1P1Q: Particle Physics Data Encoding for Machine Learning on Quantum Computers

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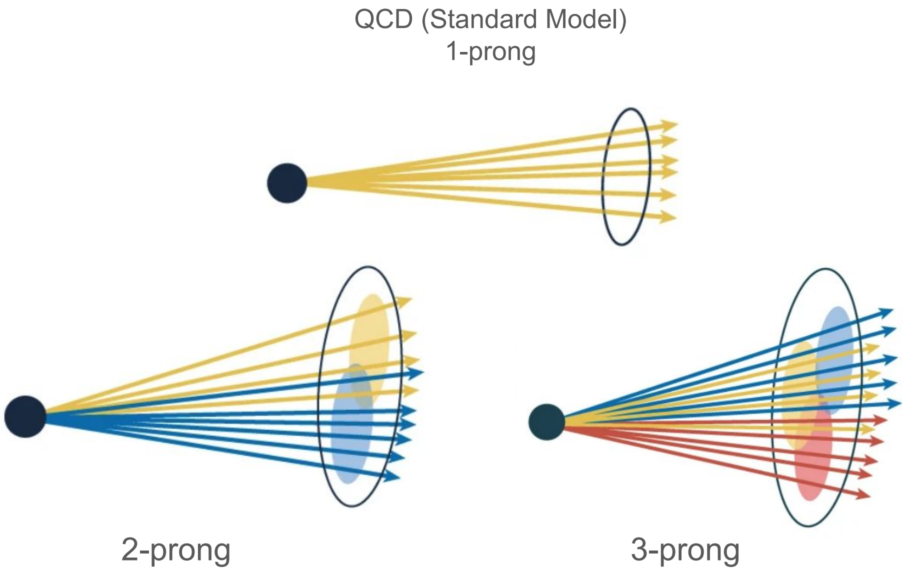
Introduction & Motivation - Anomaly Detection

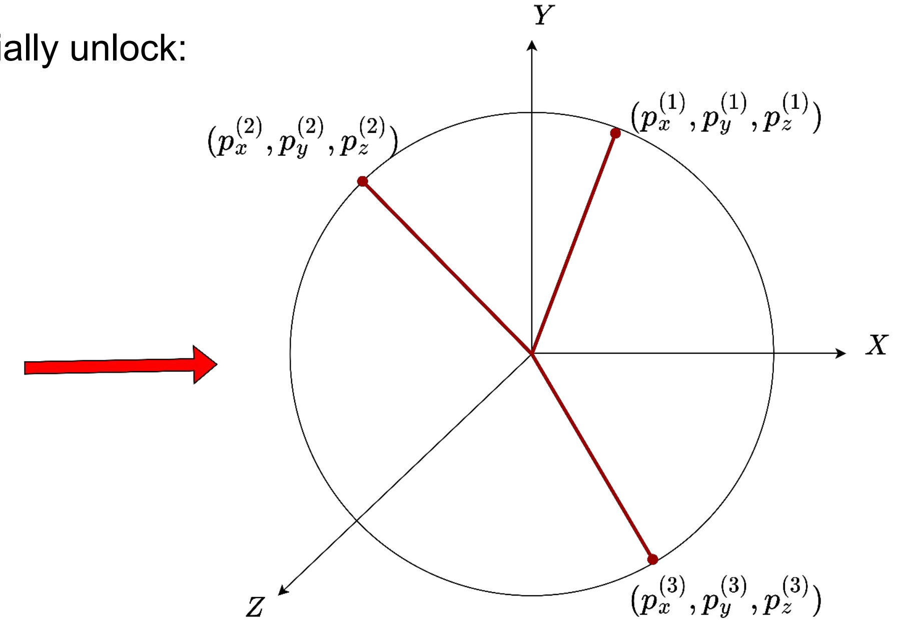


- Plenty of direct searches the past decade - no hints of new physics
- Are we missing something?
- Anomaly detection → search for outliers
- Model agnostic → wide coverage → reduce reliance on specific hypotheses

Why Quantum ML?

- Future experiments → higher data rates, faster inference requirements
- Existing **classical** techniques → could saturate in future
- Way out - newer computing paradigms → potentially unlock:
  - Better representations
  - Powerful *operations* to manipulate data?

$p_x^{(1)}$	$p_y^{(1)}$	$p_z^{(1)}$
$p_x^{(2)}$	$p_y^{(2)}$	$p_z^{(2)}$
$p_x^{(3)}$	$p_y^{(3)}$	$p_z^{(3)}$



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Why Quantum ML?

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- Quantum mechanical phenomena→ entanglement, superposition, tunneling → **no classical** equivalents → entirely **new** paradigms
    - Entanglement → uncover deeper patterns in data and capture higher order correlations

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

    - Superposition → efficient representation of multidimensional data

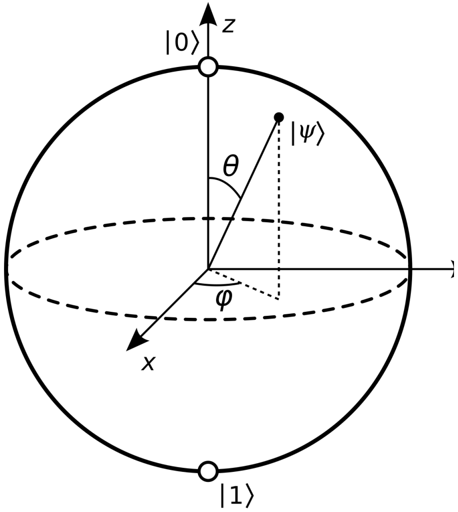
- **Quantum representations** of data →more information
- Parameter complexity advantage

$$\begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{pmatrix}$$

What is Quantum Computing?

- Building block: *qubits*
- Classical bit: either 0 or 1
- Qubit → superposition of |0⟩'s and |1⟩'s → and
- Point on unit sphere → described by two parameters (θ, ϕ)
  →same for a **qubit**



$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \quad \Longrightarrow \quad |\psi\rangle = \cos\left(\theta/2\right)|0\rangle + e^{-i\phi}\sin\left(\theta/2\right)|1\rangle$$

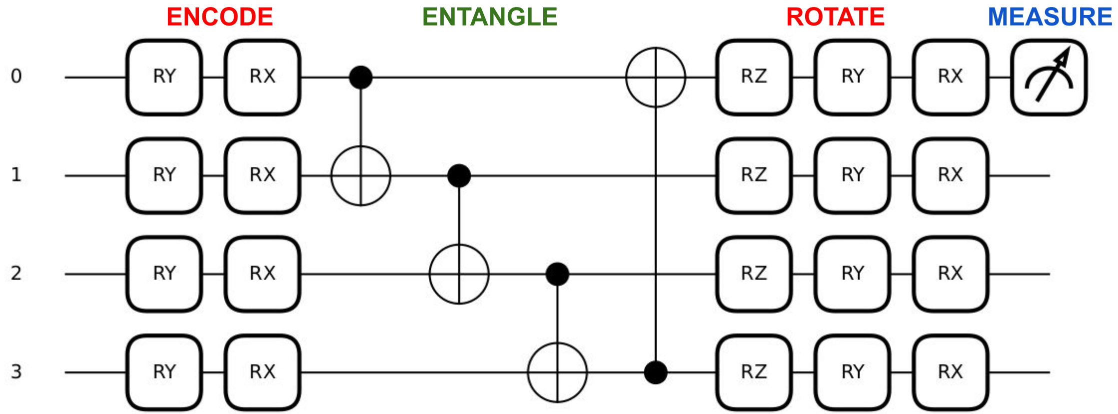
Building Quantum Circuits

- Manipulation of qubits → quantum mechanical operators (rotation, entanglement) : called **gates**
- Recipe → Encode, Entangle, Rotate, Measure

Observable

QML: makes these trainable

Most existing work focused here



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Building Quantum Circuits

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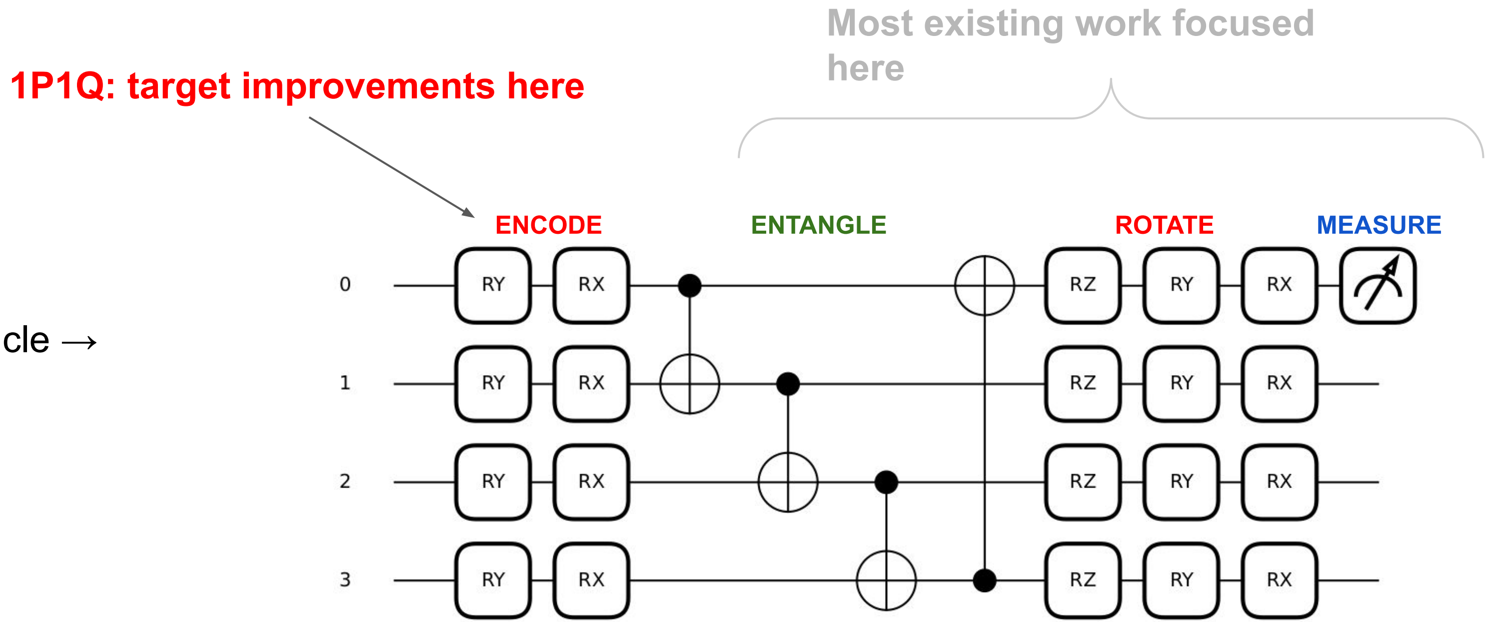
Introducing One-Particle → One-Qubit



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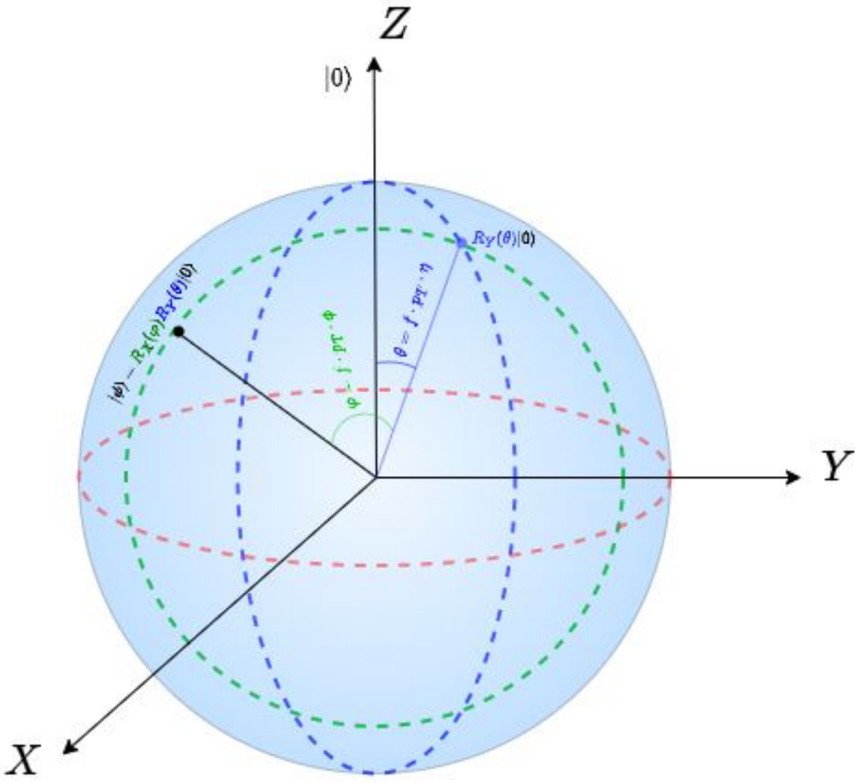
Introducing 1P1Q

- Keep it simple:
  - **1P1Q** → 1 Particle gets represented by 1 Qubit
  - Encode kinematic features (p_T , η , ϕ) per particle using rotations
  - 1 Jet → N qubits = N hardest particles

- Highly flexible encoding for **anomaly detection** and beyond

- Purely quantum → no classical pre-processing or hybrid learning approach



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Introducing 1P1Q

Scaled to lie in [-π,π]

$$(p_T, \eta) \quad \rightarrow \theta = f \cdot \frac{p_T}{p_{T,jet}}(\eta - \eta_{jet})$$

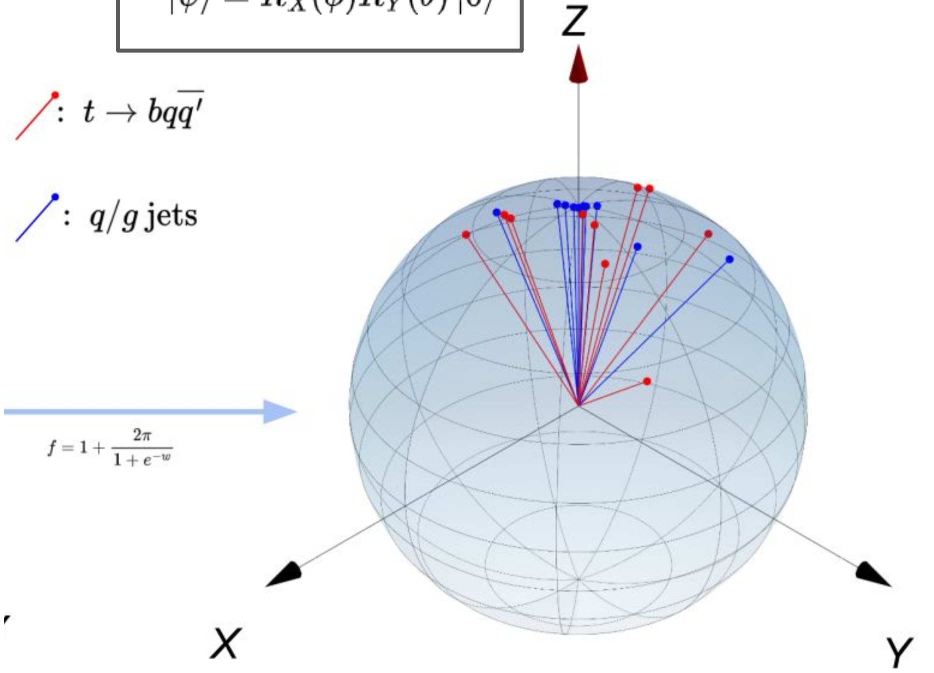
$$(p_T, \phi) \quad \rightarrow \varphi = f \cdot \frac{p_T}{p_{T,jet}}(\phi - \phi_{jet})$$

$$f = 1 + \frac{2\pi}{1 + e^{-w}}$$

trainable scale parameter → improves flexibility

ENCODING OPERATION

$$|\psi\rangle = R_X(\phi) R_Y(\theta) |0\rangle$$



Current implementation: Quantum Simulator library (Pennylane)

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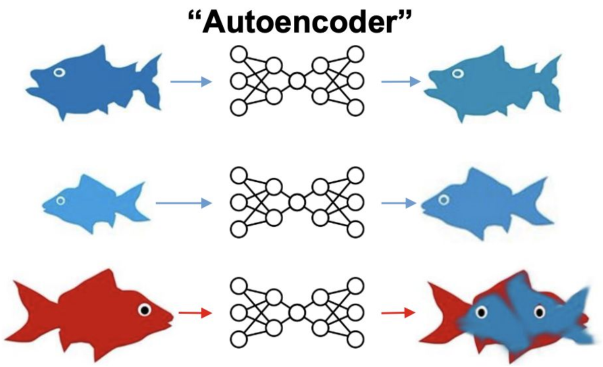
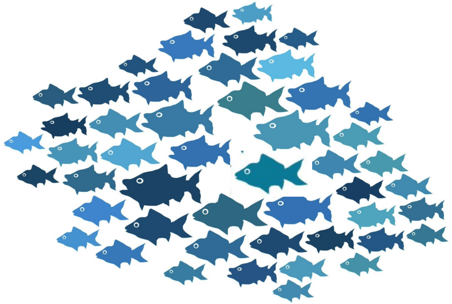
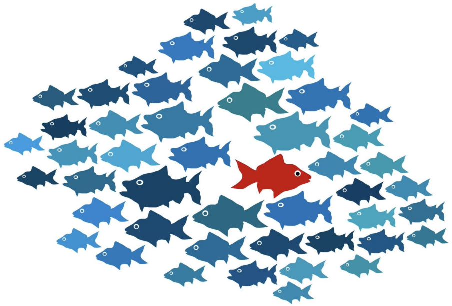
The Autoencoder Principle

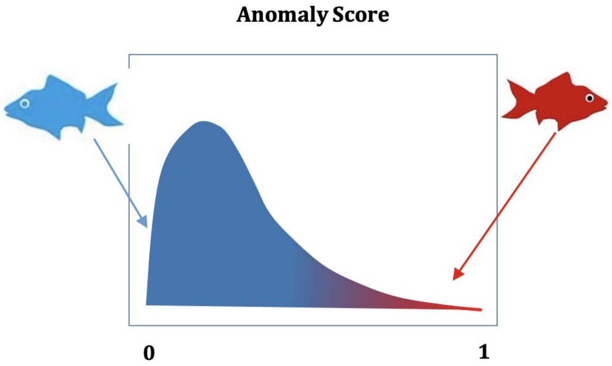
Train on non-anomalous inputs:







Apply to real-world examples



- Pass information through a **bottleneck** → retain core information
- **Reconstruct** original input
- Anomalous inputs → reconstruction performance **drops** → use as **anomaly metric**

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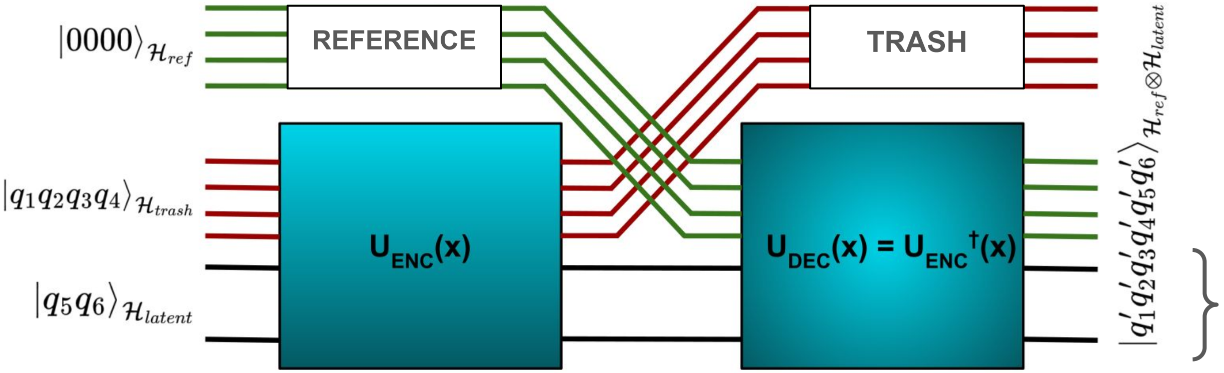
The Quantum Autoencoder (QAE)

- Compression into bottleneck → not trivial in a quantum circuit
- Unitary operators → preserve inner products
- Workaround → **replace** (some) qubits by fresh $|0\rangle$ state qubits



Bottleneck → Latent Space

The Quantum Autoencoder (QAE)

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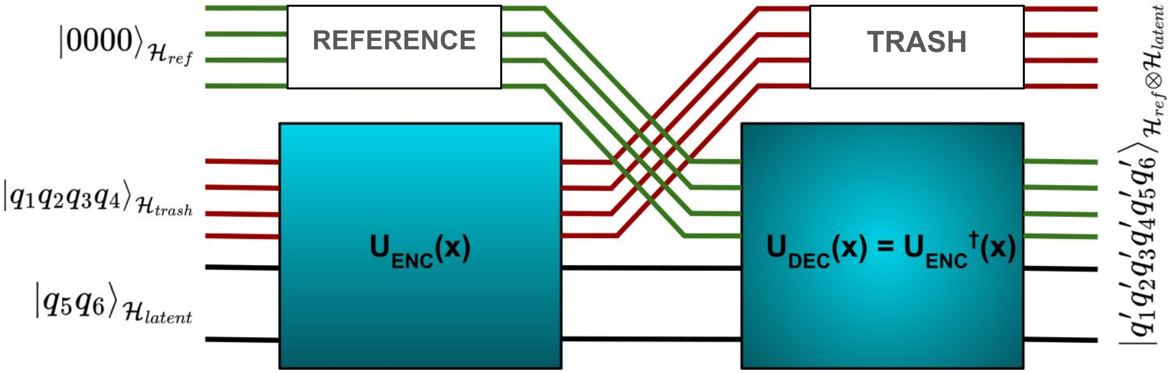
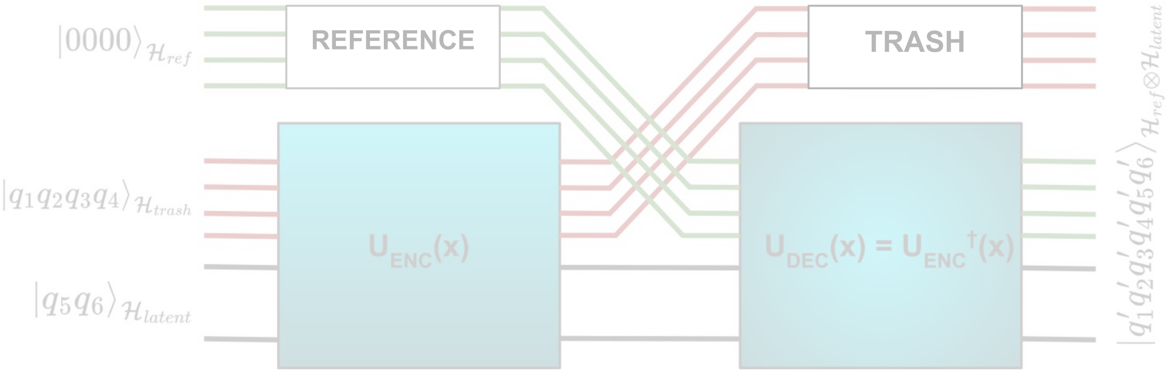
What about reconstruction quality?



Bottleneck → Latent Space

The Quantum Autoencoder (QAE)

- Compression into bottleneck → not trivial
- Unitary operators → preserve inner products
- Way out → **throw out** (some) qubits altogether



What about reconstruction quality?

Inner Product

Also known as

Quantum Fidelity

$$\langle\psi_1|\psi_2\rangle = \begin{cases} 1, & \text{when } |\psi_1\rangle = |\psi_2\rangle \\ b, & \text{otherwise} \end{cases}$$

Optimise classically (or quantum-mechanically)

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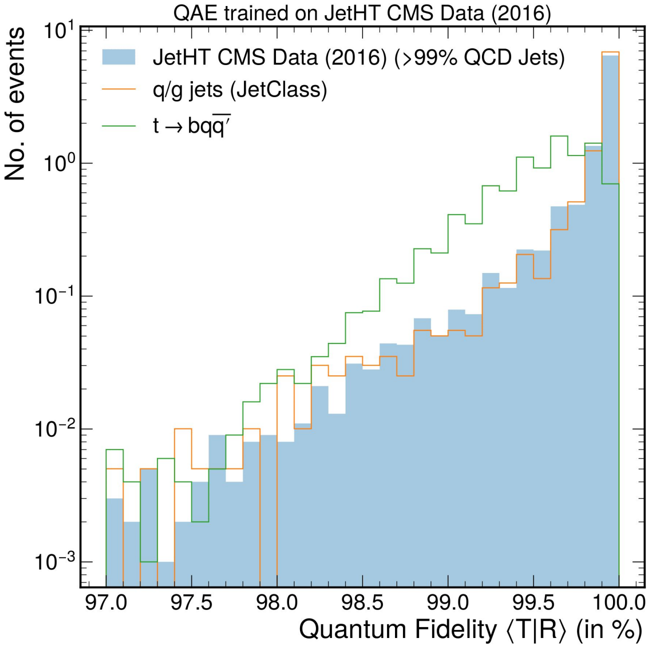
Results: Anomaly Detection Performance

- QAE is trained with:
  - only 10 jet constituents:
  - O(30) trainable parameters
- Outperforms classical autoencoders with far more parameters
- Crosscheck with open data from CMS Run 2 (**first time**)
  - similar performance on data → **robust behaviour**



Model	Signals				
	$Z \to q\bar{q}$	$W \to q\bar{q}$	$H \to b\bar{b}$	$H \to c\bar{c}$	$t \to bq\bar{q}$
QAE	**0.715**	**0.715**	**0.774**	**0.810**	**0.872**
CAE	0.676	0.675	0.739	0.767	0.858

Results: Anomaly Detection Performance

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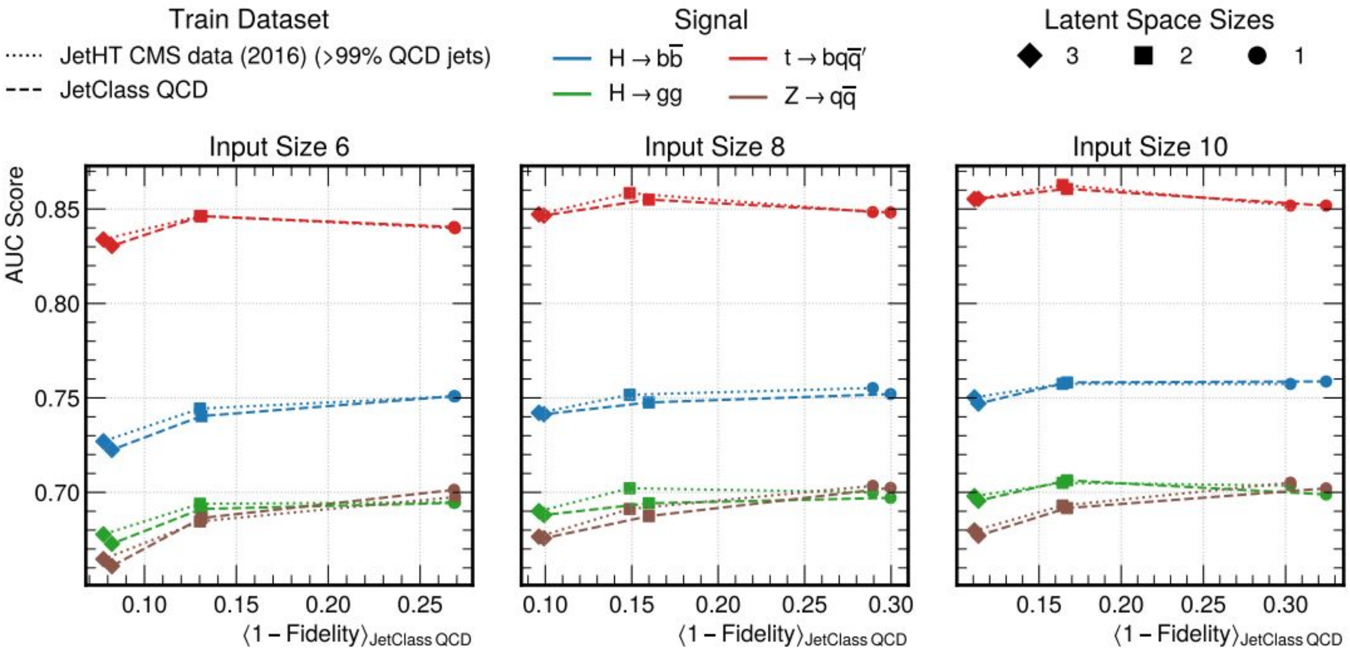
- Best performance: 2 qubit bottleneck
- QAE trained on data or simulated QCD → almost identical performance → high degree of **robustness**



Conclusion

- 1P1Q → simple and effective data encoding
  - Outperforms classical benchmarks of more complexity for anomaly detection
- Quantum ML holds promise for the future → data complexity, inference speed, etc
  - For now, classical algorithms outperform quantum as $N \to \infty$
- Deployment on real devices → work in progress
- Newer quantum computing paradigms → photonic, adiabatic, etc.

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