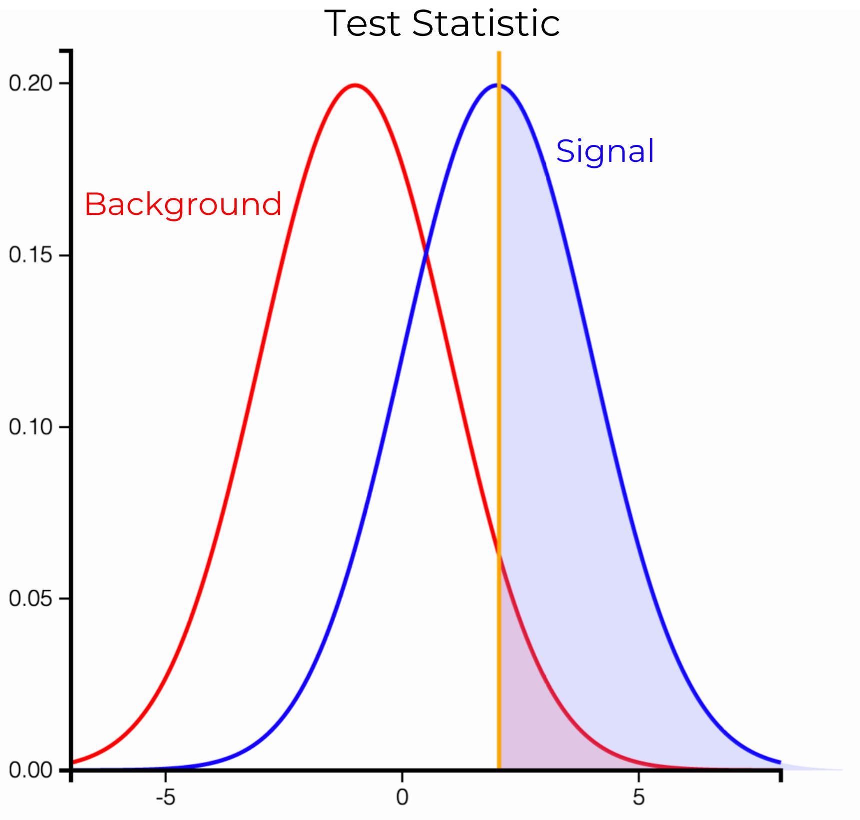

ETH zürich

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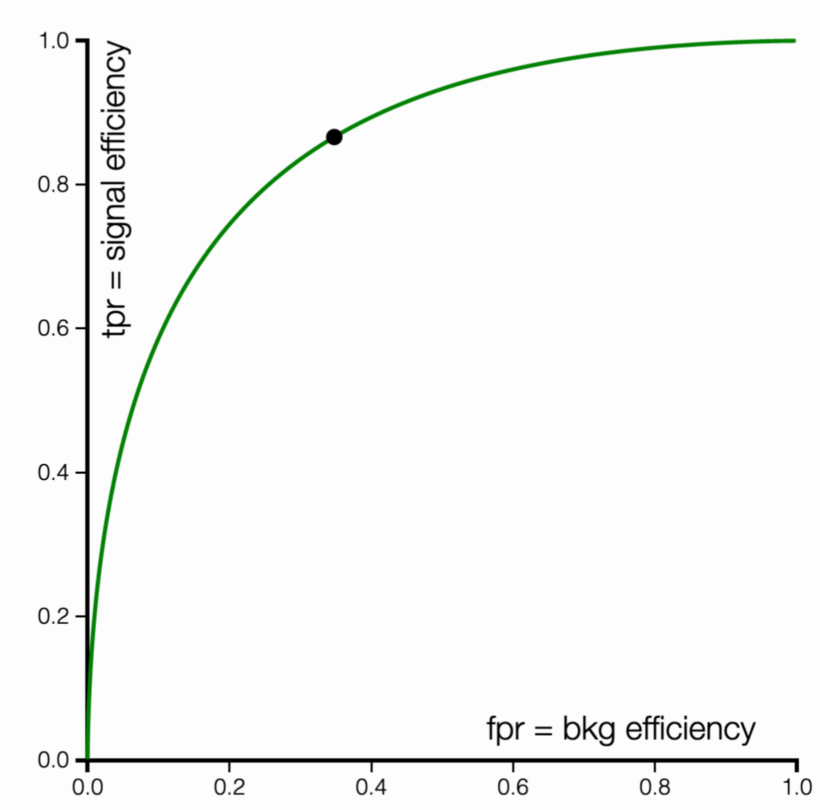

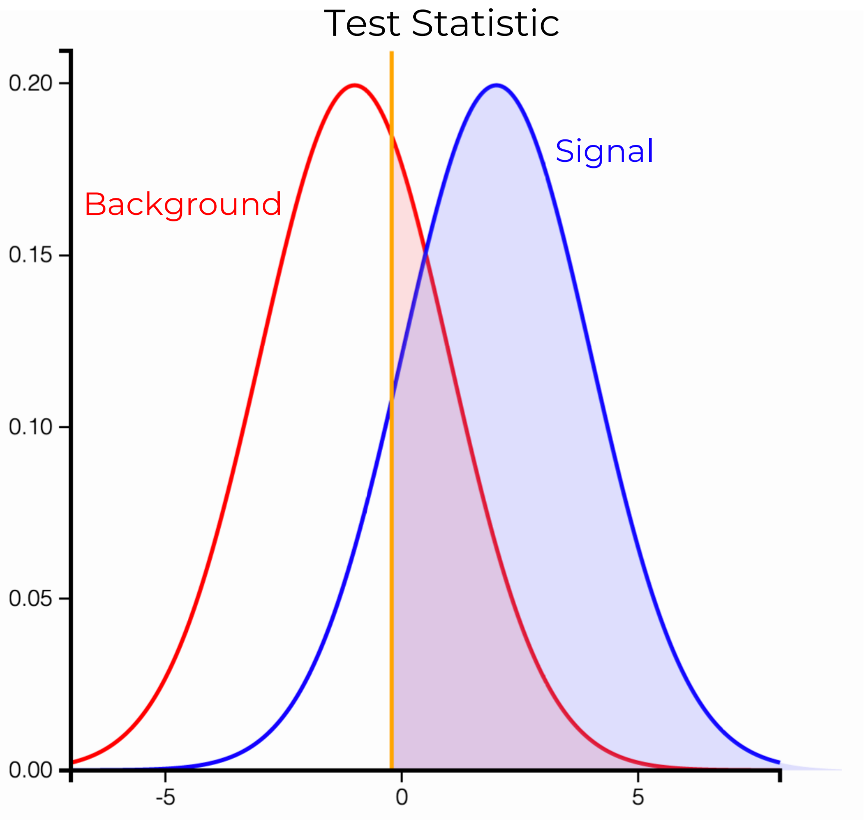

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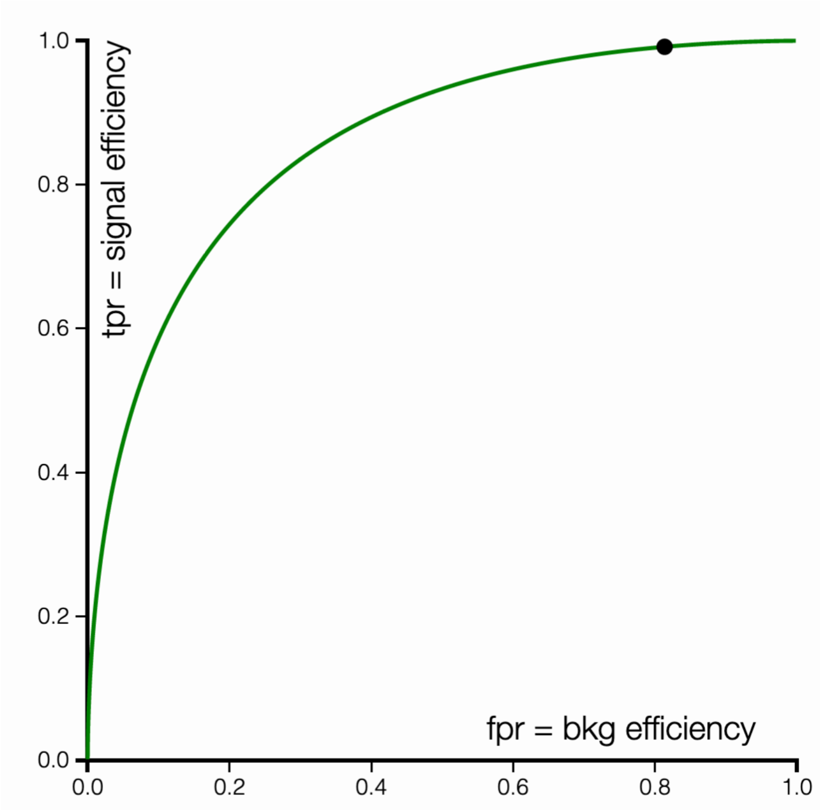
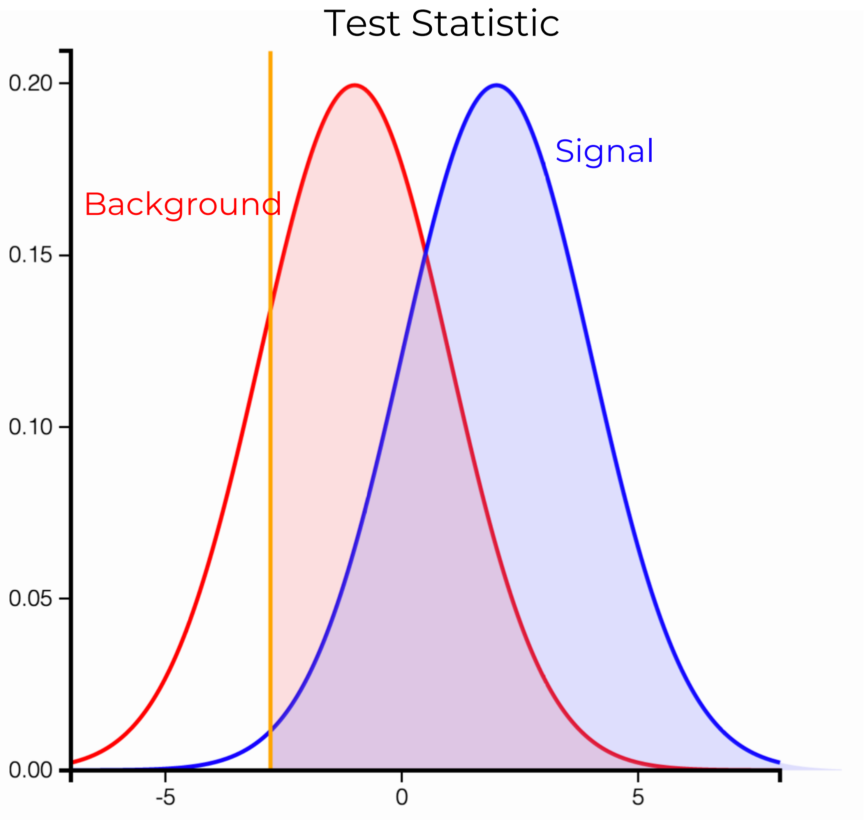
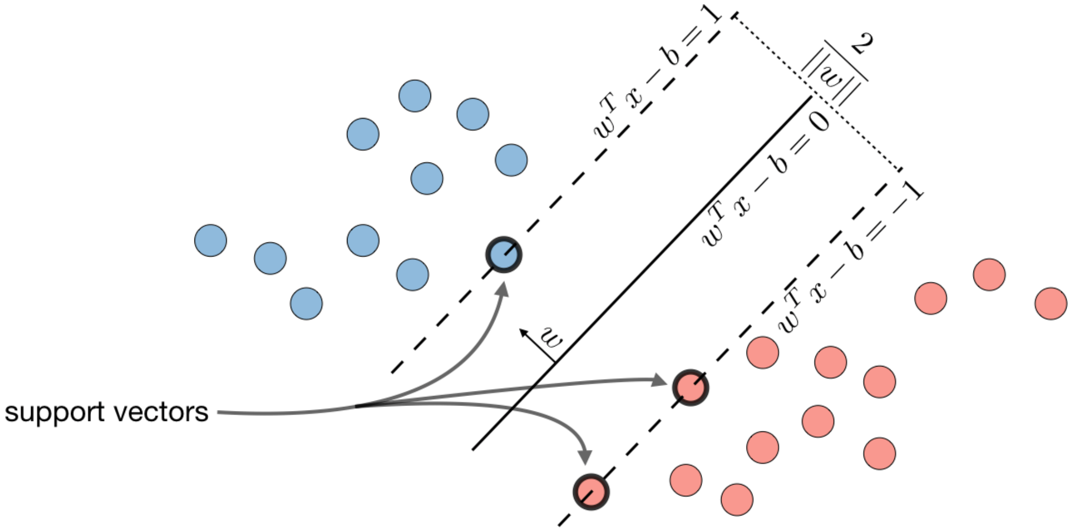




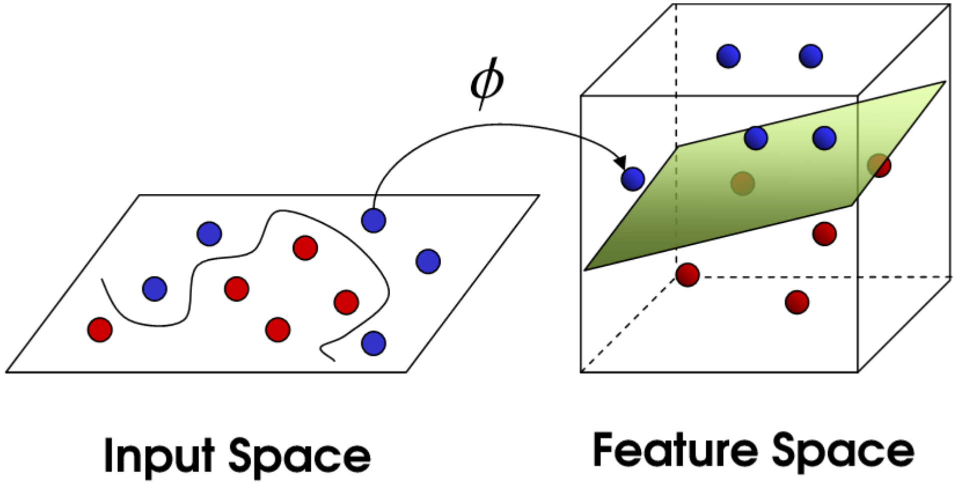
Quantum Support Vector Machines



SVM objective function is equivalent to (dual Lagrangian):

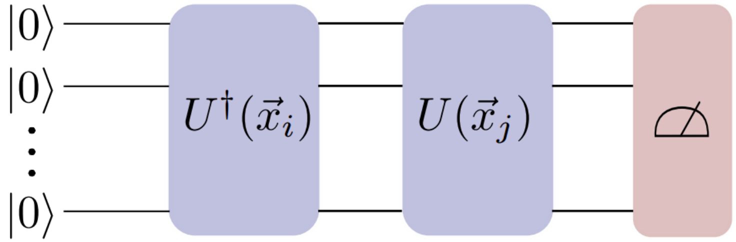
maximize $$L(c_1, \ldots, c_n) = \sum_{i=1}^{n} c_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i c_i (\vec{x}_i \cdot \vec{x}_j) y_j c_j$$

subject to $$\sum_{i=1}^{n} c_i y_i = 0, \text{ and } 0 \leq c_i \leq C, \; \forall i$$



Kernel trick: $(\vec{x}_i \cdot \vec{x}_j) \mapsto k(\vec{x}_i \cdot \vec{x}_j) = \phi(\vec{x}_i) \cdot \phi(\vec{x}_j)$

Make the kernel *quantum*

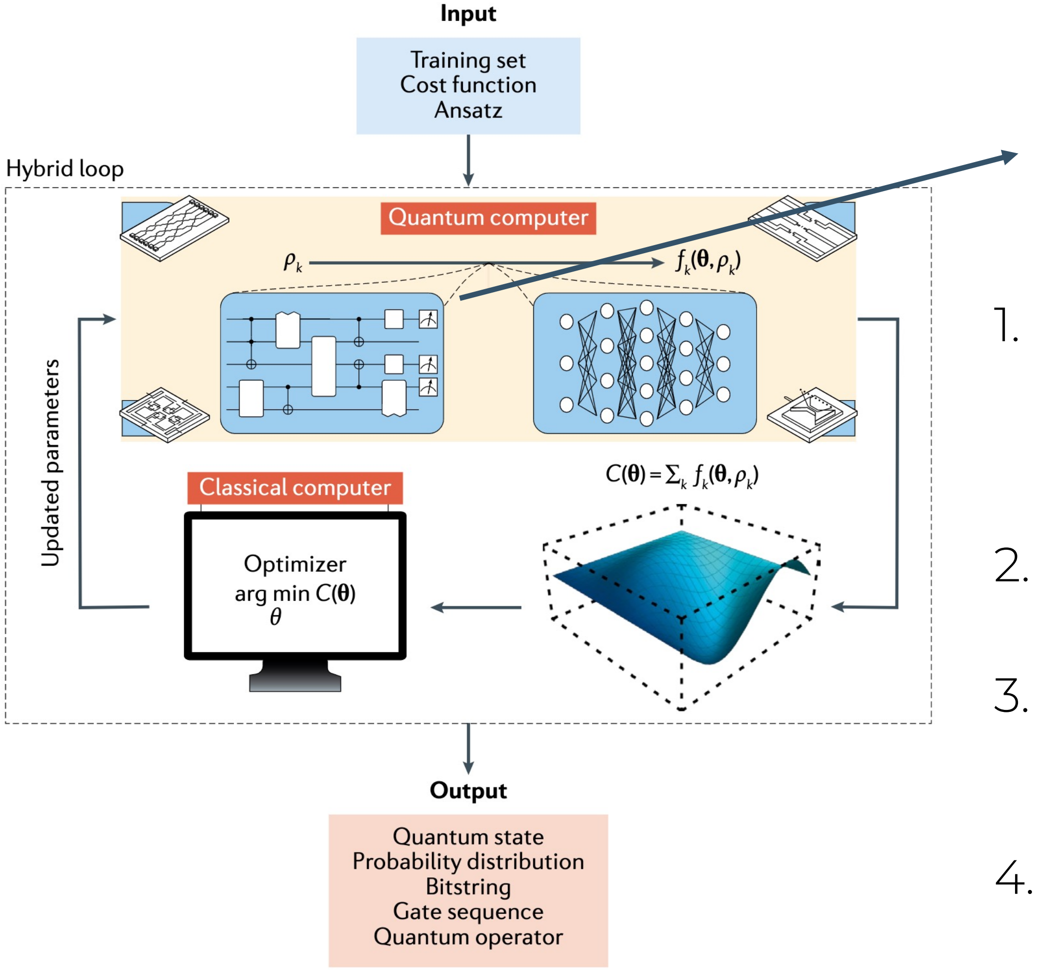


$\Rightarrow K_{ij} = |\langle 0|U^\dagger(\vec{x}_i) U(\vec{x}_j)|0\rangle|^2$

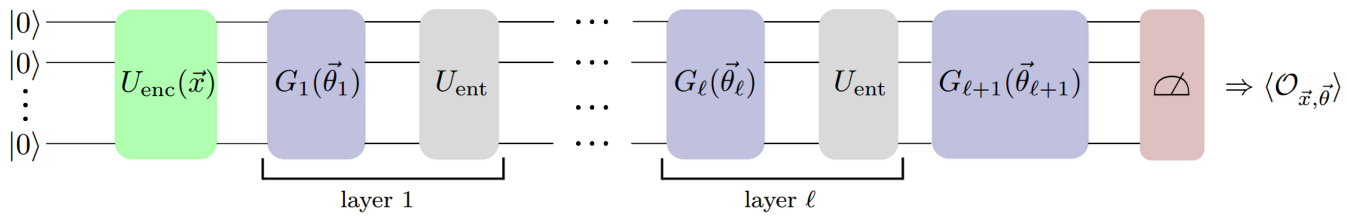
***Can be generalised to unsupervised learning**

Quantum Neural Networks

Variational quantum algorithm workflow



[M. Cerezo, et al. Nat. Rev. Phys. 3, 625–644 (2021)]



1. Choose loss function
   Task dependent: e.g. classification, reconstruction, generative modeling.

2. Embed classical data to circuit.

3. Process quantum state with parametrized quantum gates.

4. Update trainable parameters

$$\Theta_{t+1} \leftarrow \Theta_t - \eta \nabla_\Theta \mathcal{L}[\langle \mathcal{O}(x;\Theta) \rangle]$$