# Quantum anomaly detection in the latent space of proton collision events at the LHC

**Vasilis Belis**[1] [arXiv:2301.10780]

K. Woźniak[2,3], E. Puljak[2,4], P. Barkoutsos[5,*], G. Dissertori[1], M. Grossi[2], M. Pierini[2], F. Reiter[1], I. Tavernelli[5], S. Vallecorsa[2]

*currently Pasqal

23 November, CERN

QTML 2023

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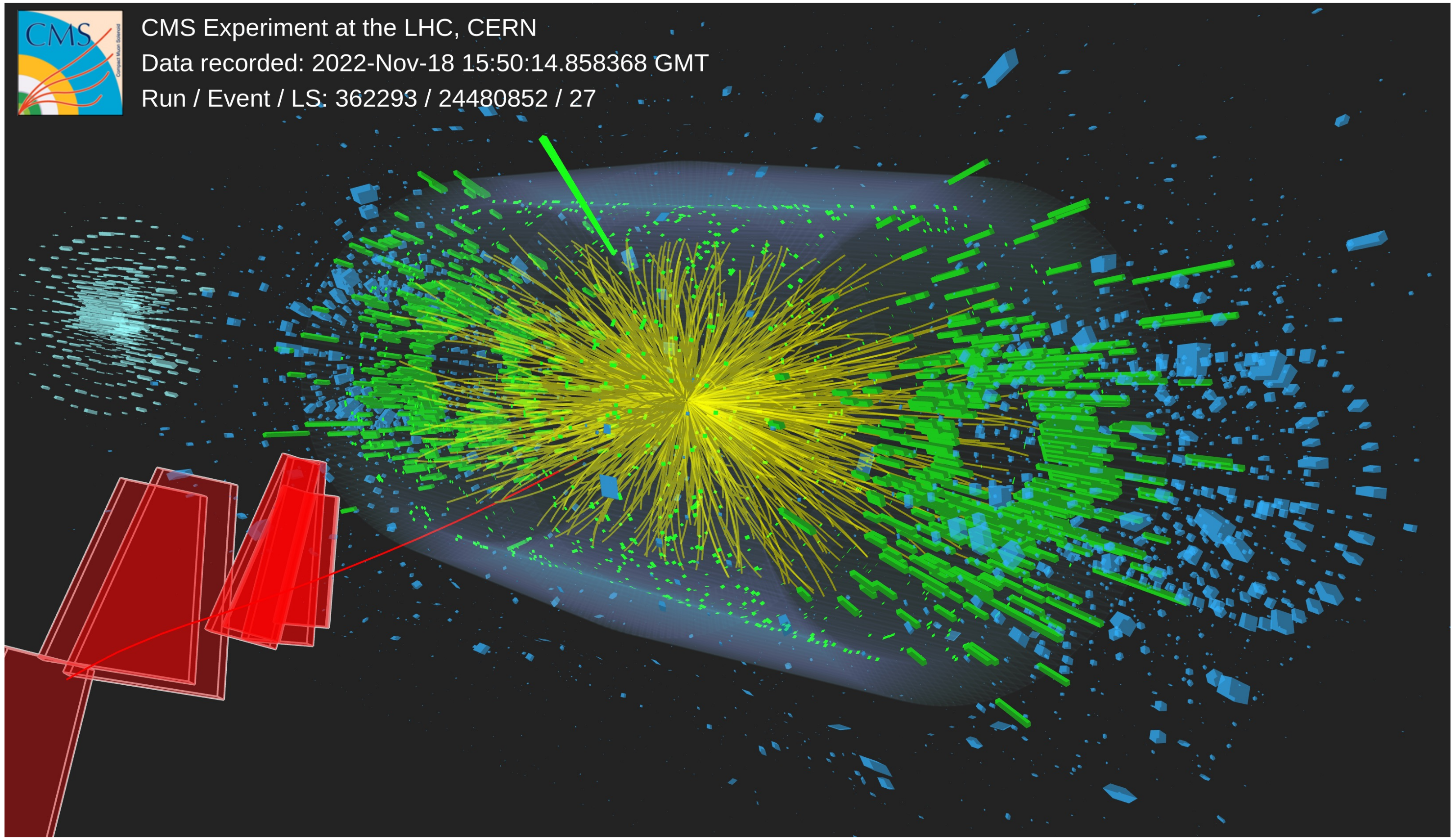
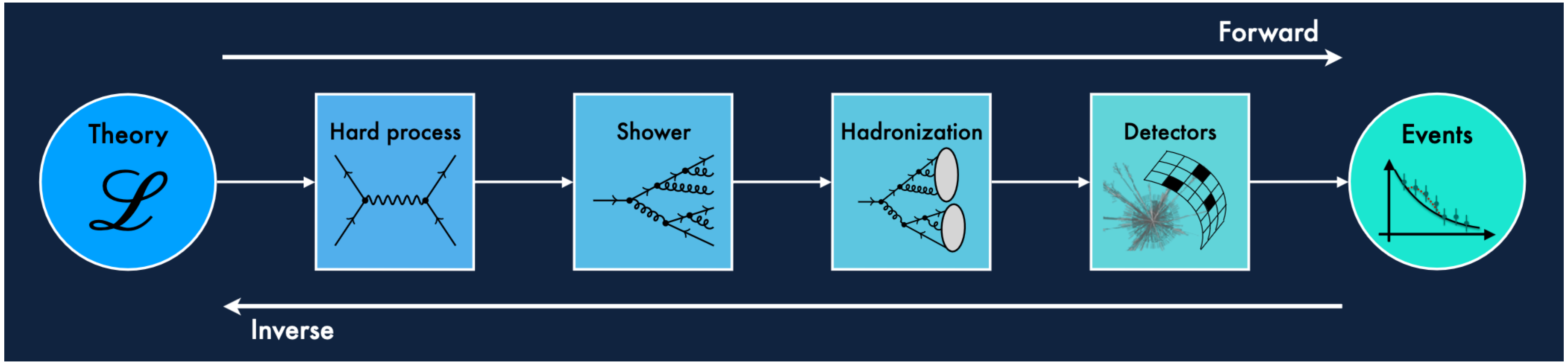


# Why QML for HEP?




**Fundamental motivation**

Utilise information and correlations inherent in HEP data.

Exploit “quantum remnants” in data.

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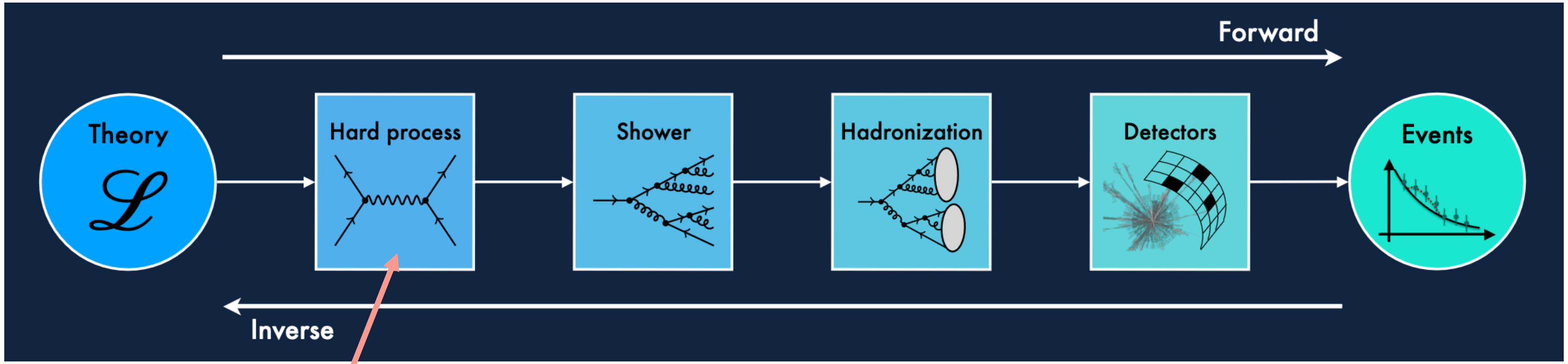


entanglement [1703.02989]

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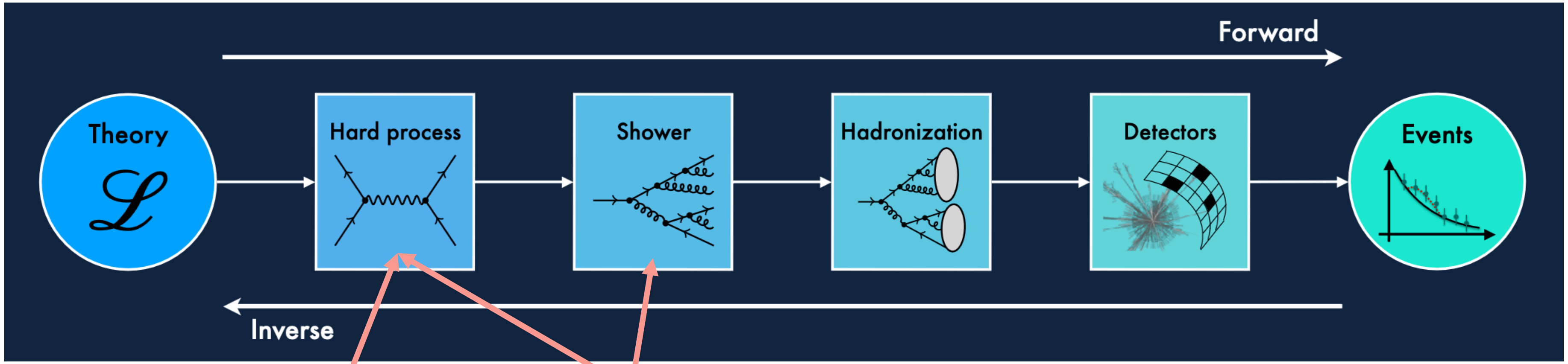


interference [2110.10112]

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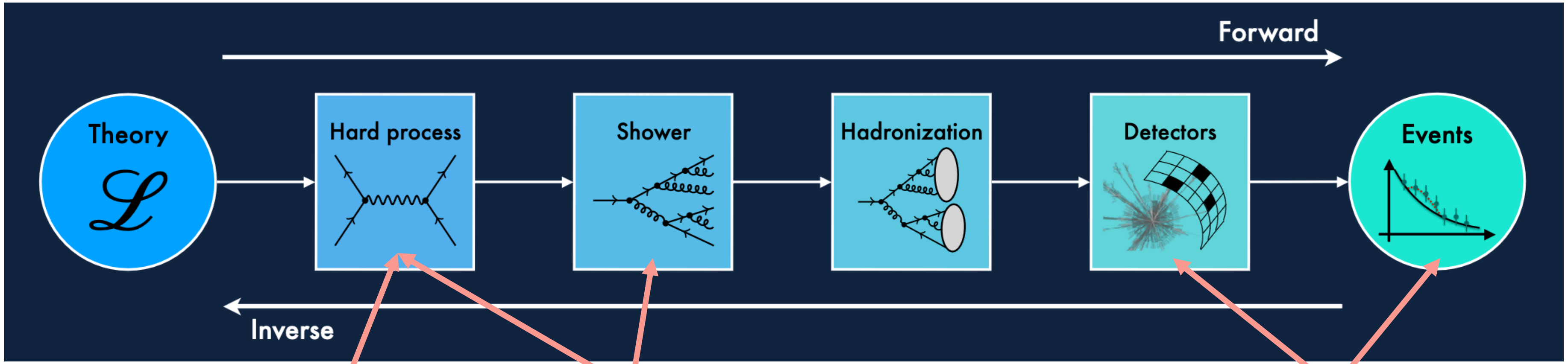


interference [2110.10112]  Bell inequalities [2102.11883, 2203.05582]

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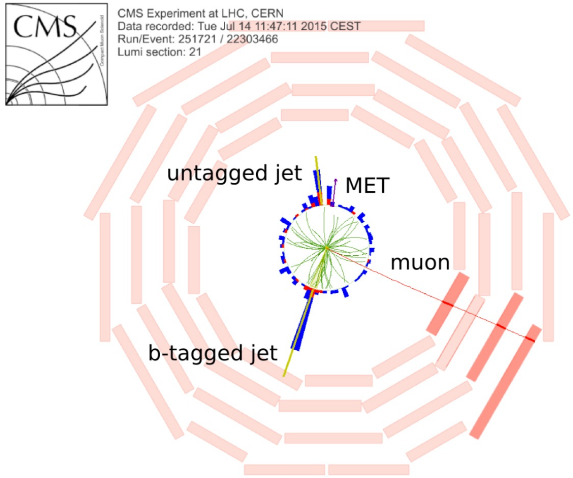
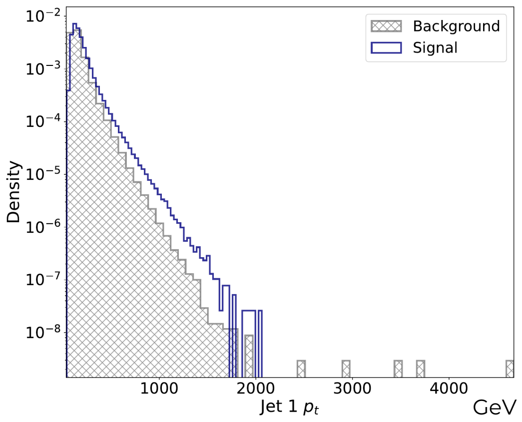
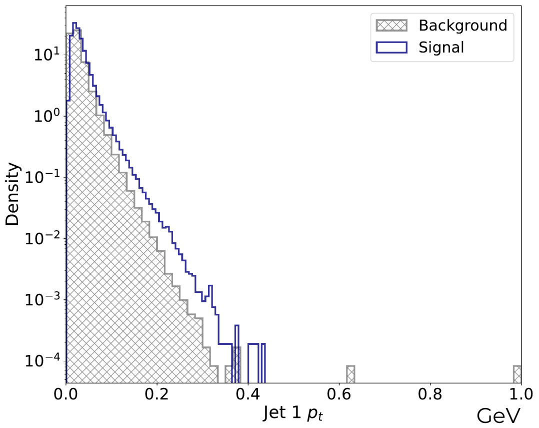



**Theory + Simulation**

compute prob. distributions




apply cuts and normalise

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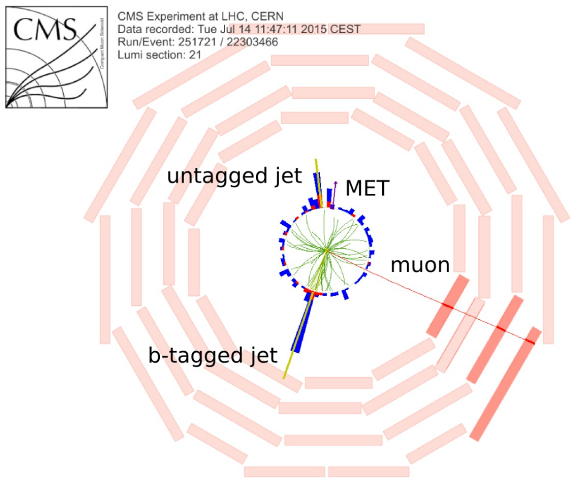


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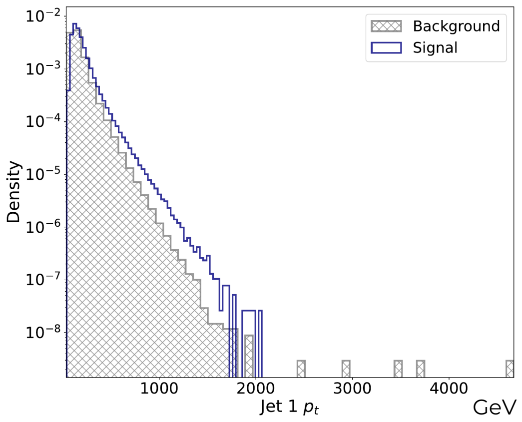


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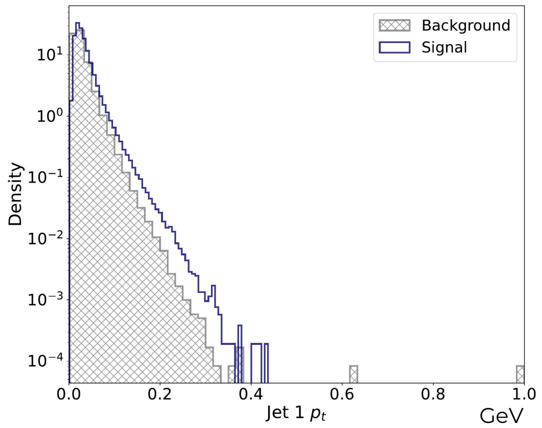


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Classifier models

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Likelihood ratio between different hypotheses

$$q = -2 \log \frac{\mathcal{L}(x|S)}{\mathcal{L}(x|B)}$$

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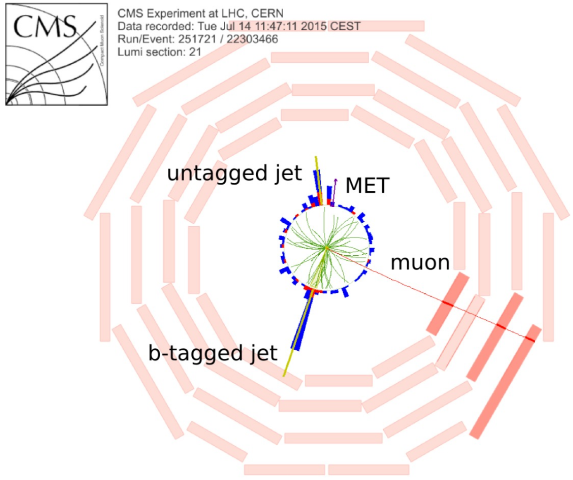


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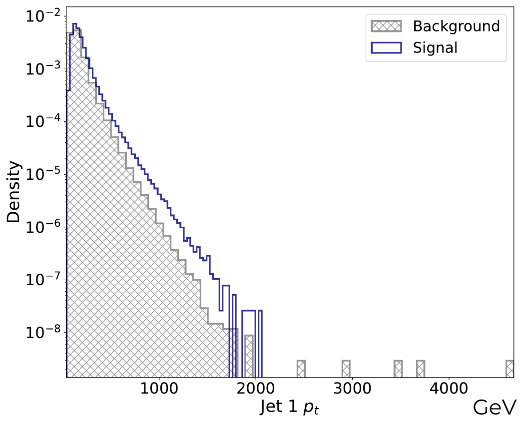


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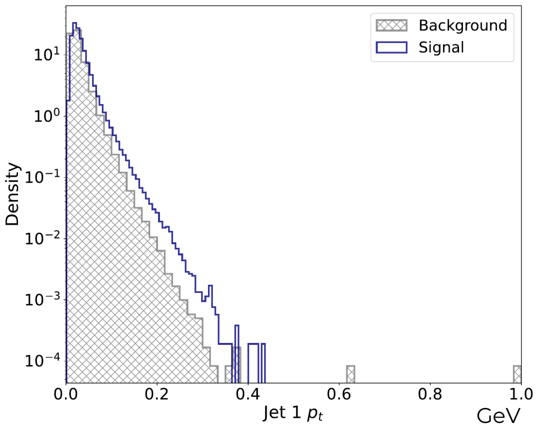


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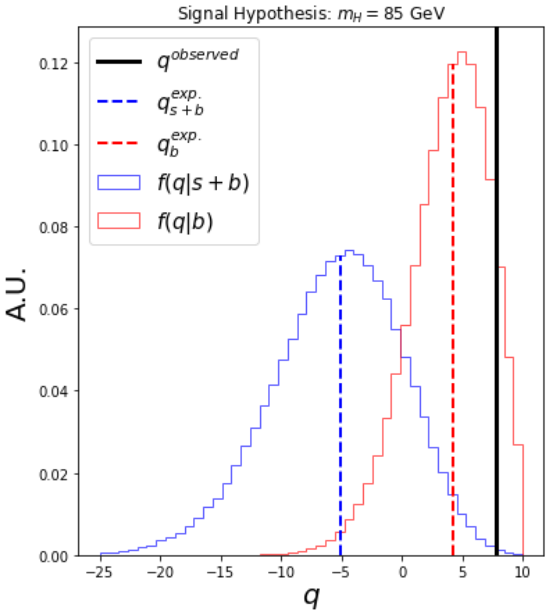

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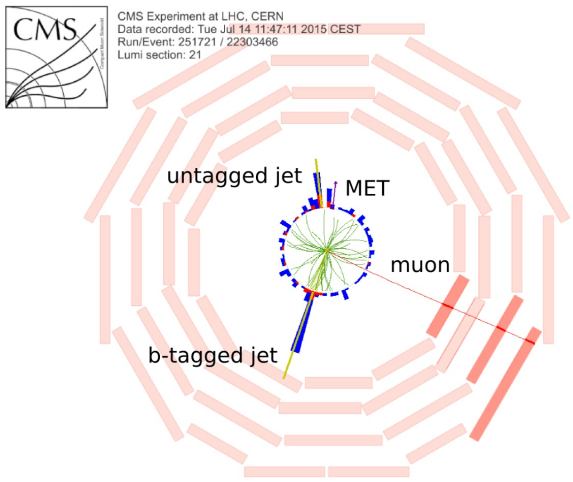


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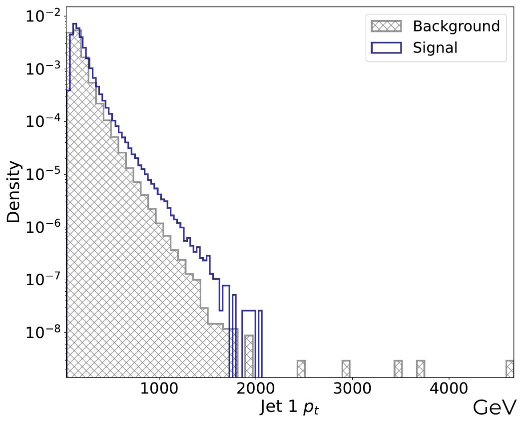


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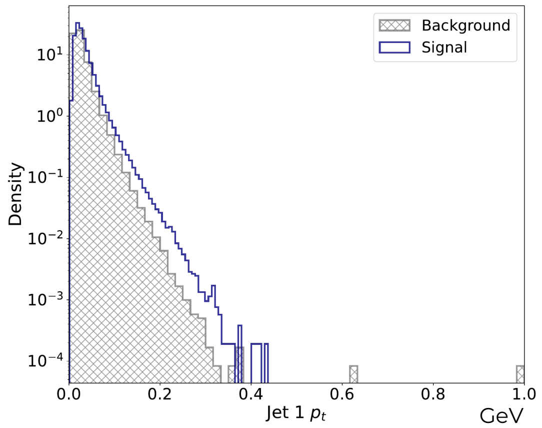


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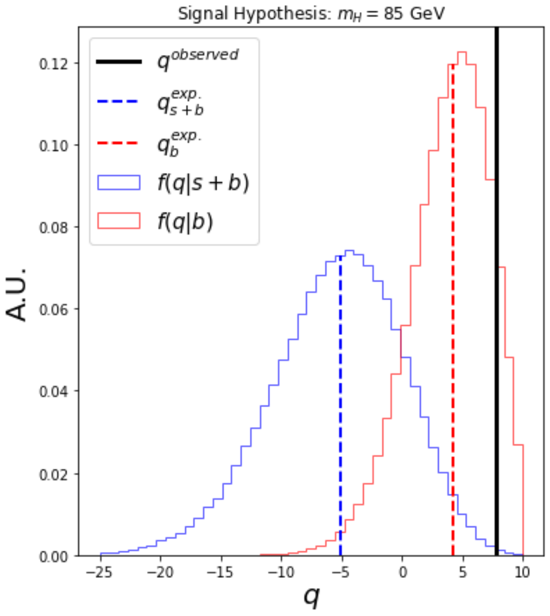



**What if you do not know the signal?**

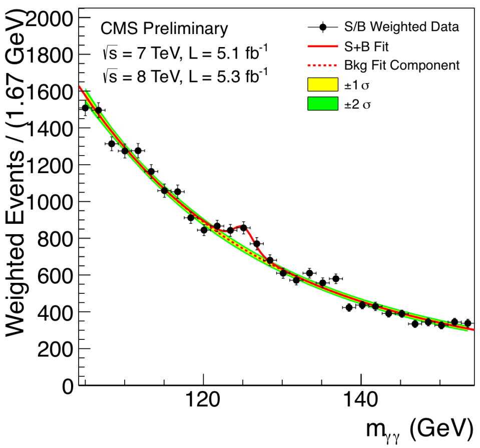
# Motivating model-independent searches

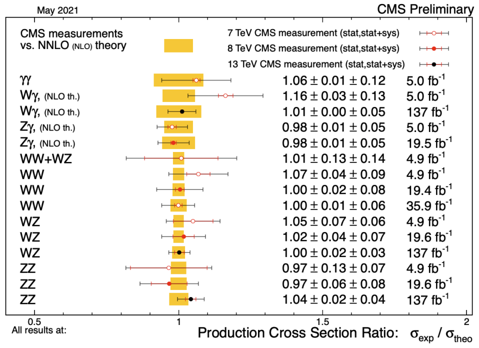
Bias is **not necessarily bad**. It can be **great!**

Higher bias ⟶ lower variance of the statistical model

[Cramér–Rao bound]

[10.1016/j.physletb.2012.08.02]




Summary SM measurements @ CMS [link]

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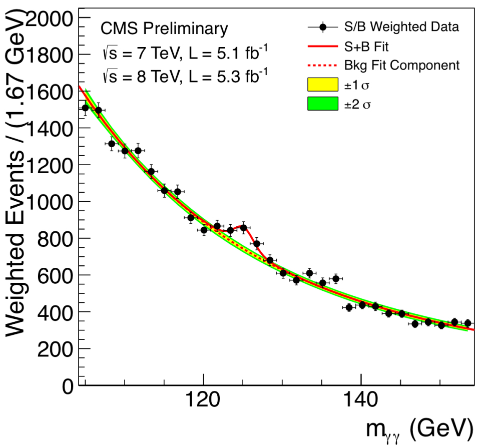


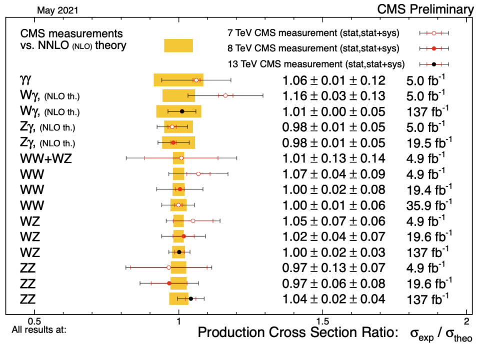


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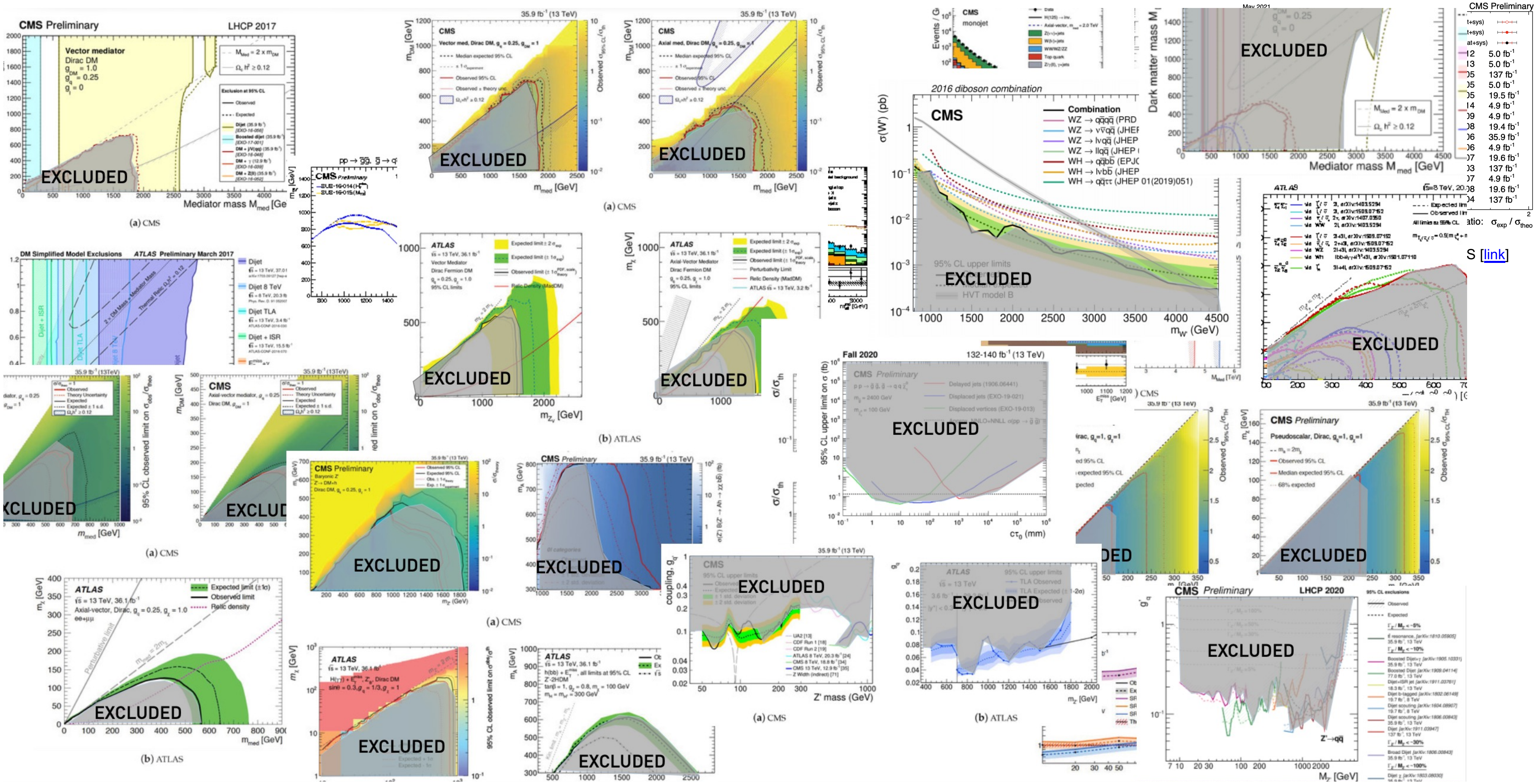

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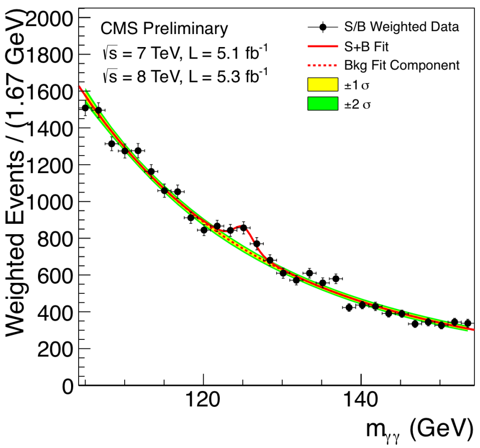


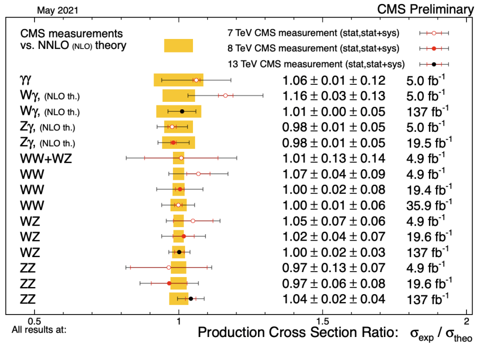


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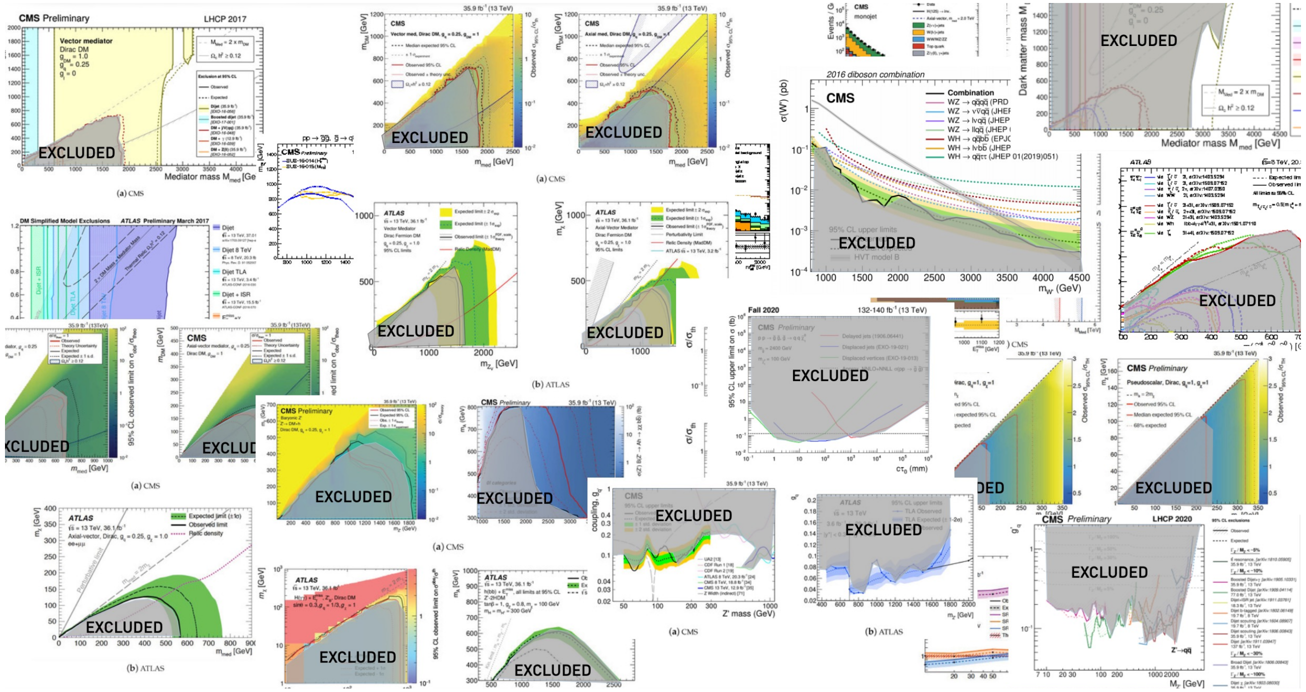

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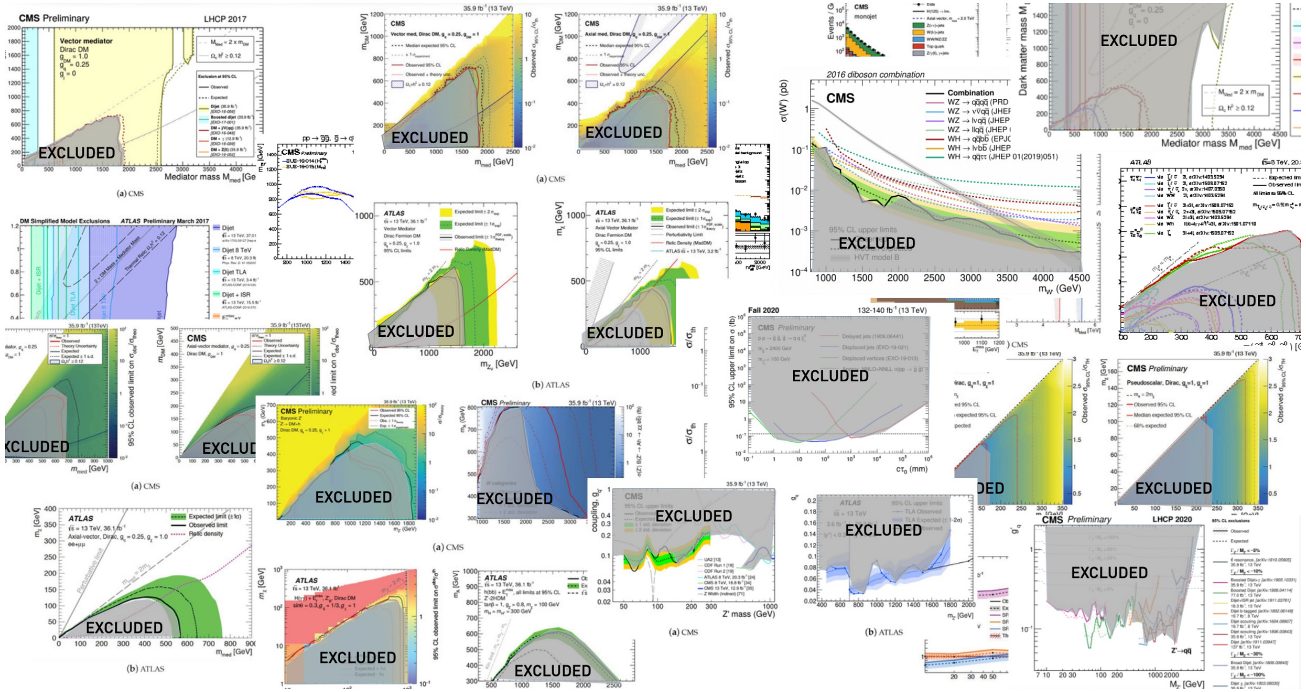


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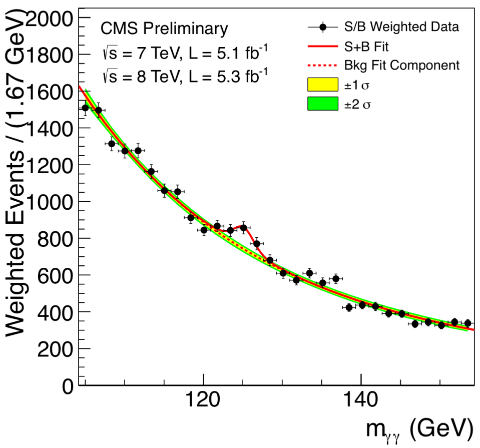


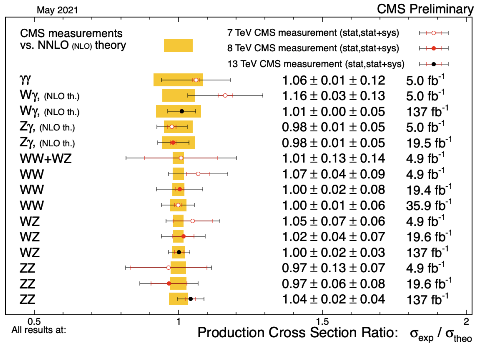


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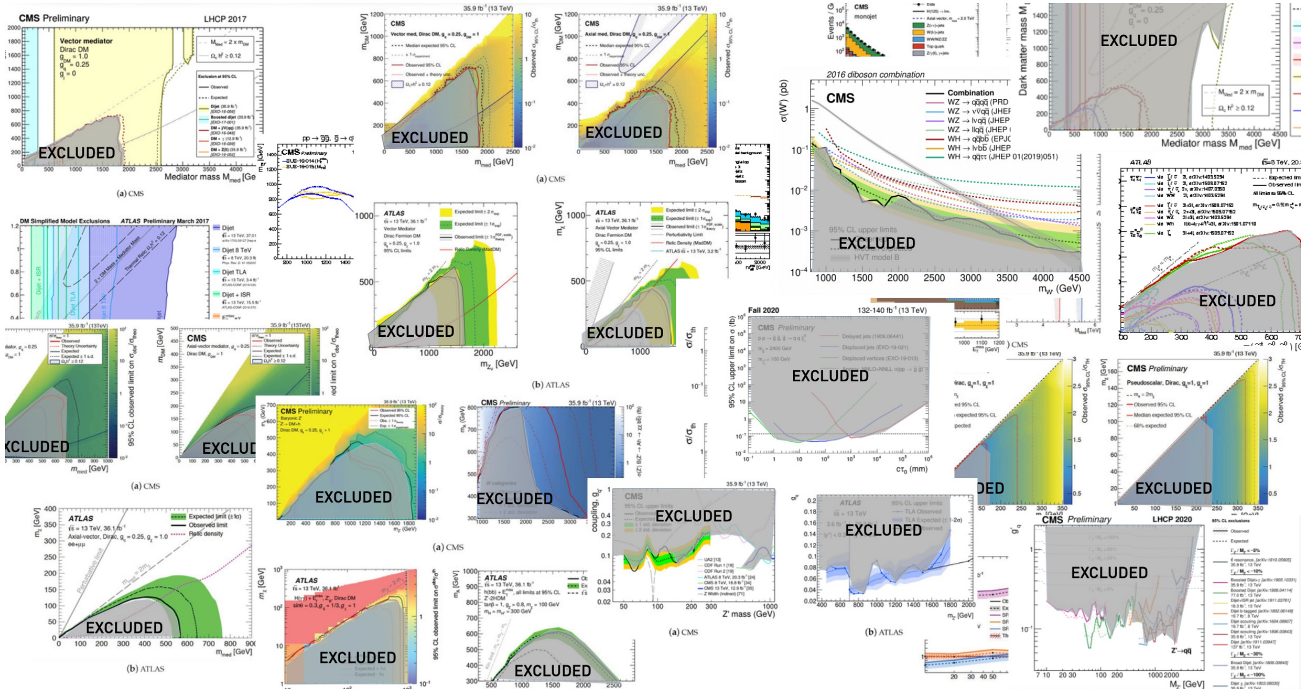

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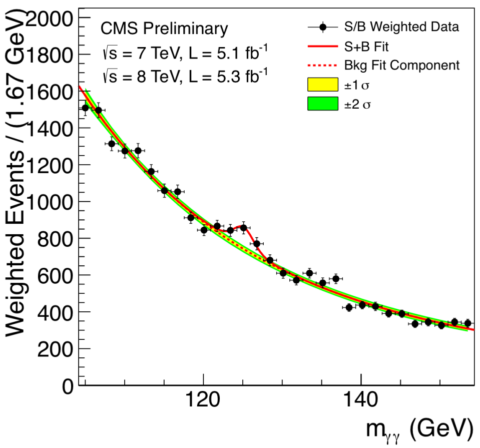


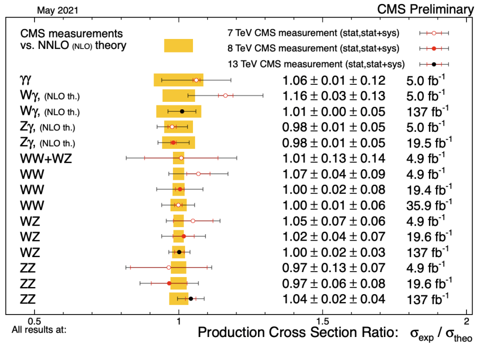


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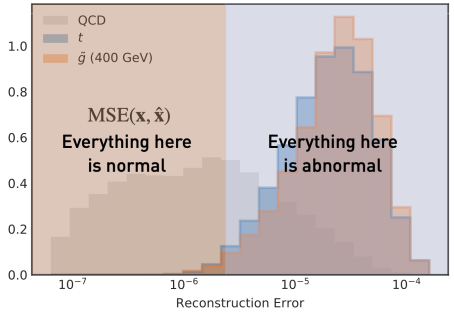
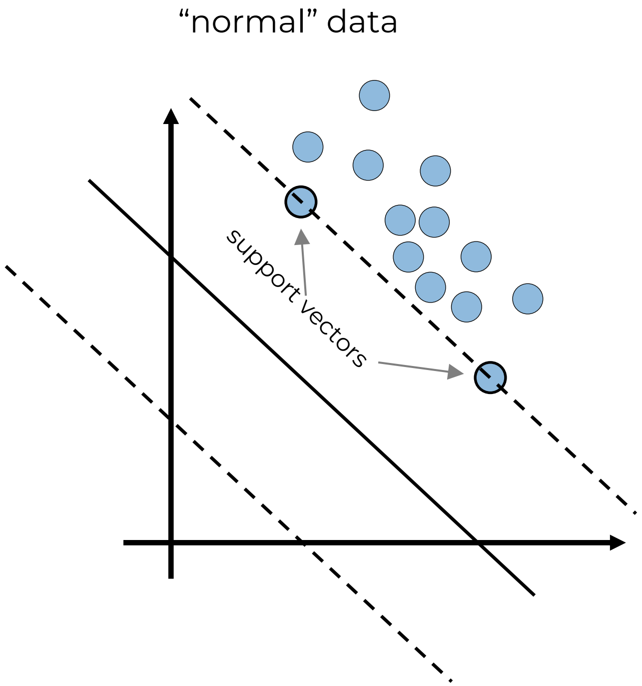
One possible solution:
**Anomaly detection**




**Unsupervised ML models**

ETH zürich

# Unsupervised quantum kernel machines




$$\min_{w\in\mathcal{H},\, \xi\in\mathbb{R}^{\mathrm{N}},\, \rho\in\mathbb{R}} \quad \frac{1}{2}||w||^2 + \frac{1}{\nu \mathrm{N}}\sum_i \xi_i - \rho$$

$$\text{subject to} \quad w\cdot\phi(x_i) \geq \rho - \xi_i,\ \xi_i \geq 0,\ \forall i$$

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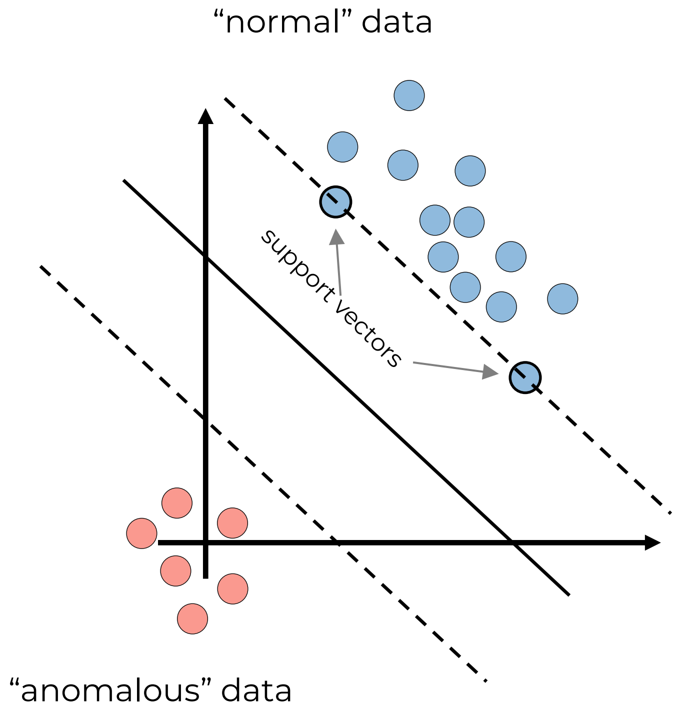


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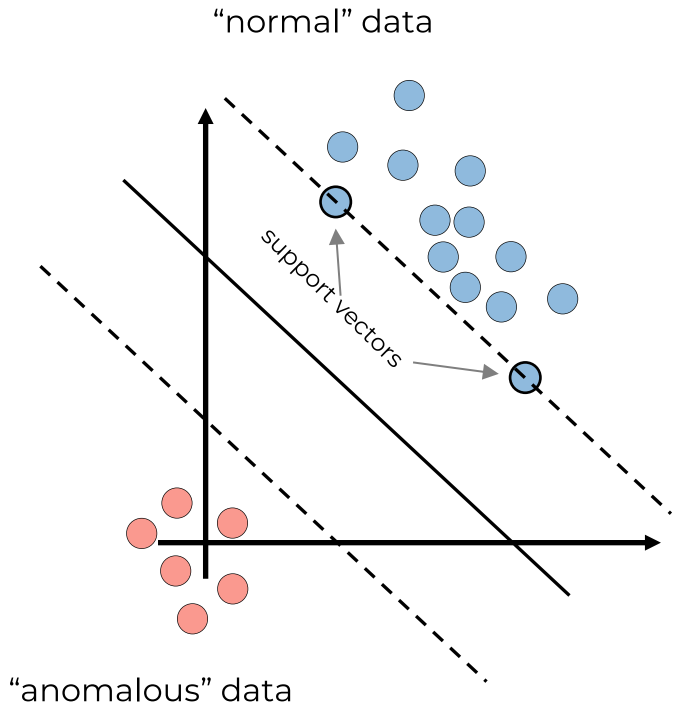


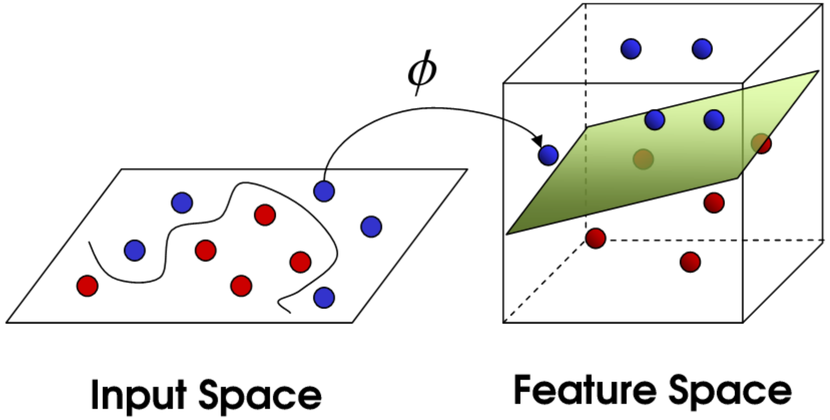


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Kernel trick:

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

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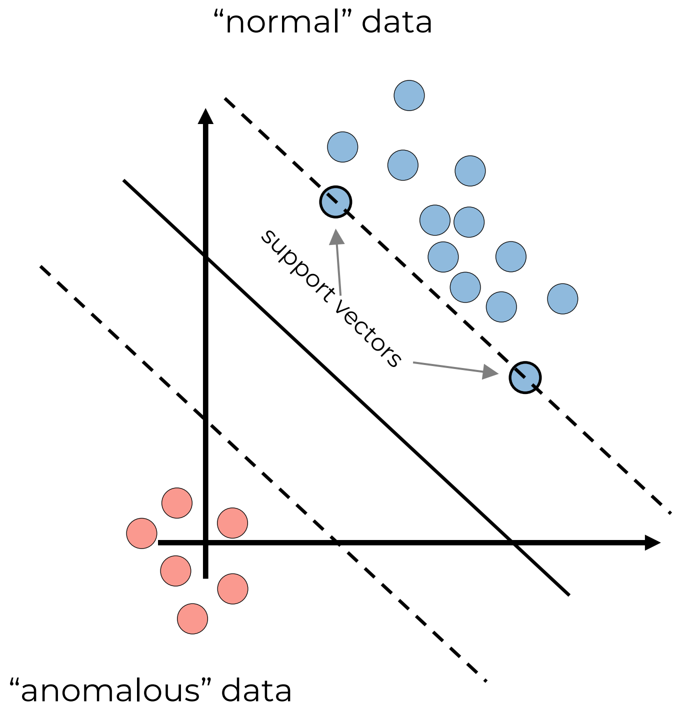


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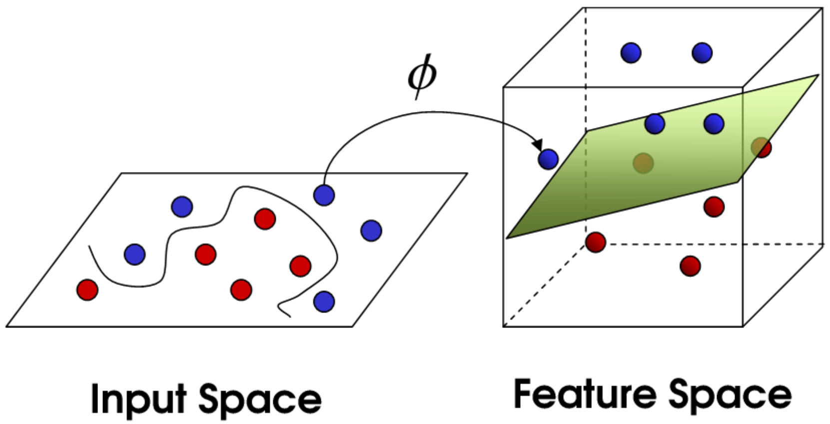


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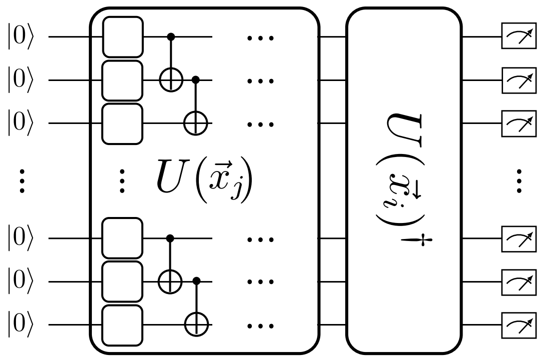


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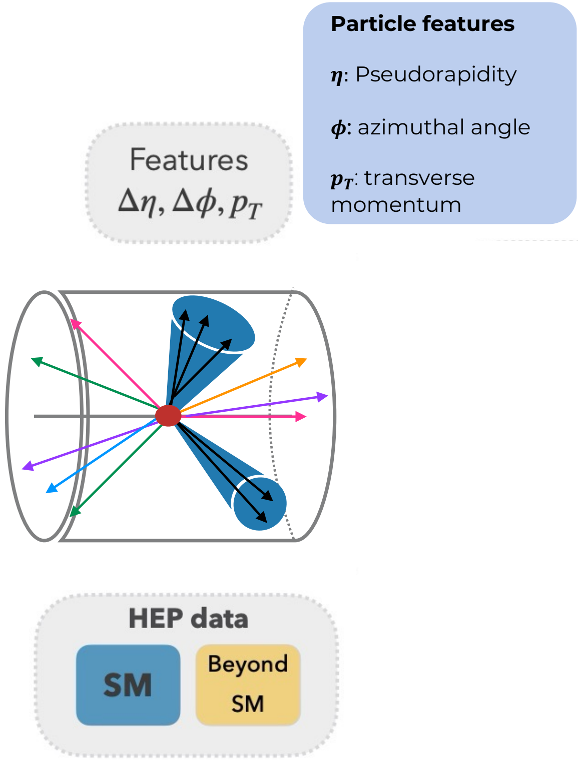
# Results

Finding new-physics in dijet events with QML

# Anomaly detection with quantum machine learning




**Background:** QCD dijet events. 600 features per event

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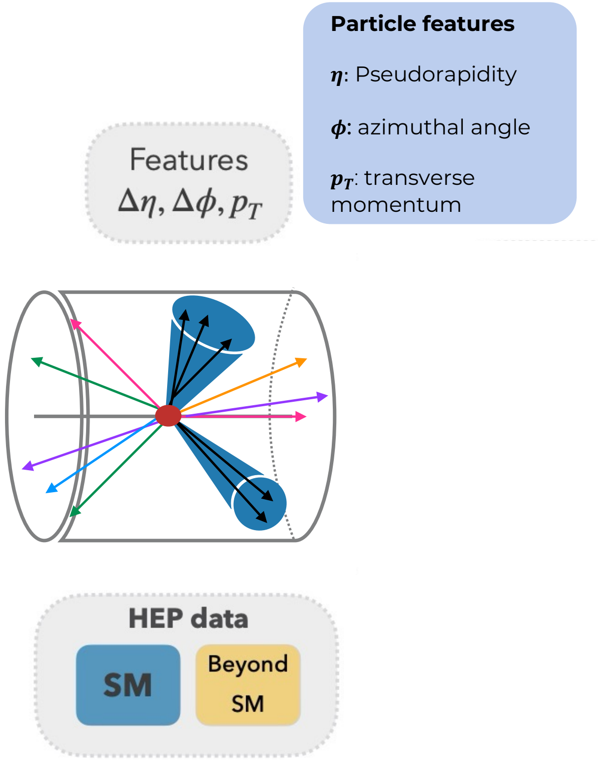


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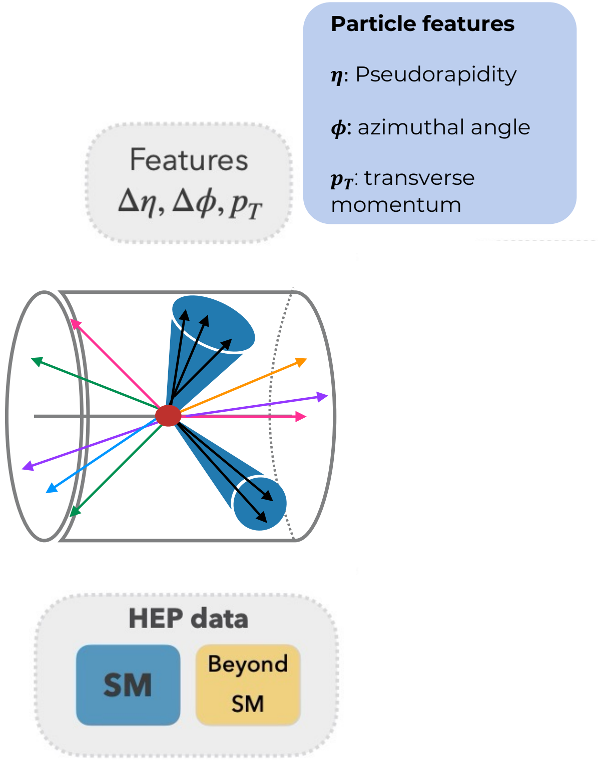


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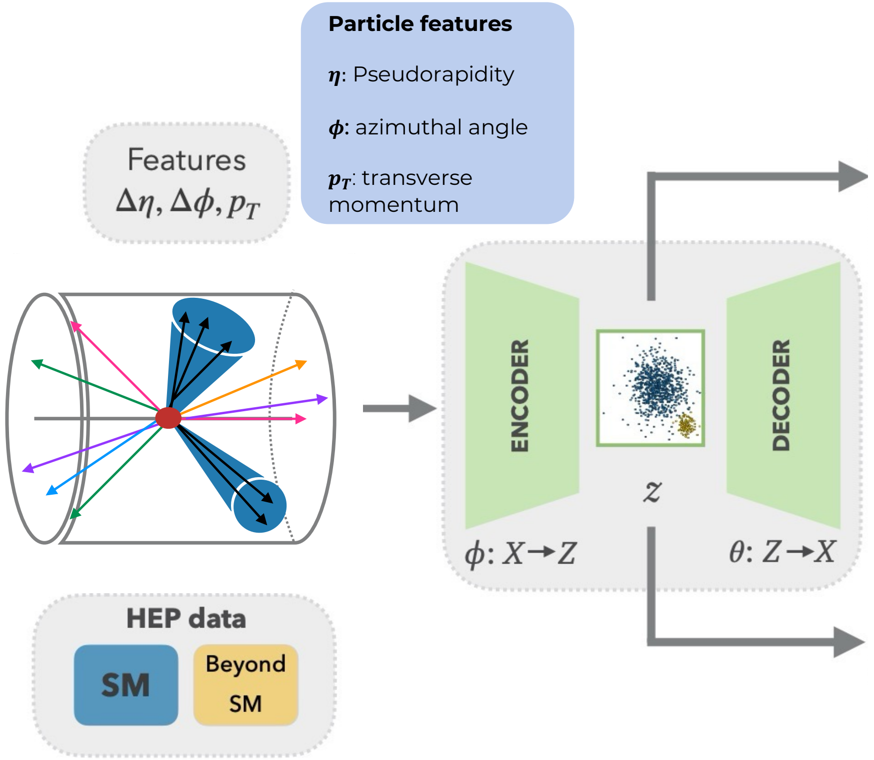


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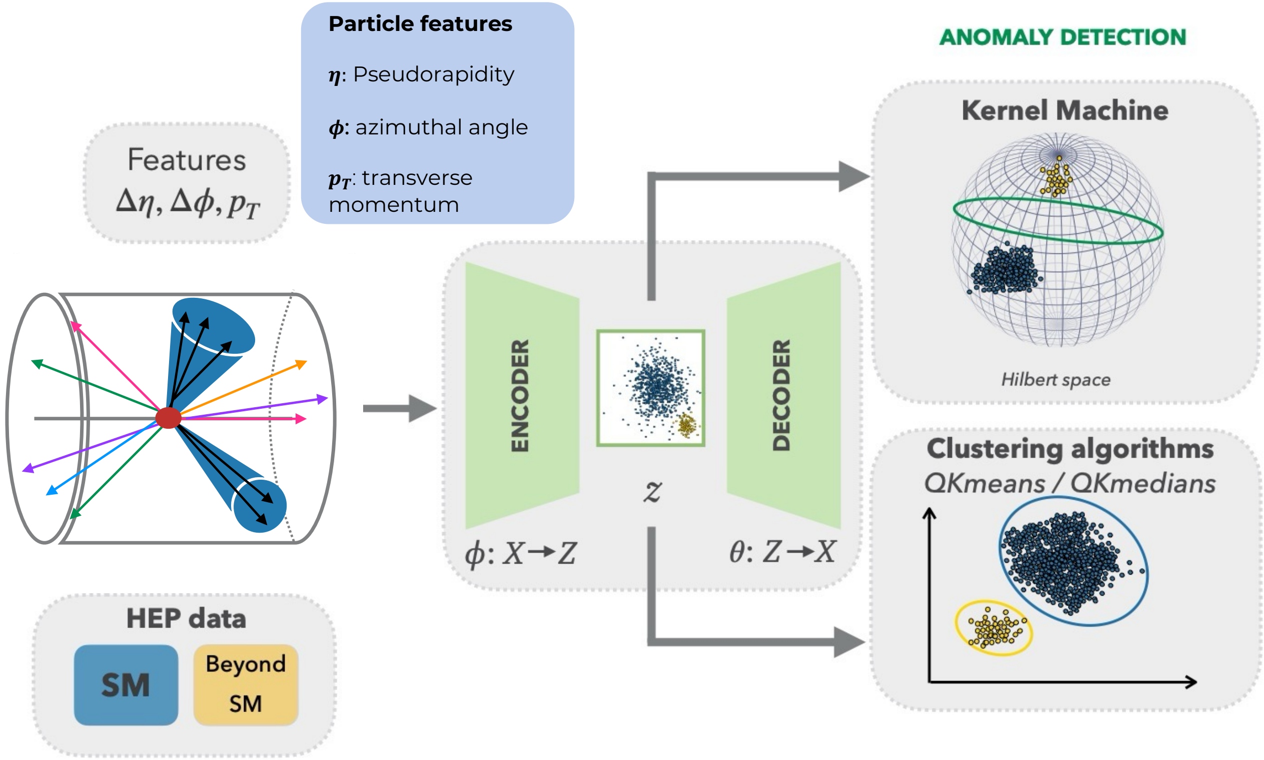


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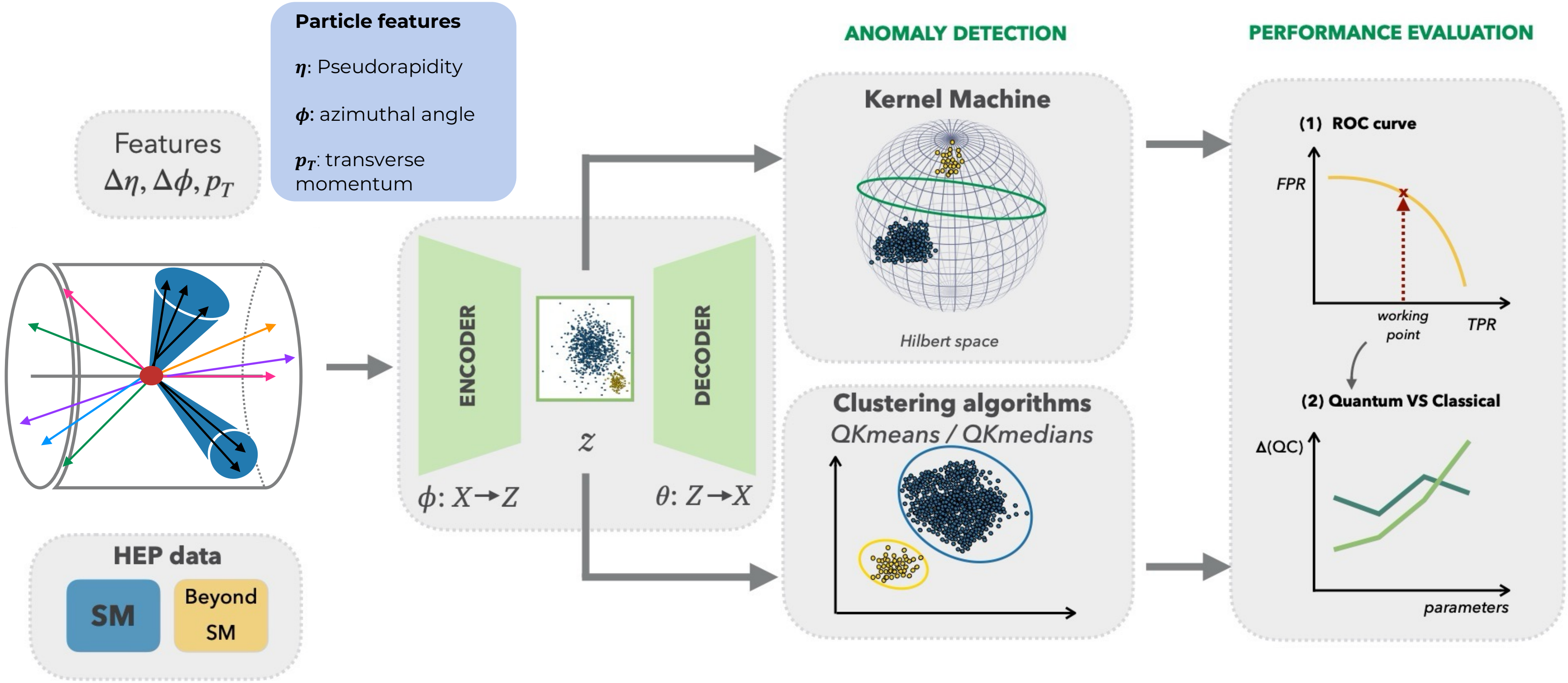


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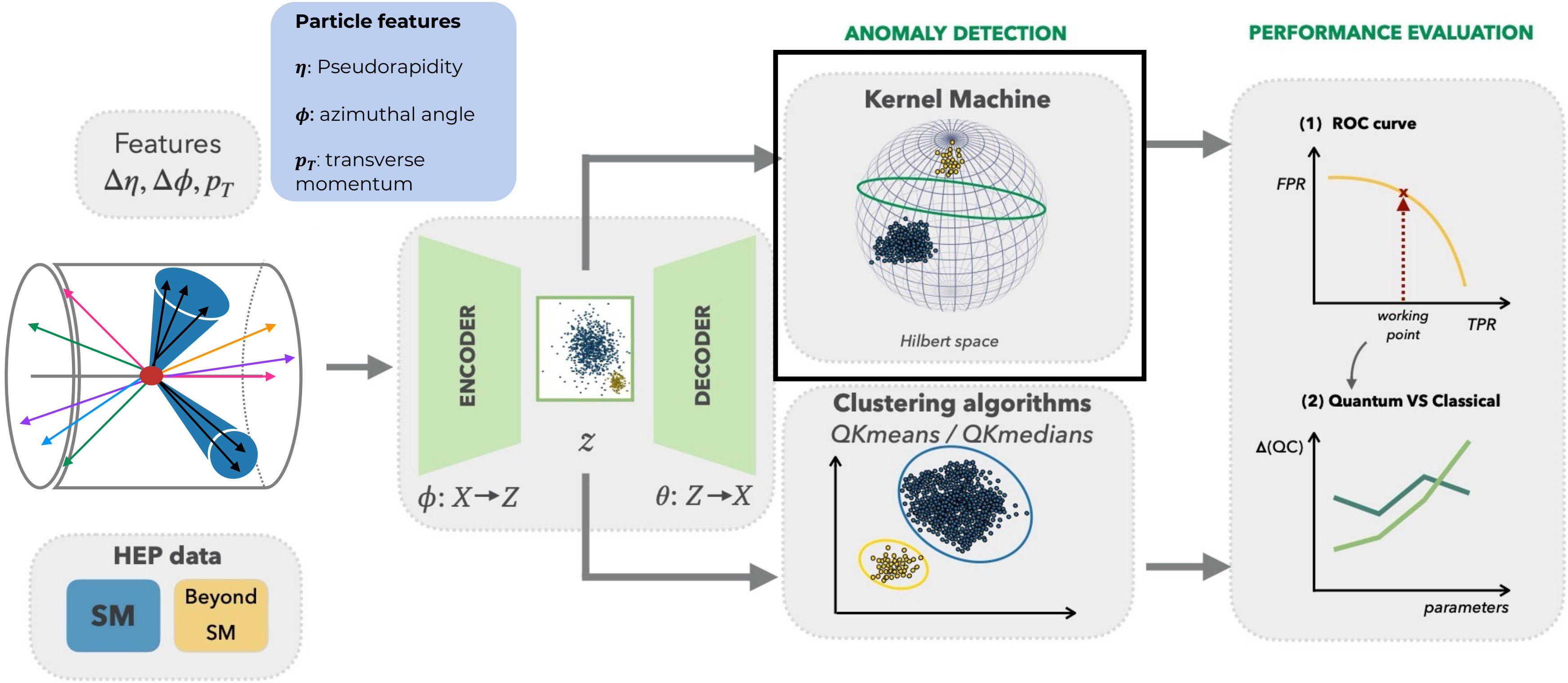


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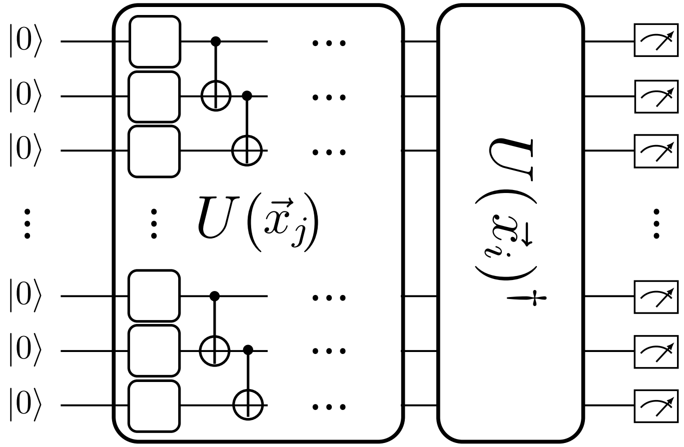


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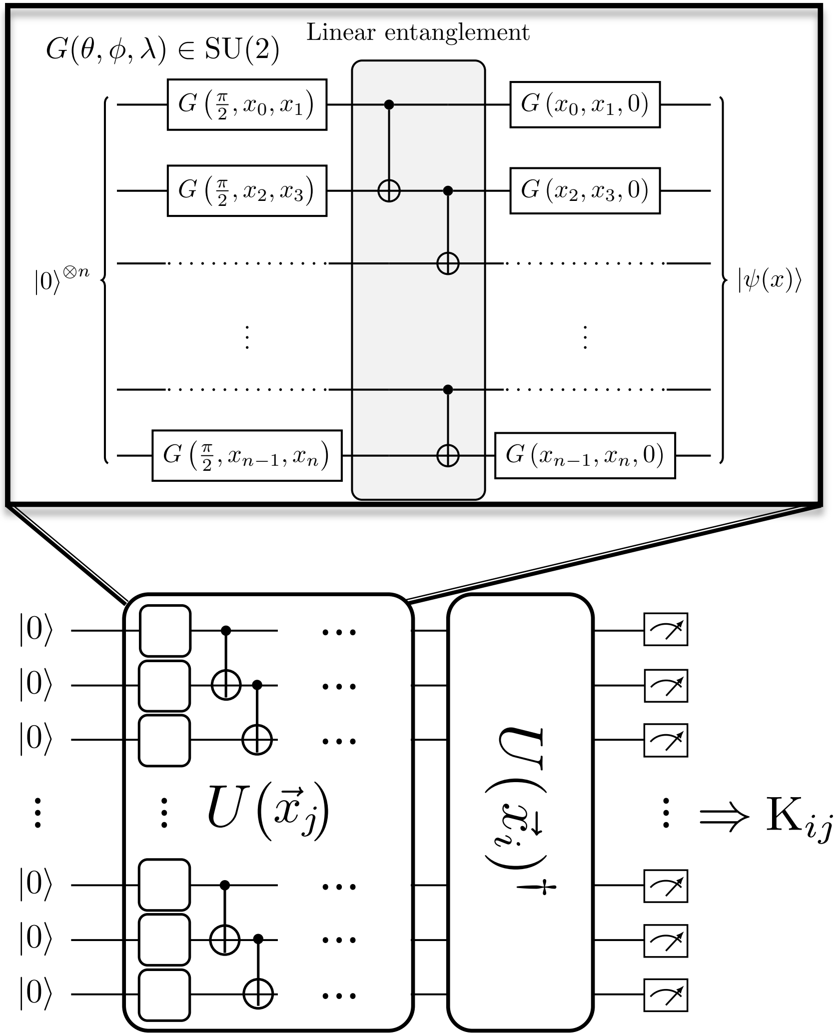


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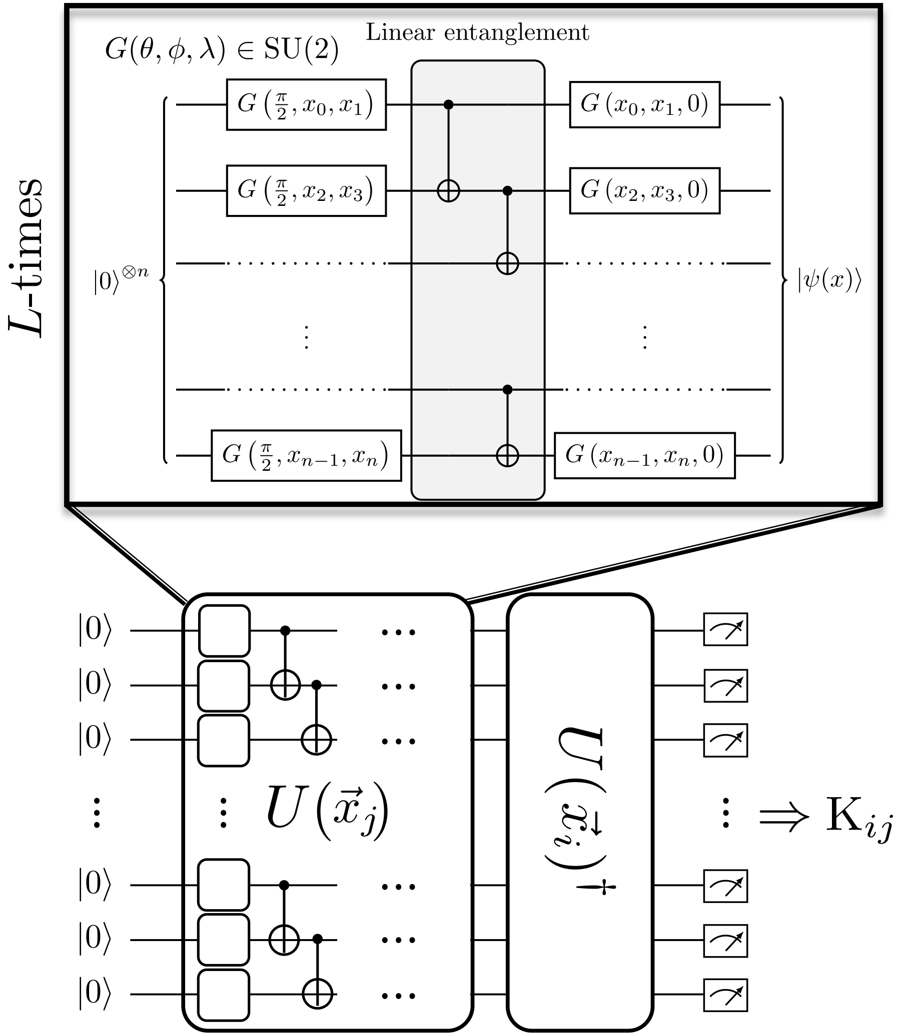


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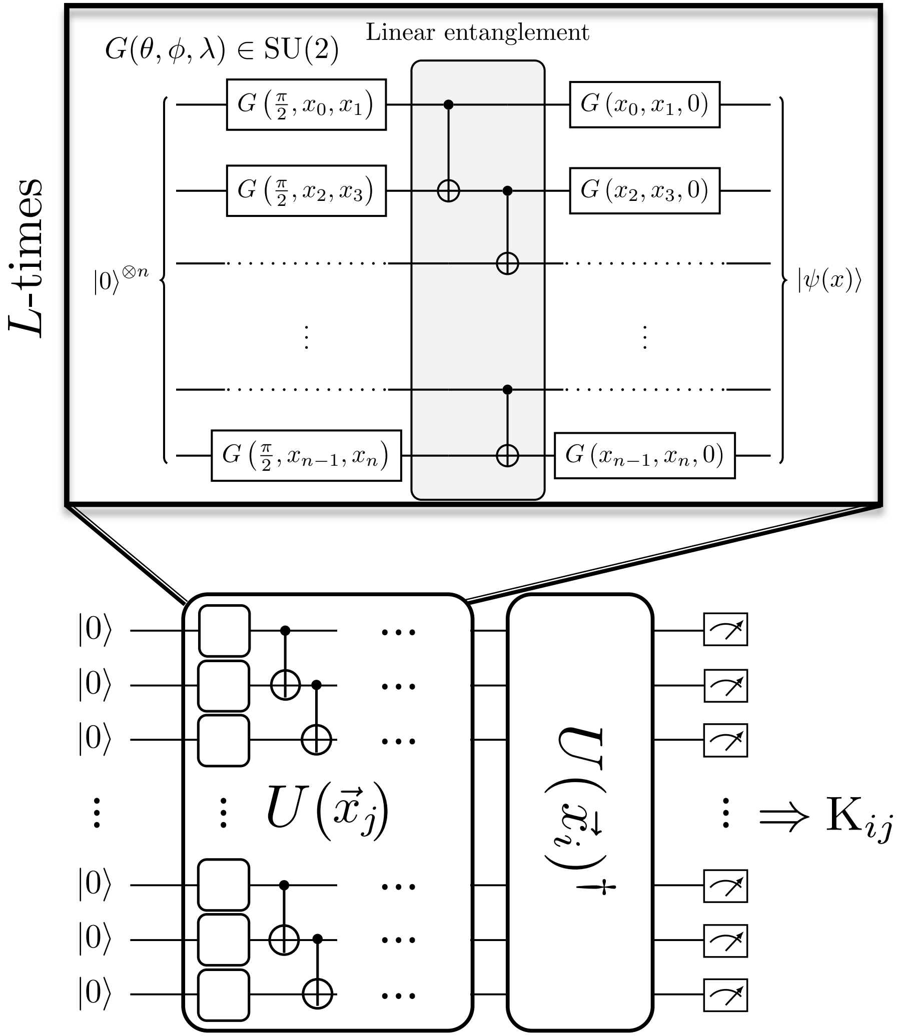


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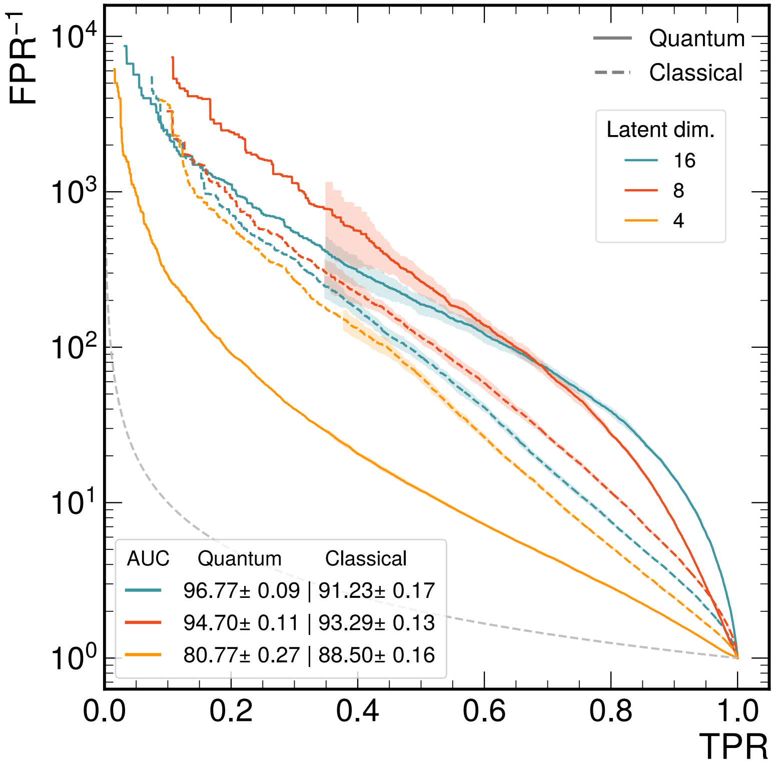
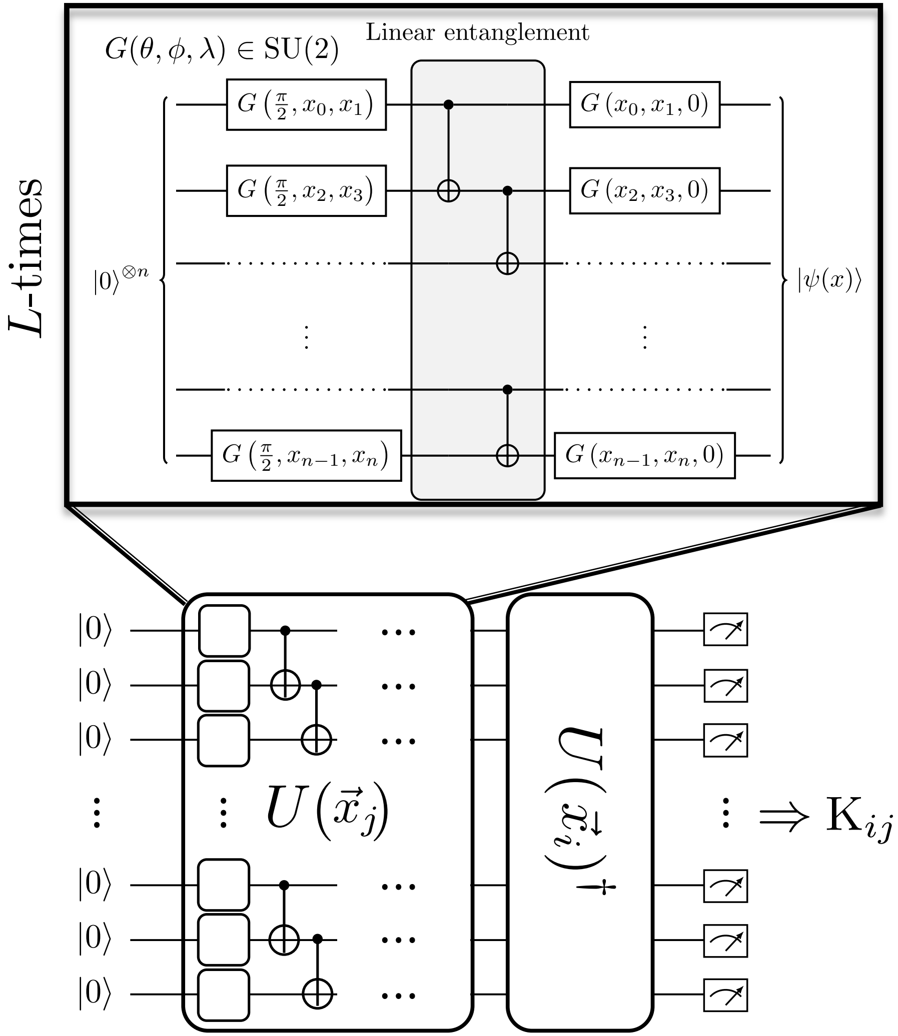
## Different qubit number



# Unsupervised quantum kernel machine

## Designed data encoding circuit

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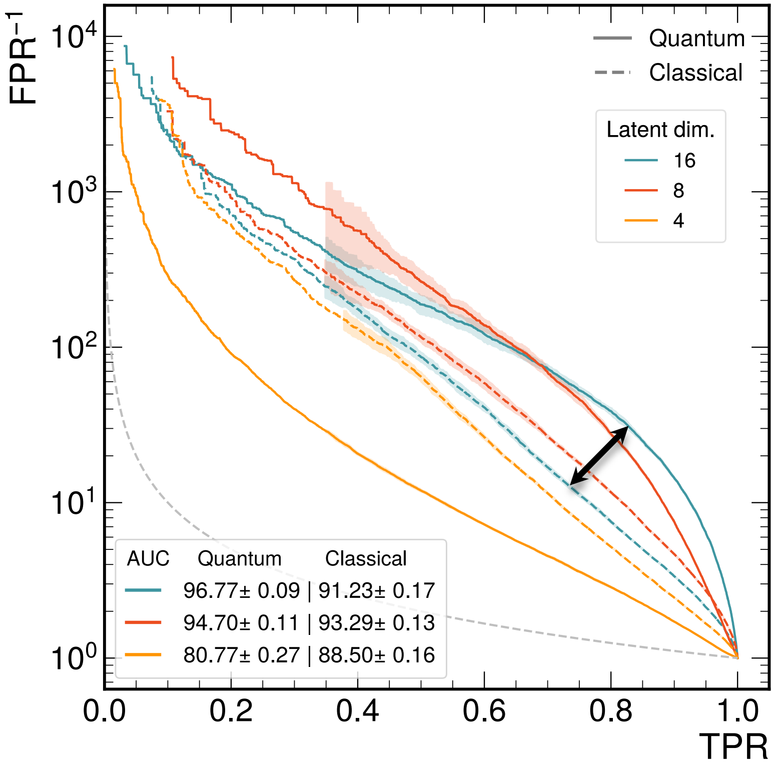

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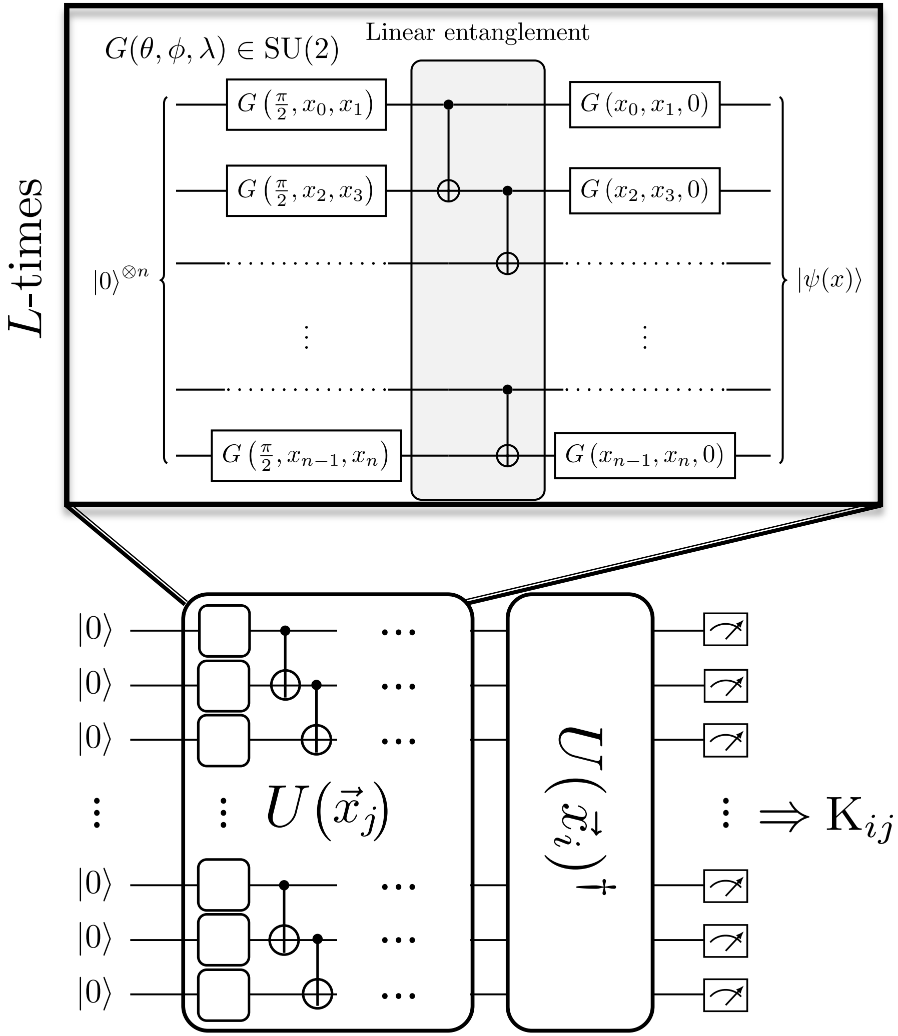


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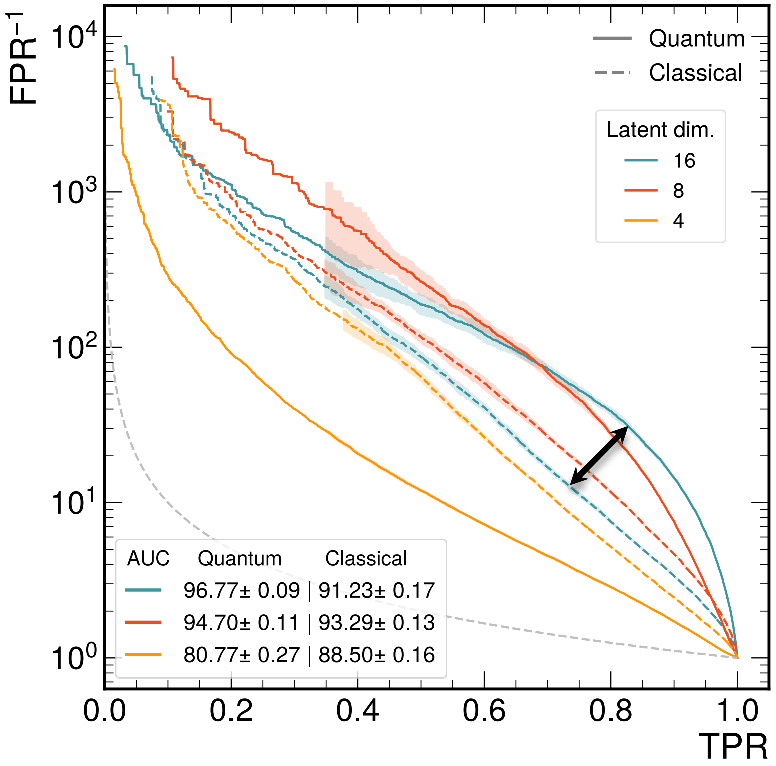


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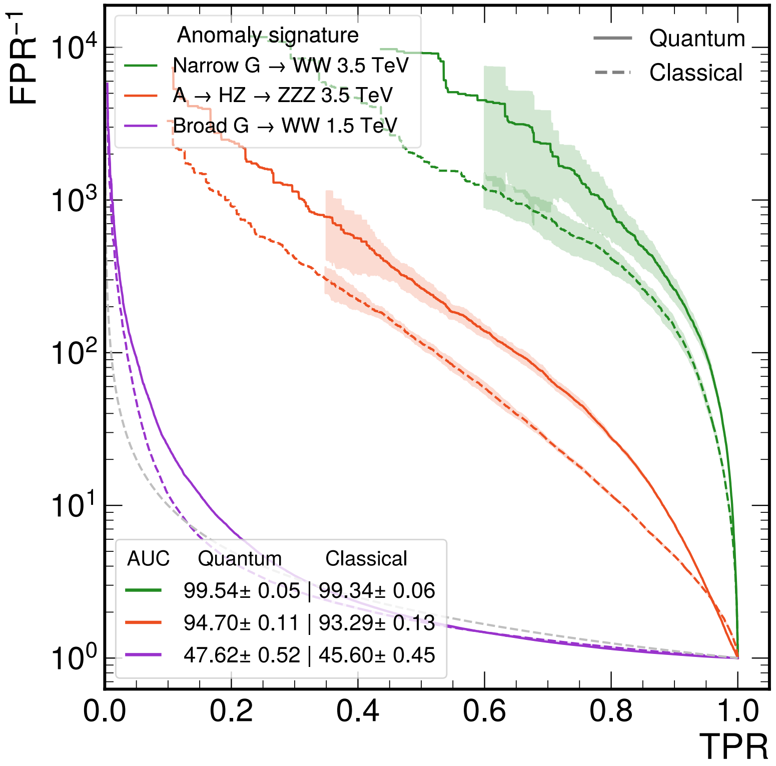

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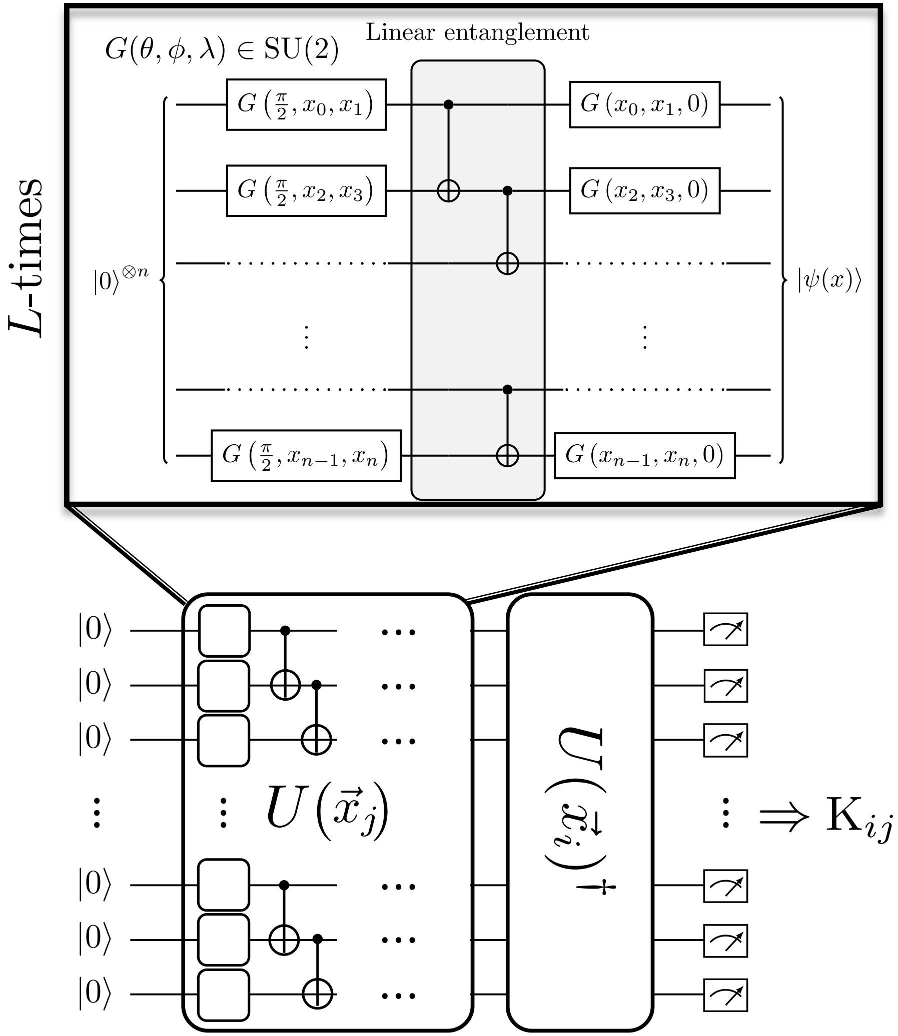


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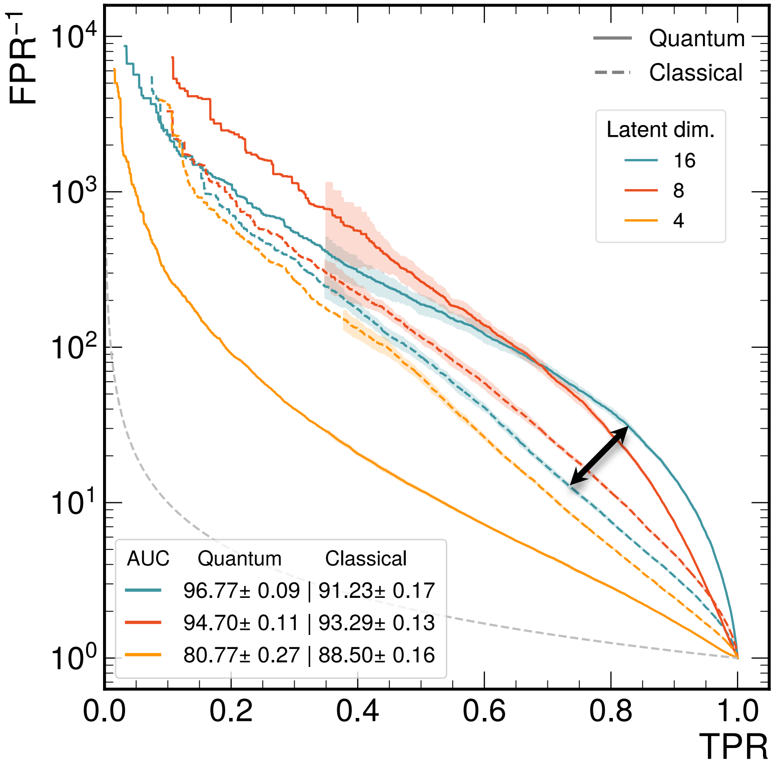


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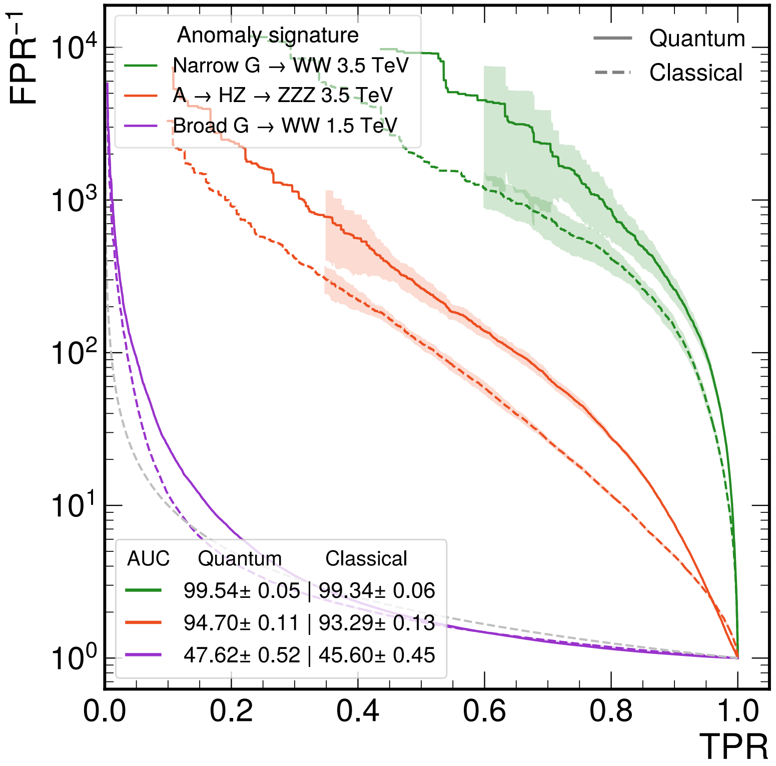


**Are quantum effects utilized by the model?**

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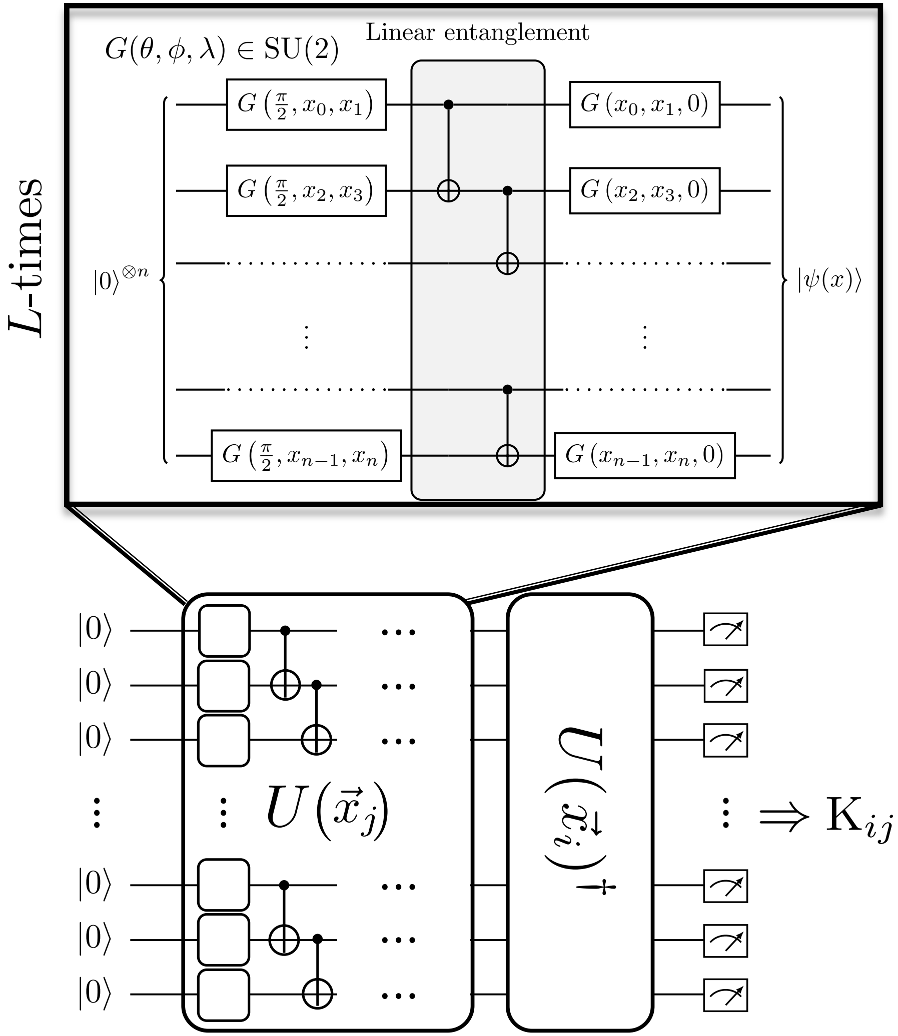


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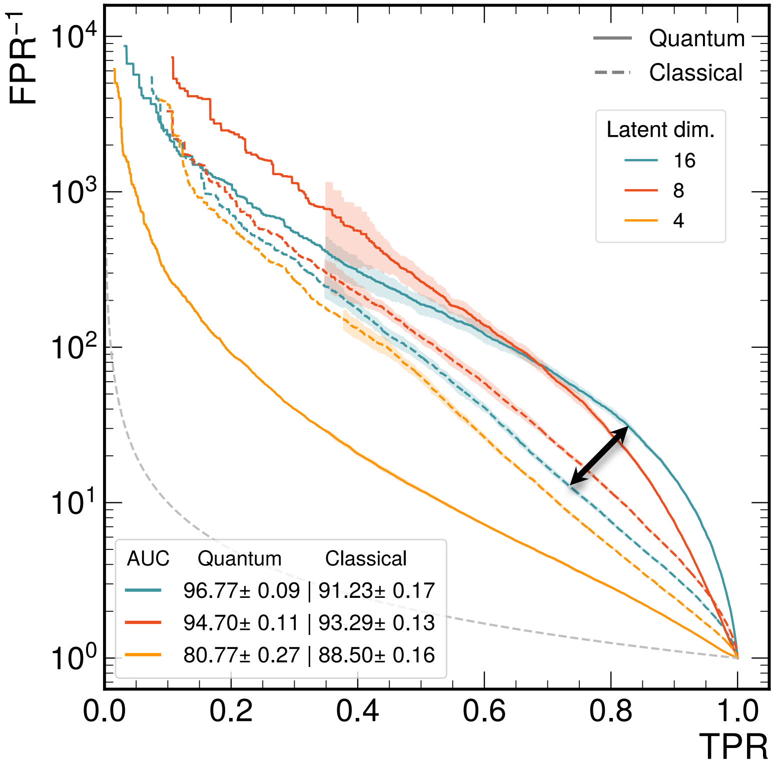


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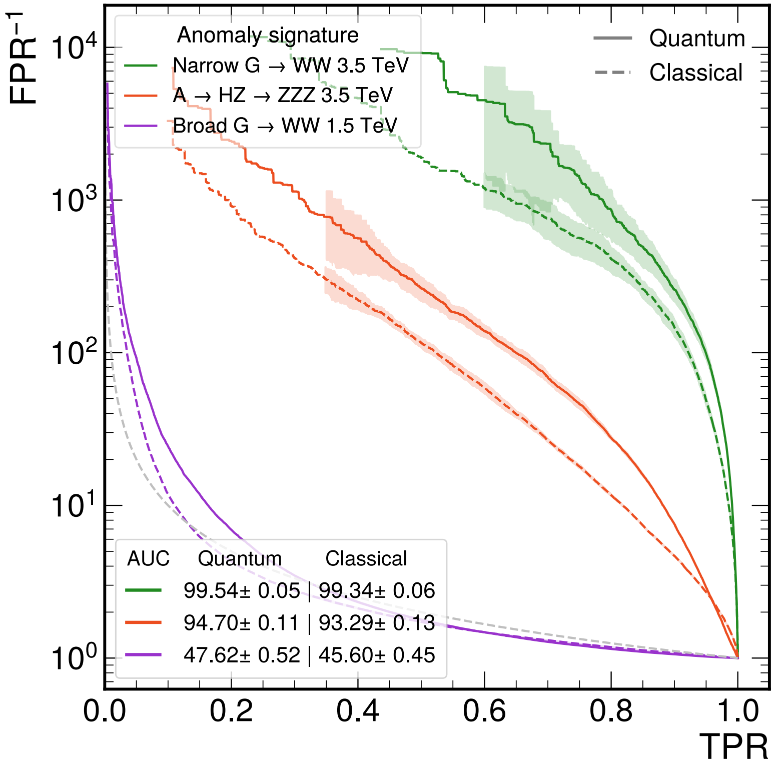


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# Quantum circuit properties vs. performance

Importance of intrinsically quantum properties of the feature map.

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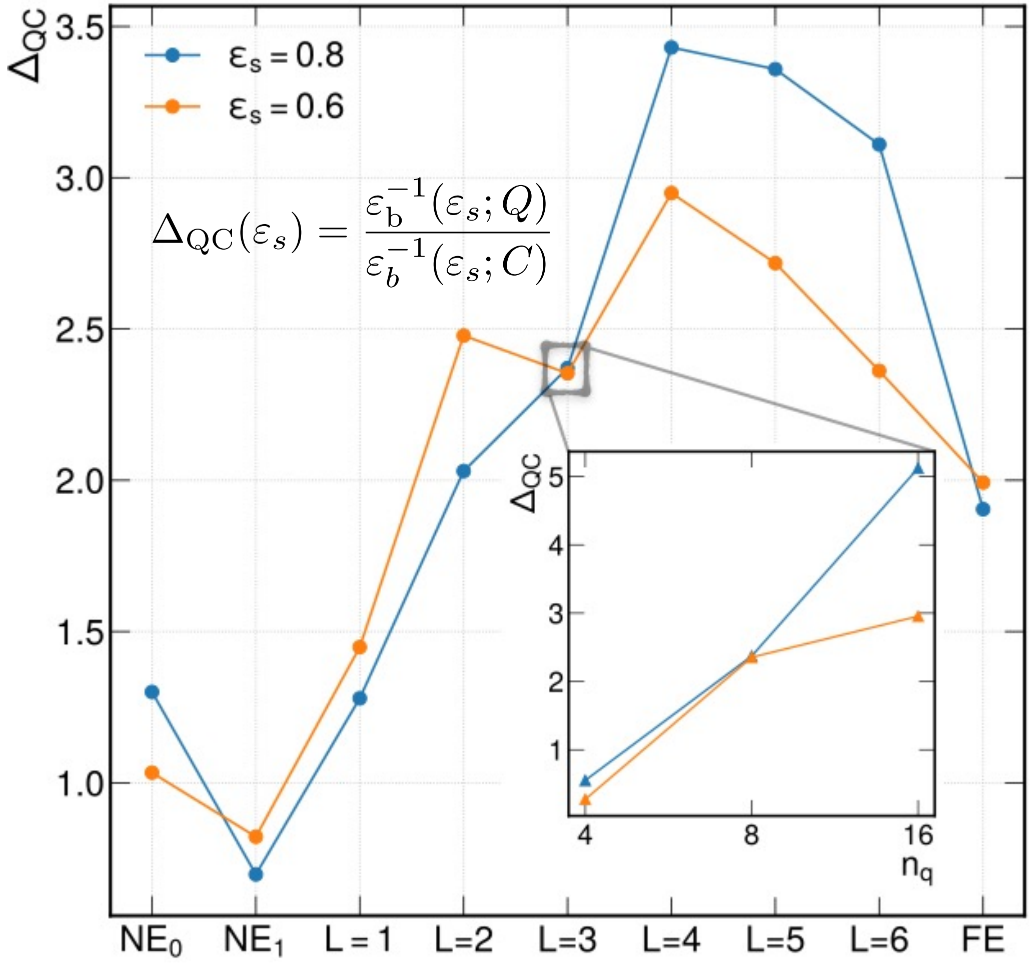


More expressive

$\varepsilon_s$ Signal efficiency = True Positive Rate (TPR)

$\varepsilon_b^{-1}$ Background Rejection = Inverse of False Positive Rate

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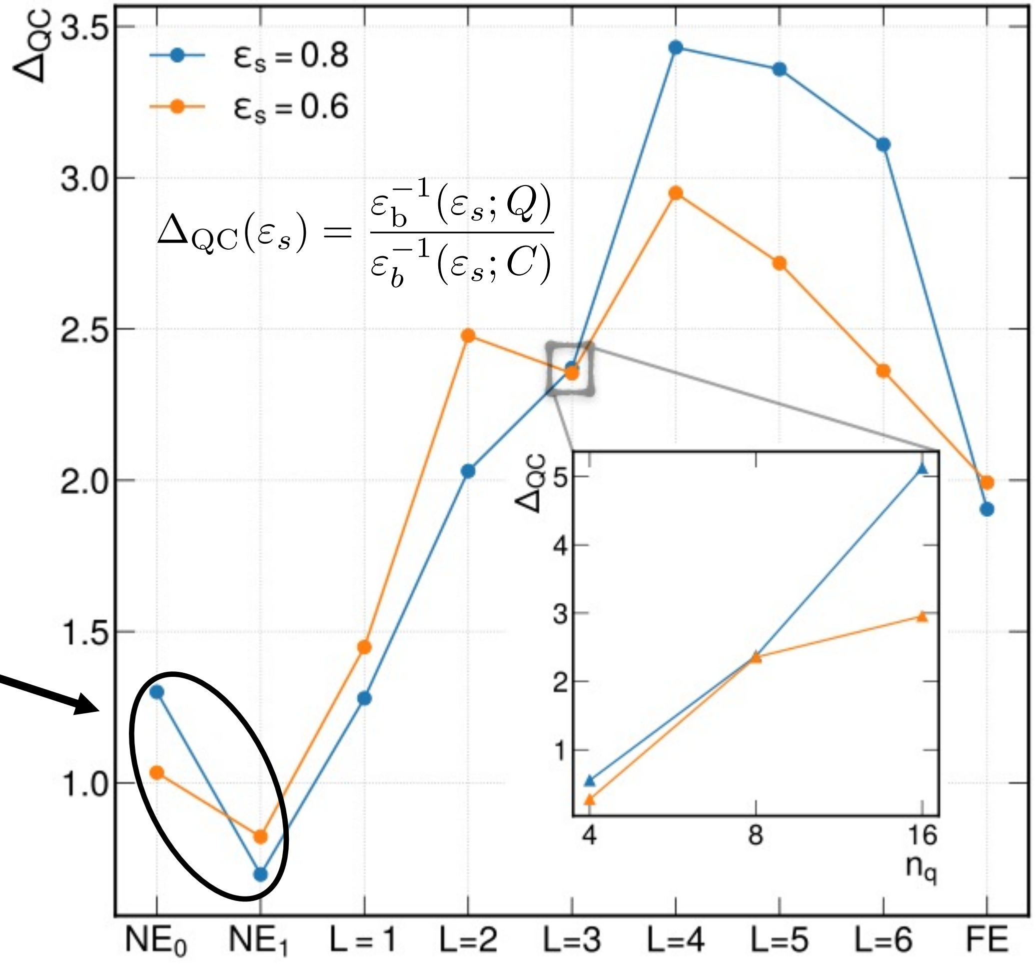


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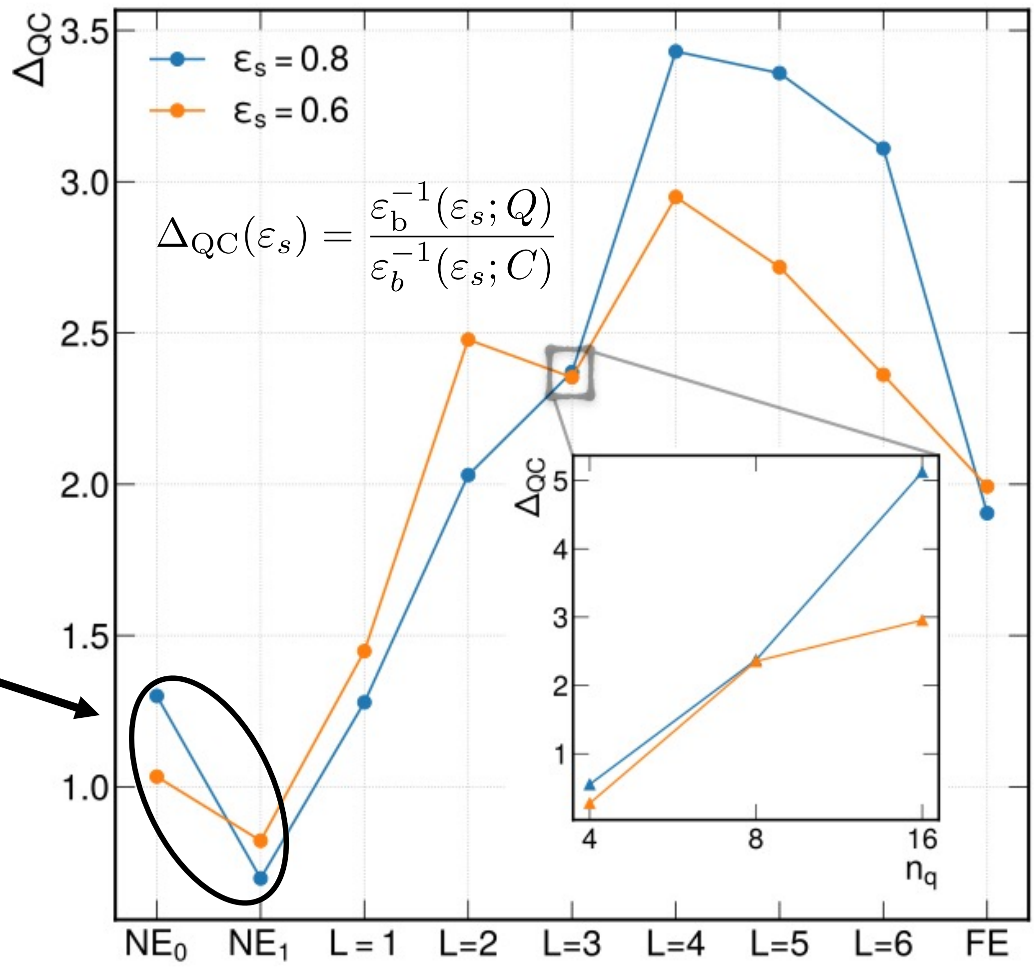
Up to **five times** the performance of the classical benchmark for 16 qubits!

No entanglement

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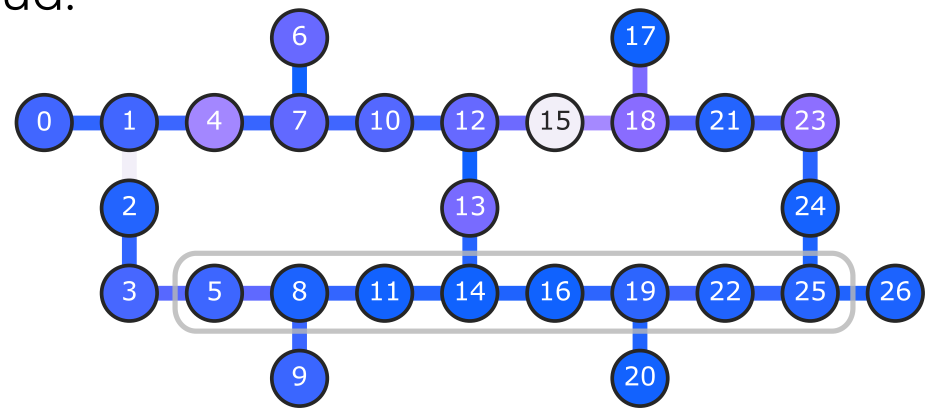
Minimal instance 100 + 100 (train + test) datapoints.




Superconducting qubits connectivity topology

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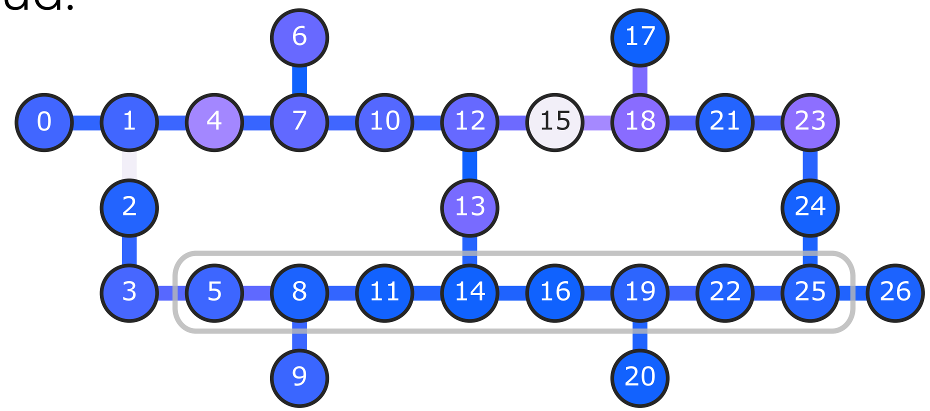

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| Kernel Machine Run | AUC | $\langle \mathrm{tr}\rho^2 \rangle$ |
|---|---|---|
| Hardware $L = 1$ | 0.844 | 0.271(6) |
| Ideal $L = 1$ | 0.999 | 1 |
| Hardware $L = 3$ | 0.997 | 0.15(2) |
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Purity of fully mixed state: $1/2^{\mathrm{n_q}} \approx 0.39 \times 10^{-2}$

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

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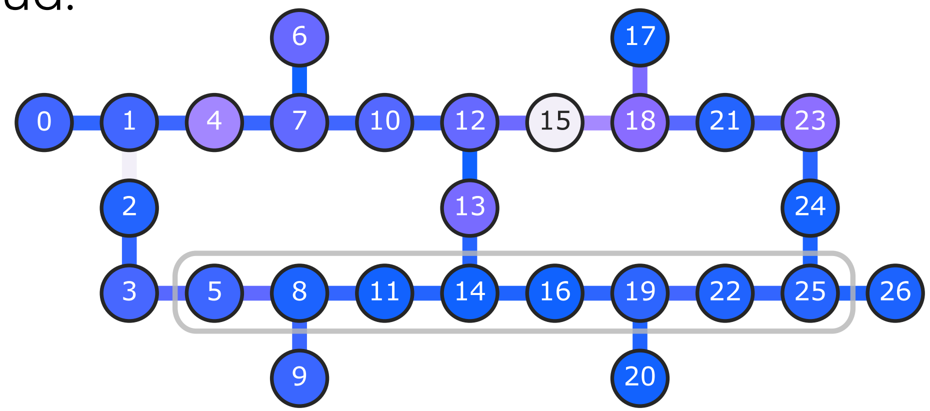


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**Proposed data encoding circuit realistic and suitable for current devices**

# Summary

QML **+** HEP : very promising results and interplay (sandbox).

- Utilize data generated by a quantum process.
- New inductive biases?

$$\mathcal{L} = -\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu} + \sum_f \bar{\psi}_f(i\gamma^\mu D_\mu - m_f)\psi_f$$
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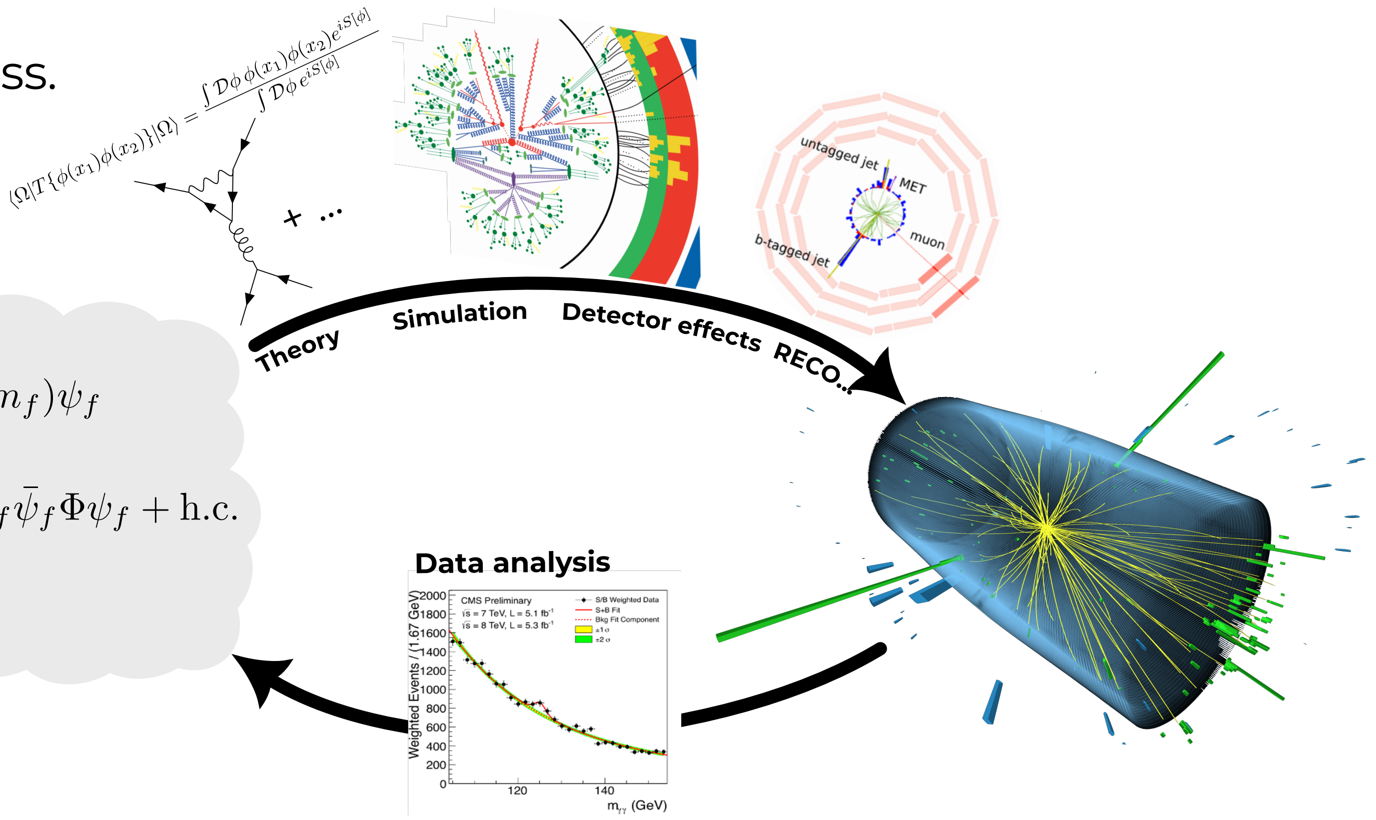
$$+\,\mathbf{BSM?}$$



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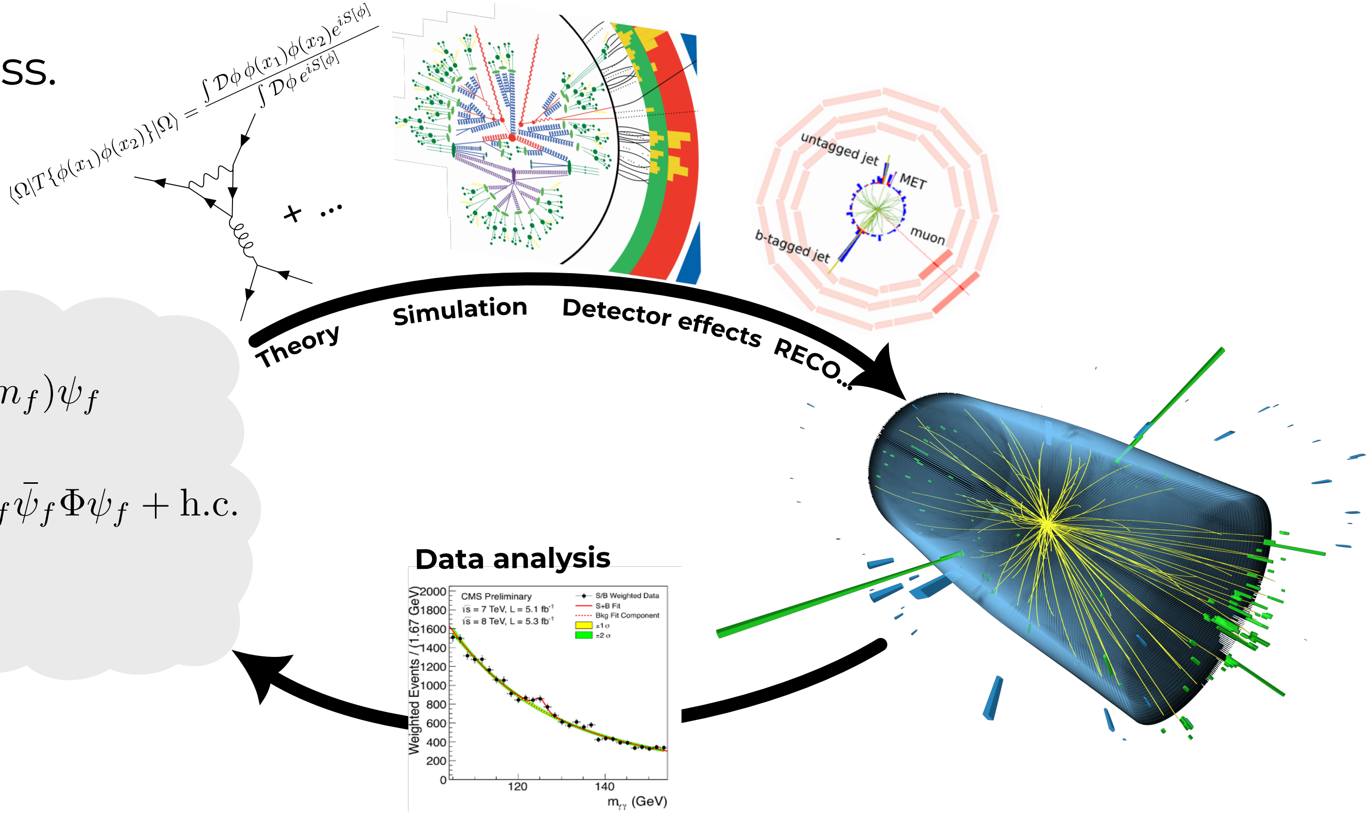


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**For more details checkout:**

[K.A. Wozniak*, VB*, E. Puljak* et al., 2301.10780]
[VB, S. González-Castillo, et al., 2104.07692]
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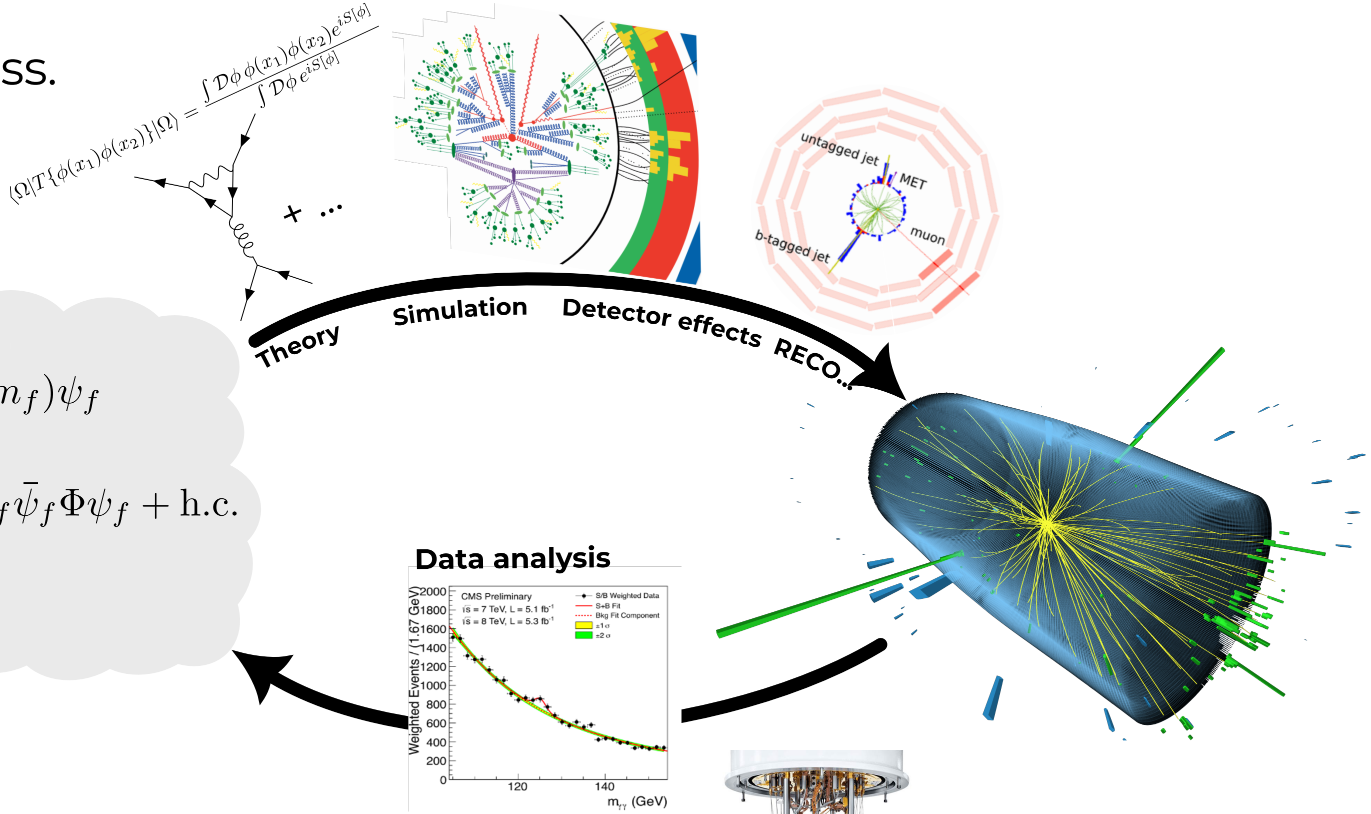


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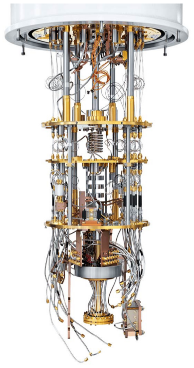
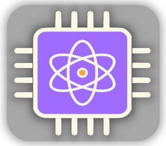
# Any cool ideas?
# Questions?

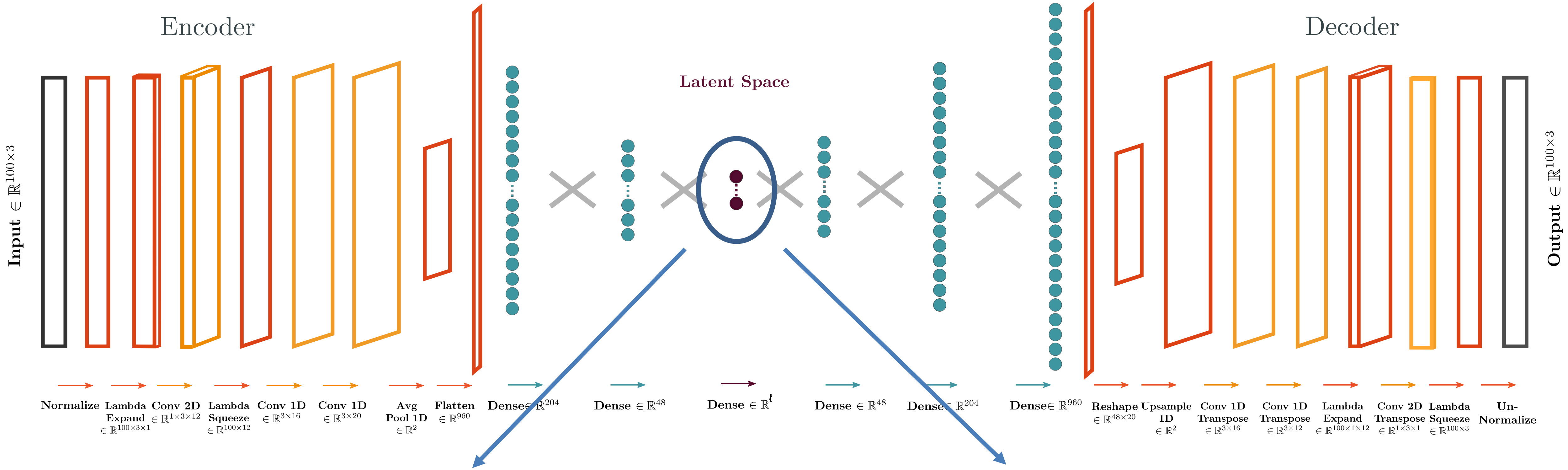




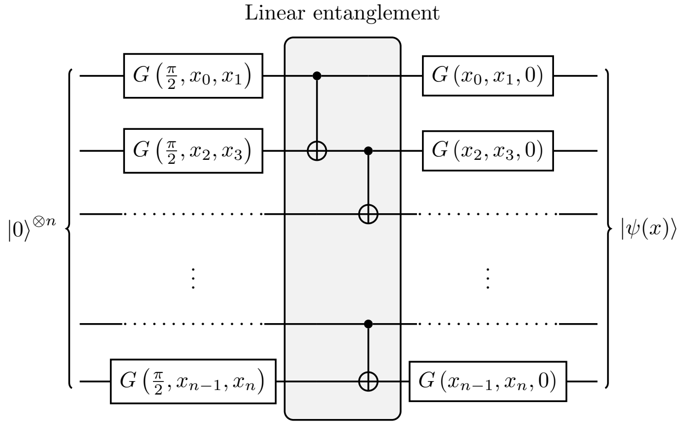
Credit: Rigetti Computing.

# Backup slides

# Convolutional autoencoder architecture



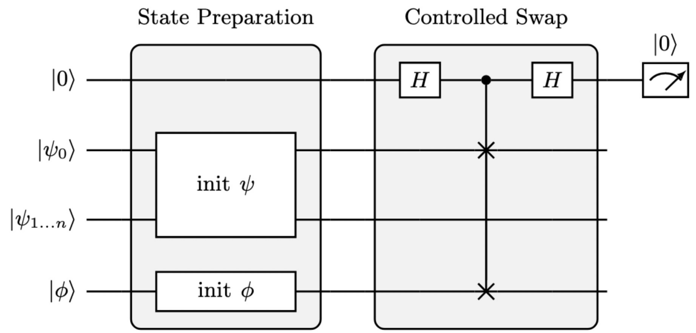

## Unsupervised kernel machine




Training size:

$\mathcal{O}(10^2) - \mathcal{O}(10^3)$

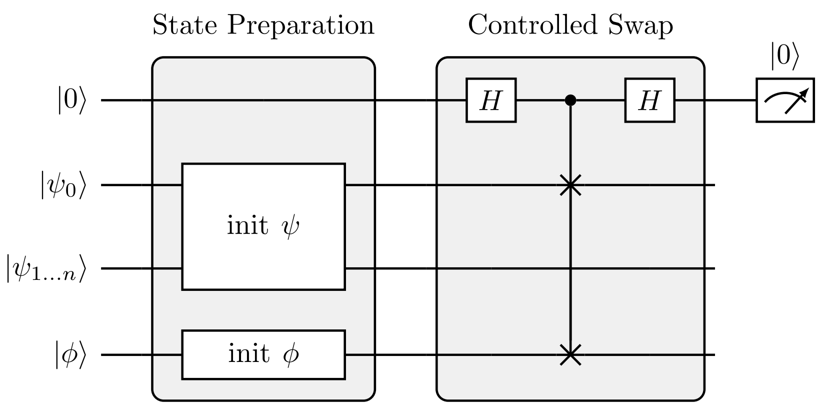
## Quantum clustering algorithms



# Quantum clustering for anomaly detection

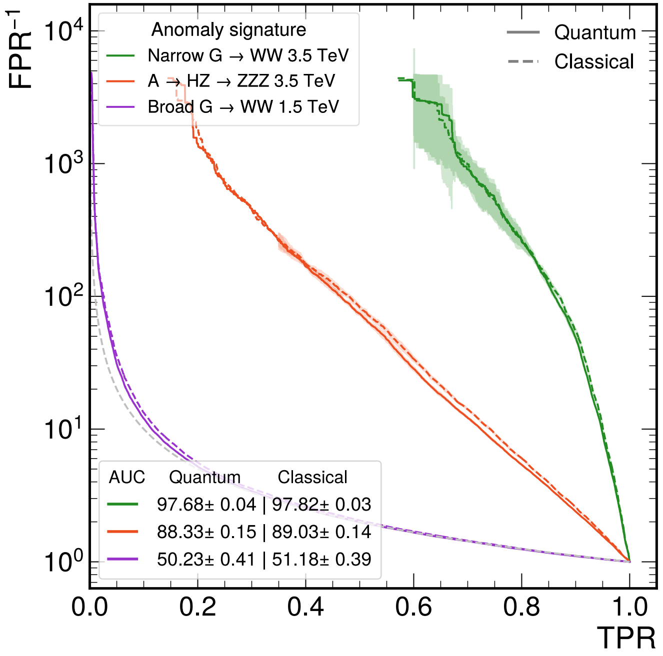
Construct clusters in the Hilbert space

Quantum distance calculation from clusters

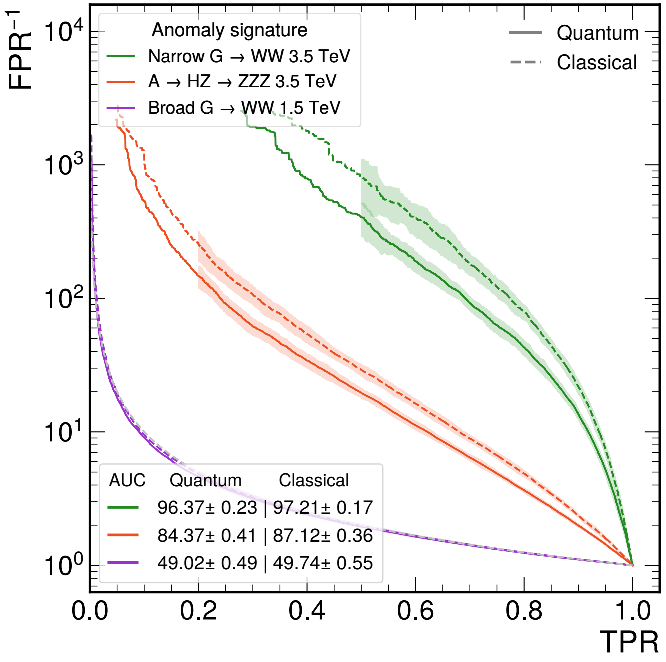



Minimise the distance with **quantum** (QK-means) or hybrid/**classical** (QK-medians) optimisation algorithms

**Quantum K-medians**




**Quantum K-means**

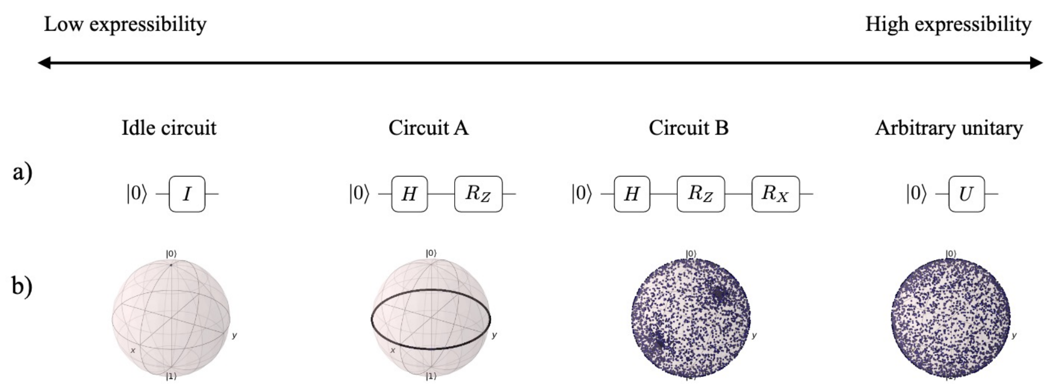



[K.A. Wozniak*, VB*, E. Puljak*, et al., arXiv: 2301.10780]

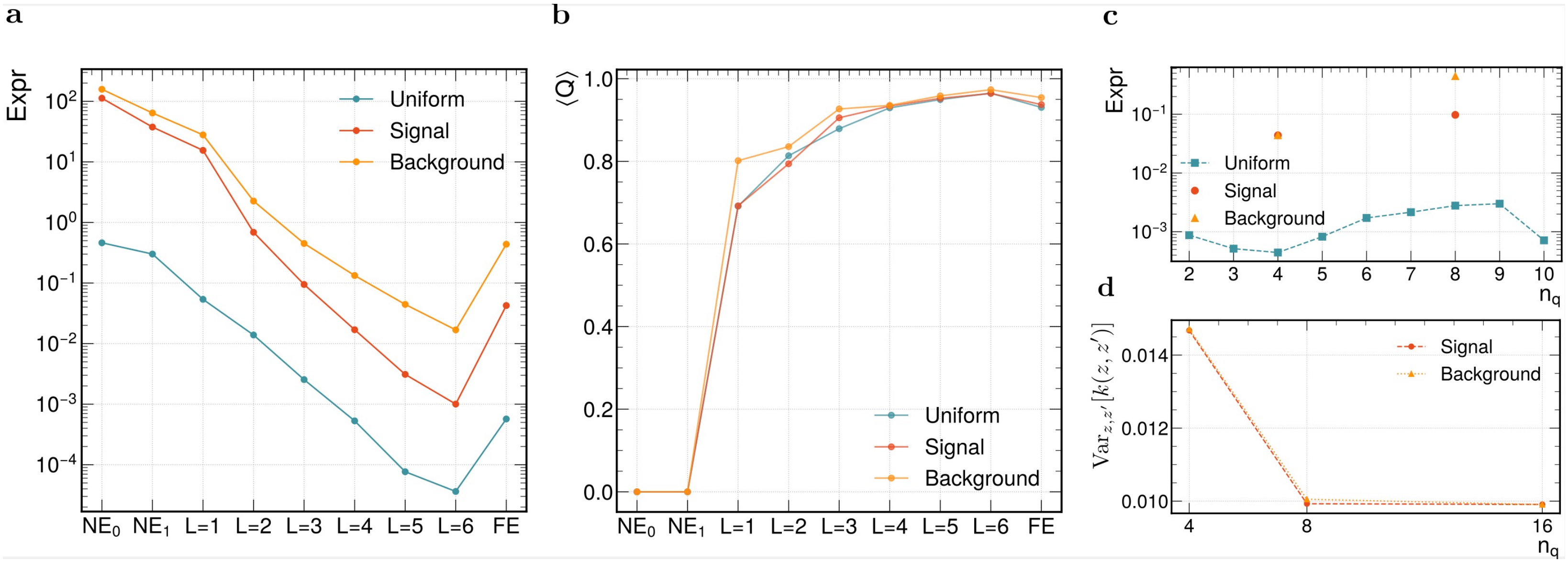
Quantum and classical anomaly detection has similar performance.

# Expressibility and entanglement capability

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

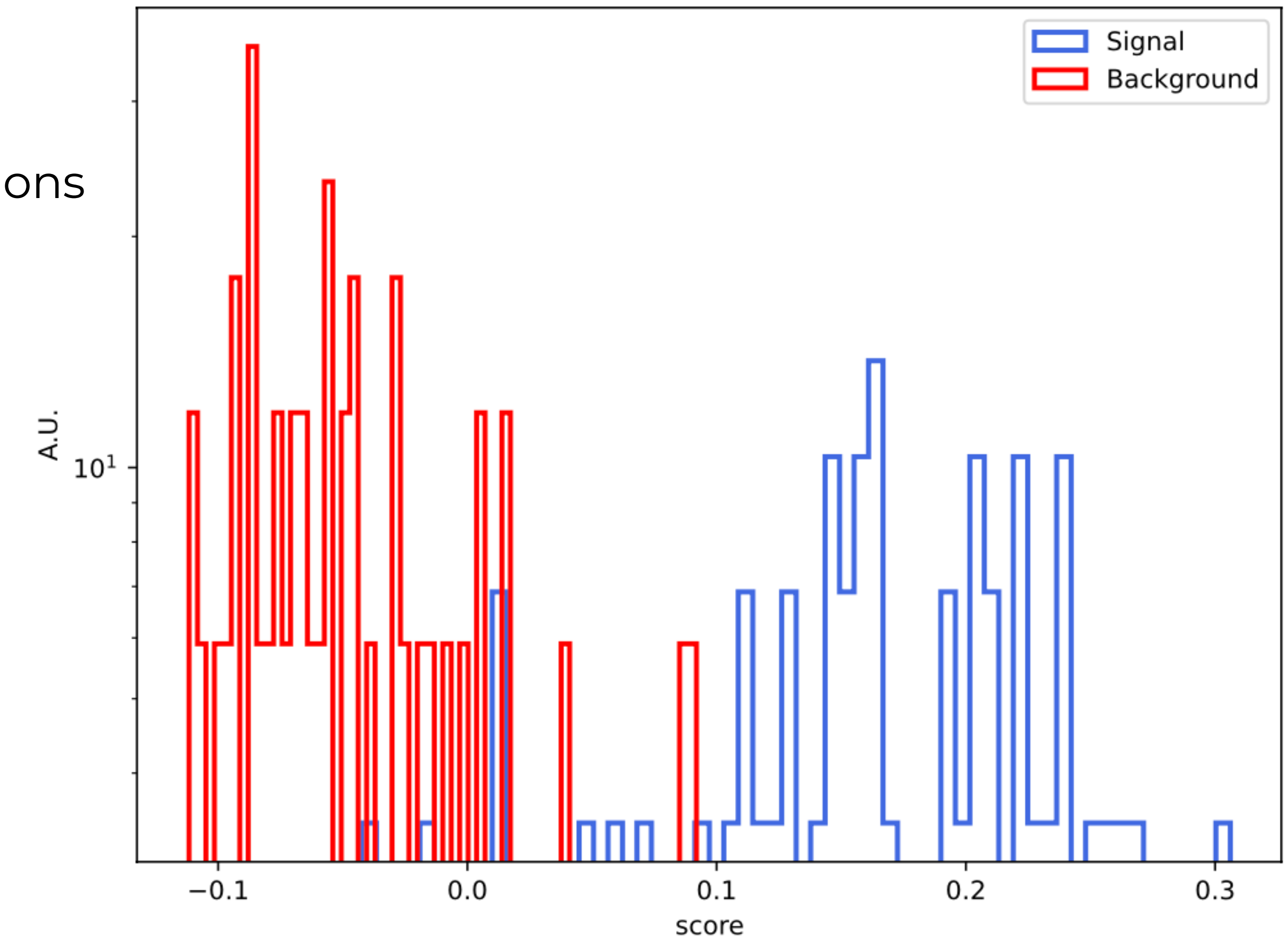



**Expressibility & Entanglement capability** of our data encoding circuit



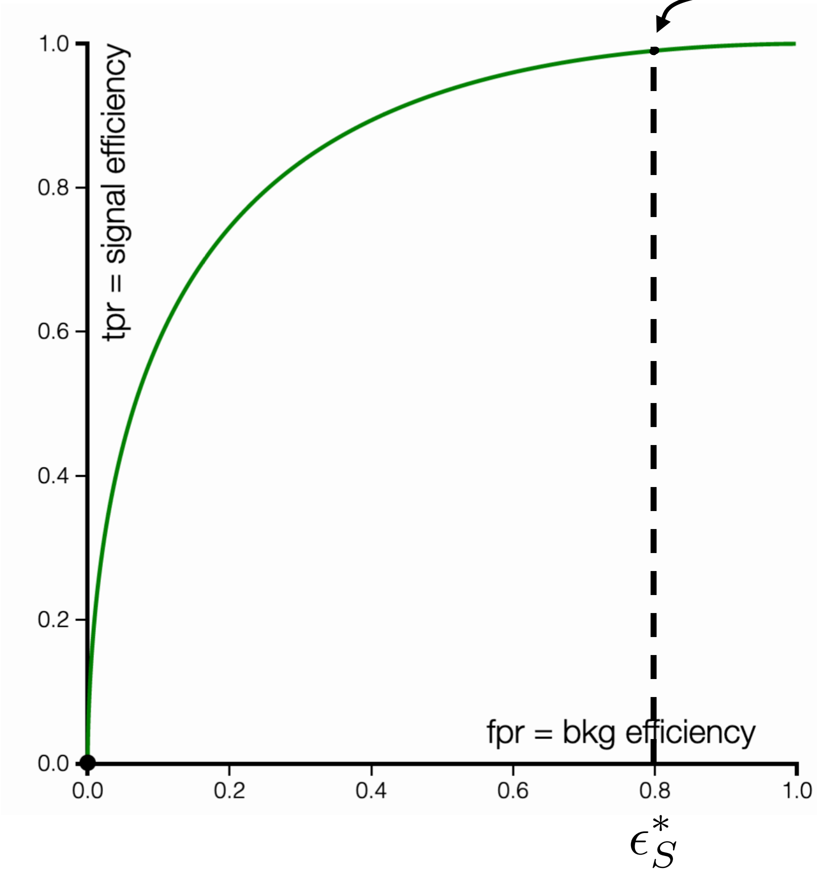
# Sparsity of the distributions in hardware

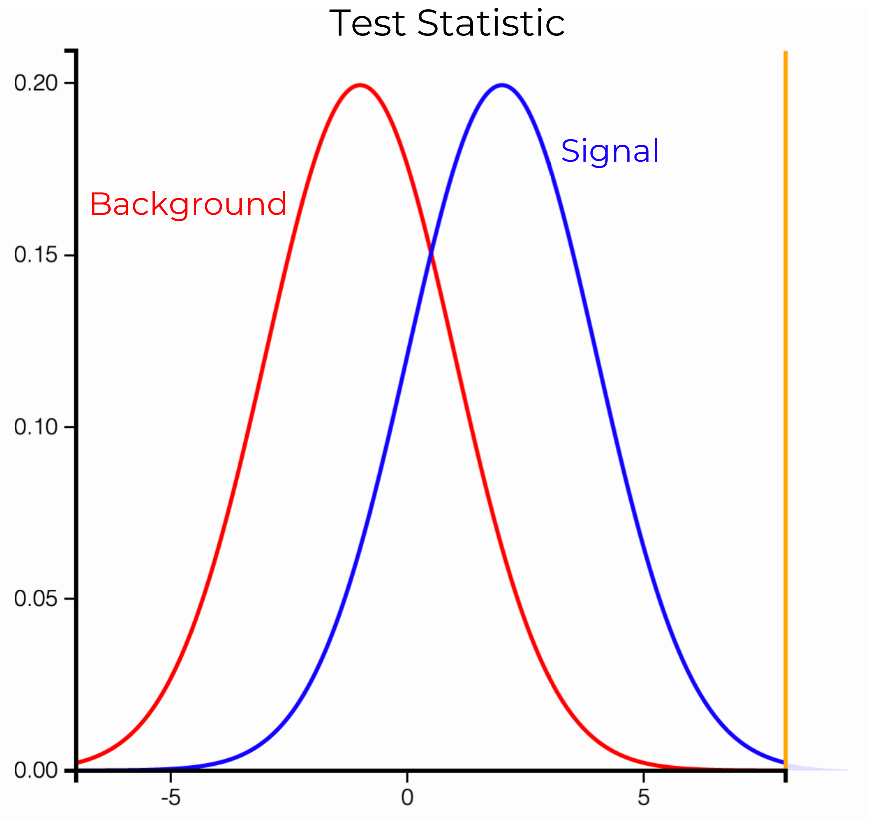
All models have sparse output distributions when training size is low.



# 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 $\epsilon_B(\epsilon_S^*)$




ETH zürich

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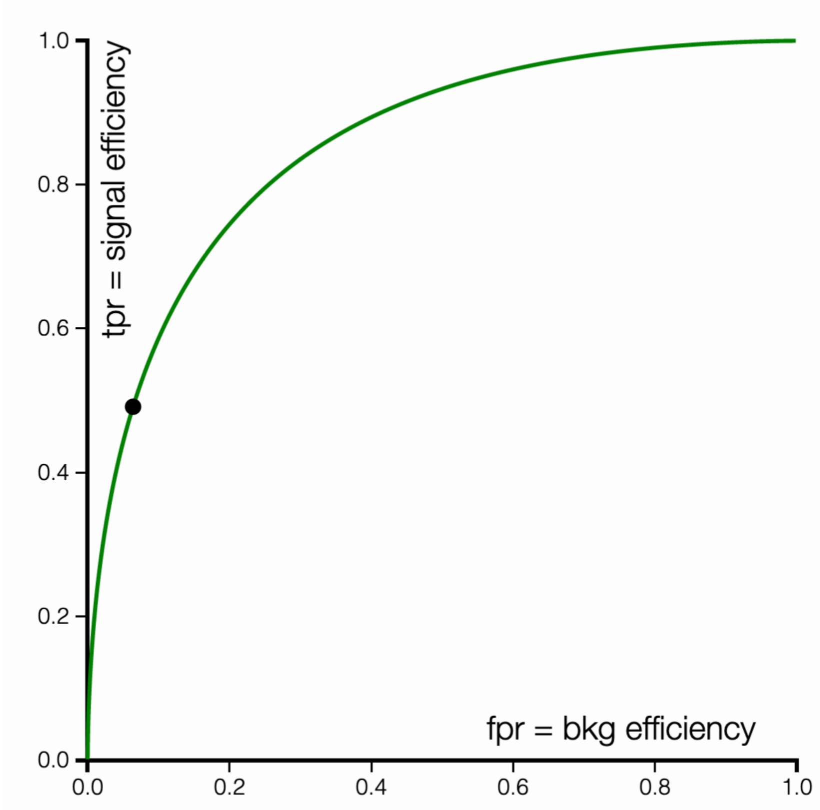


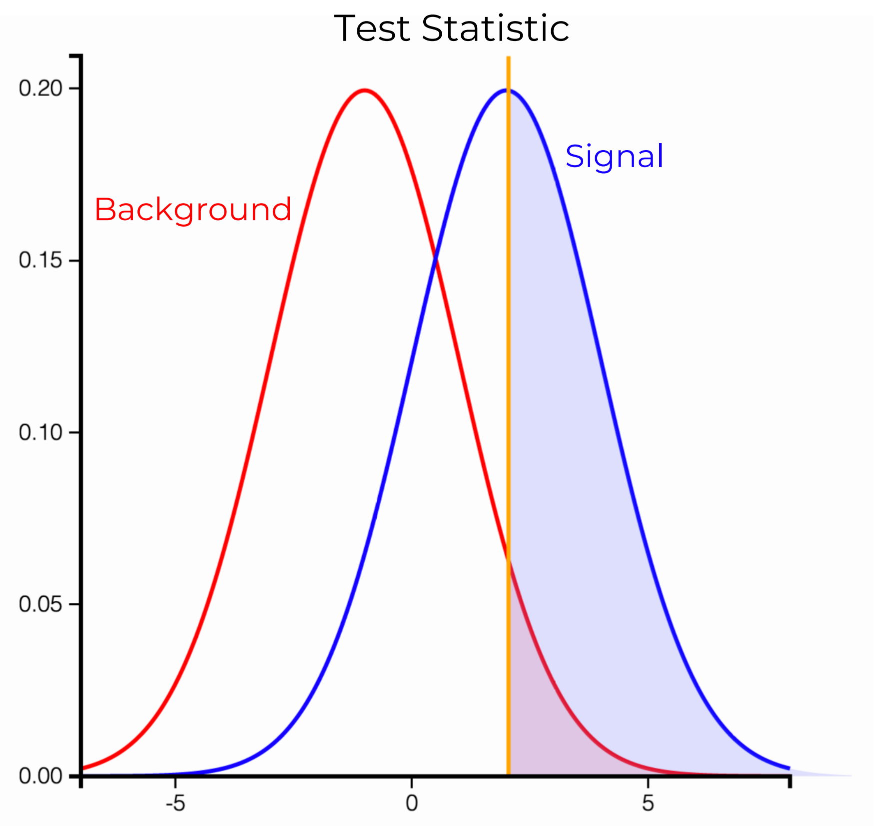

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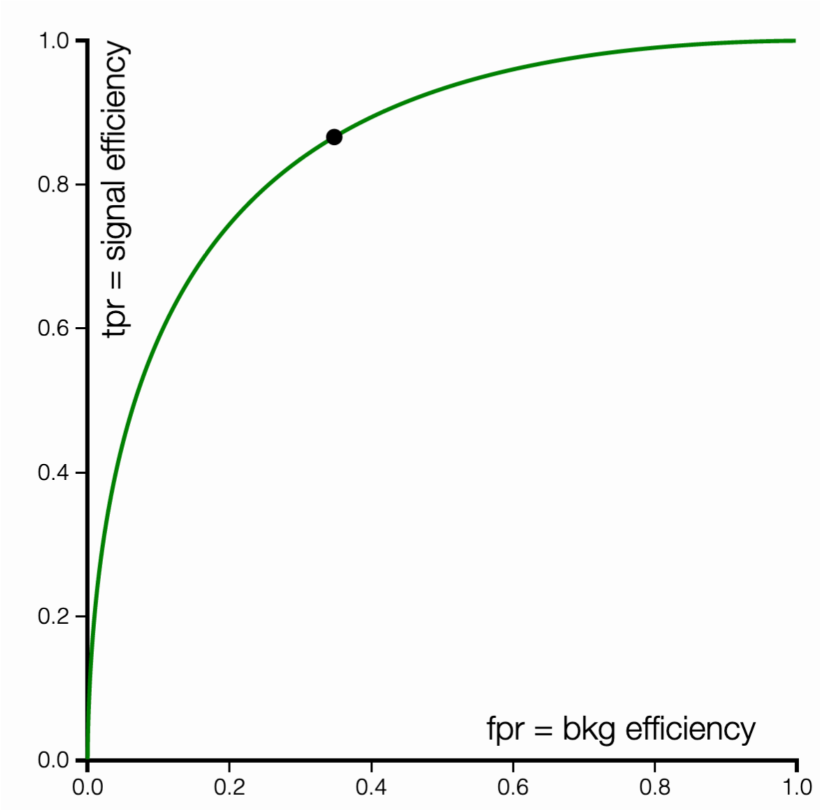


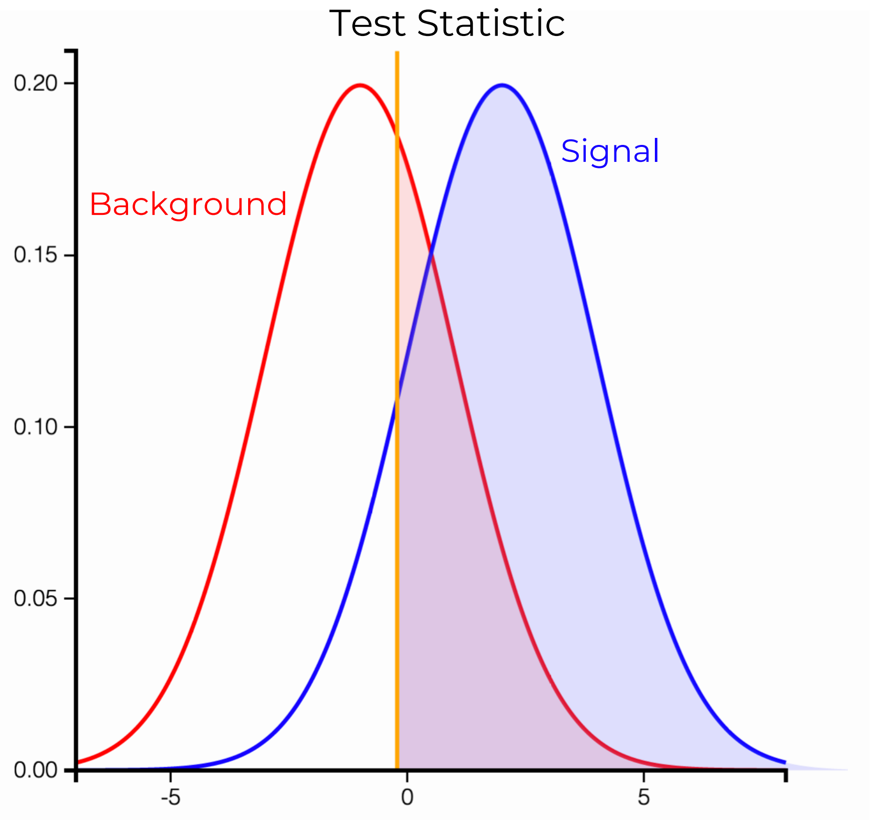

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