QML and Particle Physics

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Overview

1. Simulating Physics with Computers
2. Quantum Optimization Algorithms
3. Quantum Annealing

Can Quantum Computers really perform better when it comes to tasks related to natural sciences ?

Discretization Problem

Continuous processes are allowed to be divided into extremely small units (e.g., 10^{-15} s), leading to an enormous computational burden.

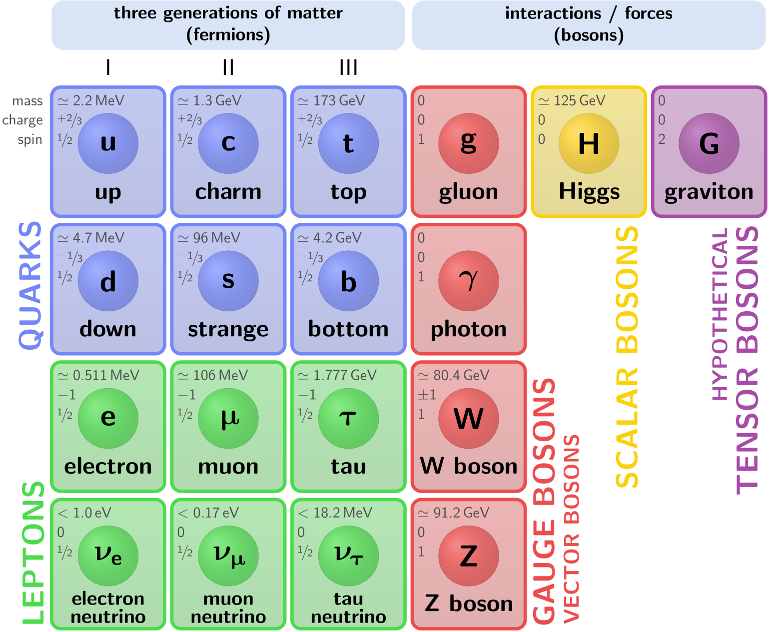
Randomization

Quantum mechanics naturally operates with probabilistic outcomes, while classical simulations must artificially mimic these probabilities. Classical systems generate pseudo randomness, quantum systems can produce true randomness.

Reversible Operations

Quantum processes are reversible (unitary), classical systems are made of non reversible elements

[Feynman, 1982]


three generations of matter
(fermions)
interactions / forces
(bosons)
I
II
III
mass
charge
spin
≃ 2.2 MeV
+2/3
1/2
u
up
≃ 1.3 GeV
+2/3
1/2
c
charm
≃ 173 GeV
+2/3
1/2
t
top
0
0
1
g
gluon
≃ 125 GeV
0
0
H
Higgs
0
0
2
G
graviton
QUARKS
≃ 4.7 MeV
−1/3
1/2
d
down
≃ 96 MeV
−1/3
1/2
s
strange
≃ 4.2 GeV
−1/3
1/2
b
bottom
0
0
1
γ
photon
SCALAR BOSONS
HYPOTHETICAL
TENSOR BOSONS
≃ 0.511 MeV
−1
1/2
e
electron
≃ 106 MeV
−1
1/2
μ
muon
≃ 1.777 GeV
−1
1/2
τ
tau
≃ 80.4 GeV
±1
1
W
W boson
LEPTONS
< 1.0 eV
0
1/2
ν_e
electron neutrino
< 0.17 eV
0
1/2
ν_μ
muon neutrino
< 18.2 MeV
0
1/2
ν_τ
tau neutrino
≃ 91.2 GeV
0
1
Z
Z boson
GAUGE BOSONS
VECTOR BOSONS

Unravelling physics beyond the standard model with classical and quantum anomaly detection

Supervised Learning

- Model is trained on labeled data.
- Labels typically obtained via simulations based on BSM theories.
- Effective only if the signal type is known and correctly modeled.
- Limited generalization to unknown or unexpected signals.

[Schuhmacher et al., 2023]

Unsupervised Learning:

- Model is trained without labels, learning the structure of mostly SM data.
- Identifies anomalies as outliers in the learned distribution.
- Higher generalization capability—can detect unknown signals.
- Lower accuracy for specific signals due to absence of prior knowledge.

Data Scrambling : Middle Ground

- **Goal:** Combine the strengths of supervised and unsupervised learning for BSM event detection.
- **Strategy:**
  - Use **supervised learning**, but without relying on specific BSM models.
  - Create artificial signal events by **scrambling** Standard Model (SM) background data.
  - Scrambling introduces controlled perturbations while respecting physical laws and detector constraints.
- **Advantages:**
  - Minimizes physically-inspired bias in signal assumptions.
  - Increases generalization while preserving some accuracy.
  - Does not rely on prior BSM simulations.
- **Implementation:**
  - Binary classification task solved using **Support Vector Classifier (SVC)**.
  - Positioned as a middle ground between fully supervised and fully unsupervised approaches.

[Schuhmacher et al., 2023]

Quantum SVC

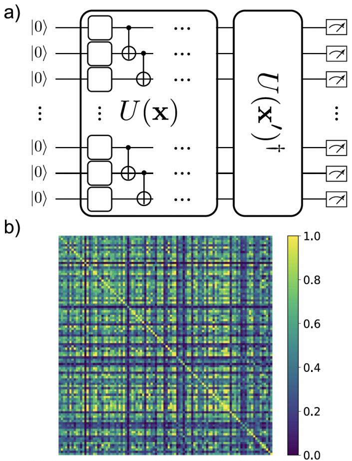


Figure 3. (a) Quantum circuit used by the quantum support vector classifier (QSVC) to measure the overlap between two encoded quantum states. The feature vector $\boldsymbol{x}$ is encoded into a quantum state through the parameterized unitary $U(\boldsymbol{x})$. (b) Kernel matrix for the classification between SM events and artificial anomalies calculated on the IBM quantum processor *ibm_cairo* using 6 features (corresponding to 6 qubits).

[Schuhmacher et al., 2023]

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

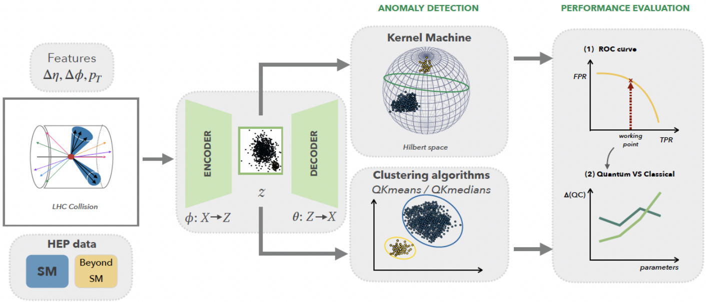
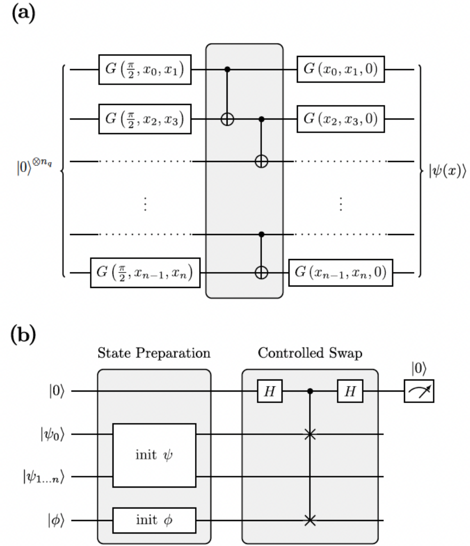


FIG. 1. *Classical-quantum pipeline.* LHC collision data (simulation) are passed through an autoencoder for dimensionality reduction followed by the quantum anomaly detection models: *unsupervised quantum kernel machine* and *quantum clustering algorithms* (QK-means/QK-medians). Each jet contains 100 particles, each particle is described by three features ($\Delta\eta, \Delta\phi, p_T$) where Δ represents a distance from the jet axis. Hence, a dijet collision event is described by 300 features. The quantum models are trained on Standard Model data and learn to recognise anomalies in unseen data. All models are evaluated by calculating the Receiver Operating Characteristic (ROC) curve and metrics appropriate for anomaly detection tasks, and are compared to their classical counterparts (see "Evaluation of model performance" subsection in the Results).

[Belis et al., 2024]

Stage	What Happens	Why It Is Done
Raw LHC event	Simulated proton–proton collision produces $\mathcal{O}(10^2)$ particles.	Goal = find very rare BSM events hidden in vast SM background.
Feature extraction	Each jet keeps three jet–centric variables $\Delta\eta$, $\Delta\phi$, p_T. 100 particles 300 features / event.	Compact, physics-motivated description of particle kinematics.
Classical autoencoder (AE)	Encoder $f : X \to Z$ compresses 300-D input to latent z. Decoder $g : Z \to X$ reconstructs input.	Latent space captures "normal" SM structure; anomalies stand out in Z.
2*Quantum anomaly detector	**(i) Quantum kernel machine**: uses quantum feature map to compute kernel and flag outliers.	24.3cmQuantum feature maps+entanglement may reveal subtle patterns with fewer parameters than classical methods.
	(ii) Quantum clustering (QK-means/QK-medians): quantum distance used for cluster assignment; isolated points = anomalies.	
Performance evaluation	ROC curve $\to$ choose working point; compute background rejection. Plot $\Delta QC = \epsilon_b^{-1}(Q)/\epsilon_b^{-1}(C)$ vs qubits/depth.	Quantifies quantum gain; $\Delta QC > 1$ = quantum outperforms classical.



[Belis et al., 2024]

Results

Performance Metric:

- ROC curves and AUC (Area Under Curve)

Quantum Advantage:

- Achieved when $n_q > 4$ qubits and circuit depth $L \geq 1$
- Entanglement in the encoding circuit is essential — absence leads to drastic performance drop
- Quantum kernel machines outperform classical models in background suppression (higher ϵ_b^{-1})

Quantum anomaly detection for collider physics

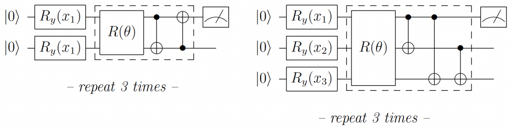


Figure: VQC

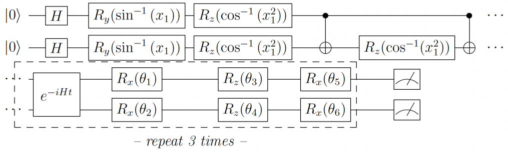


Figure: QCL

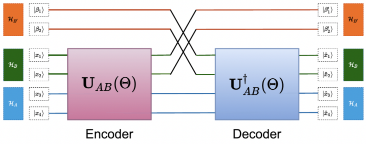
[Alvi et al., 2023]

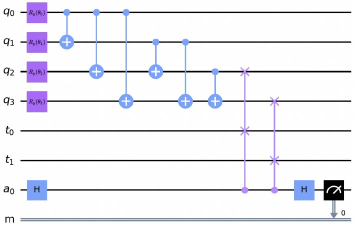
1D	Model	Parameters	Time (h:mm:ss)	Optimization Method	Optimization Steps
	VQC	18	0:56:42	Vanilla GD	50
	QCL	18	0:00:45	COBYLA	30
	NN Low	97	0:03:25	Adam	50
	NN High	1217	0:03:40	Adam	50
3D					
	VQC	27	1:57:35	Vanilla GD	50
	QCL	54	0:01:07	COBYLA	20
	NN Low	97	0:06:40	Adam	50
	NN High	1217	0:03:35	Adam	100

Table 1. A summary of the hyperparameters chosen for each classifier and average running (training and testing) time. The times were evaluated using the Perlmutter computer at NERSC, which has nodes consisting of A100 NVIDIA GPUs (used for NNs) and Milan AMD CPUs.

[Alvi et al., 2023]

Anomaly detection in high-energy physics using a quantum autoencoder





[Ngairangbam et al., 2022]

Source	Model	AUC (Example)	Params	Runtime	Optimization Algorithm
belis2024quantumanomaly	QKM	0.844 / 0.997	n_q, L	–	Classical obj. opt + quantum kernel eval
	Classical RBF SVM	0.998	SV-based	–	Quadratic Prog (SVM)
	QK-means / medians	–	circuit-dependent	–	Grover (QK-means), hybrid iter. (QK-medians)
duffy2024unsupervised	QAE (new, 6f)	**0.983**	6–32	–	Adam (LR=0.005)
	CAE (deep, 6f)	0.971	up to 540+	–	Adam (LR=0.001)
alvi2023quantumanomaly	VQC (3D)	–	27	1h 57m	Vanilla Gradient Descent
	QCL (3D)	–	54	1m 7s	COBYLA
	NN High (3D)	–	1217	3m 35s	Adam
ngairangbam2022anomaly	QAE	–	$\sim$10	–	Quantum Gradient Descent
	CAE	–	$\sim$1000	–	Adam
schuhmacher2023unravelling	QSVC (Graviton, 8f)	**0.997**	Qubits + circuit	$\sim$16 ms (QPU only)	Quantum kernel est. + hyperparam fixed
	SVC (Graviton, 8f)	0.944	SV-based	Fast	SMO (typical) + hyperparam tuned

Problems with existing work

- Not leveraging quantum optimization
- classical optimization is time consuming

Quantum Optimization Algorithms

Algorithm	**Type**	**Example Use Cases**
Grover's Search	Unstructured Search	MAX-SAT, Graph Problems
QAOA (NISQ)	Combinatorial (Approx.)	Max-Cut, Scheduling, Logistics
Quantum Annealing (NISQ)	Combinatorial (Exact)	Routing, Resource Allocation
VQA (NISQ)	General (Hybrid)	Portfolio Opt., ML, Chemistry
Gibbs Sampling	Probabilistic/Statistical	Boltzmann Machines, Energy Mode
Phase Estimation	Eigenvalue-Based	Convex Programming, SDP

Table: Summary of Quantum Optimization Algorithms

[Guerreschi et al., 2023]

Problem Classes & Quantum Algorithms

Problem Class	Quantum Optimization Algorithms
Discrete Optimization	Grover's Search, QAOA, Quantum Annealing (QA), Variational Quantum Algorithms (VQA)
Continuous Optimization	Variational Quantum Algorithms (VQA), Quantum Gradient Descent, Quantum Natural Gradient Methods
Mixed-Integer Programming	QAOA extensions, Hybrid Classical-Quantum Solvers, Discrete-encoded QA
Convex Optimization	Quantum Interior-Point Methods, Semidefinite Programming (SDP) Solvers, Quantum Linear Systems (HHL)
Dynamic Programming	Grover-enhanced Bellman updates, Early-stage Quantum Dynamic Programming
Optimal Control	Quantum Trajectory Optimization, Quantum Control Theory, Reinforcement Learning-based methods
Robust Optimization	Stochastic VQAs, Sampling-based Quantum Methods with Uncertainty Modeling
Multi-objective Optimization	Quantum Pareto Sampling, Multi-output VQAs, Quantum Genetic Algorithms

[Guerreschi et al., 2023]

Hamiltonian

Hamiltonian

Operator corresponding to the total energy of a quantum system described by Hermitian matrix

$$H = H^{\dagger}$$

Energy of system in state $|\psi\rangle$ given by expectation value

$$E(|\psi\rangle) = \langle\psi|H|\psi\rangle$$

Ground State

The lowest energy state $|\psi^*\rangle$ of a quantum system

$$|\psi^*\rangle = \underset{|\psi\rangle\in\mathcal{H}}{\operatorname{argmin}} E(|\psi\rangle)$$

'https://www.youtube.com/watch?v=YpLzSQPrgSct=649s'

QUBO

- Optimization problems with quadratic objective function and linear and quadratic constraints
- Special case: Quadratic Unconstrained Binary Optimization (**QUBO**)
  - Quadratic objective function
  - No variable constraints
  - Binary optimization variables

$$\text{minimize} \quad x^T Q x + c^T x$$

$$x \in \{0,1\}^n \quad Q \in \mathbb{R}^{n \times n} \; c \in \mathbb{R}^n$$

$$\text{subject to} \quad \begin{aligned} Ax &\leq b \\ x^T Q_i x + a_i^T x &\leq r_i \\ l_j \leq x_j &\leq u_j \end{aligned}$$

'https://www.youtube.com/watch?v=YpLzSQPrgSct=649s'

QUBO for Portfolio Optimization

Objective: Minimize portfolio risk under return and budget constraints.

Binary variable $x_i = 1$ if asset i is selected, 0 otherwise.

QUBO Form:

$$\min \left(\lambda_0 \cdot x^\top \Sigma x + \lambda_1 \left(\sum_{i=1}^{N} x_i - n \right)^2 + \lambda_2 \left(\mu^\top x - R^* \right)^2 \right)$$

- $x \in \{0, 1\}^N$: decision vector
- Σ: covariance (risk) matrix
- μ: expected return vector
- n: number of assets to be selected
- R^*: minimum return threshold
- $\lambda_0, \lambda_1, \lambda_2$: penalty weights for tuning

[Phillipson and Bhatia, 2020]

Formulating a QUBO Model: A High-Level Overview

QUBO Definition:

$$\min_{x \in \{0,1\}^n} x^\top Q x$$

- x: Binary decision vector
- Q: Symmetric matrix encoding the objective function and constraints

Formulation Steps:

1. **Identify Decision Variables:** Define binary variables representing problem decisions.
2. **Construct Objective Function:** Express the goal (e.g., cost, profit) as a quadratic function of binary variables.
3. **Incorporate Constraints:** Transform constraints into penalty terms and add them to the objective function.
4. **Assemble Q Matrix:** Combine coefficients from the objective and penalty terms into a symmetric matrix Q.

[Glover et al., 2018]

Common Penalty Transformations:

- **Equality Constraint ($x + y = 1$):** Add penalty term $P(1 - x - y + 2xy)$
- **Inequality Constraint ($x + y \leq 1$):** Add penalty term $P(xy)$

Applications:

- Portfolio Optimization
- Graph Problems (e.g., Max-Cut, Vertex Cover)
- Machine Learning Model Training

[Glover et al., 2018]

From QUBO to Hamiltonian

Goal: Find Hamiltonian operator H_C that encodes cost function $C(x)$

$$H_C|x\rangle = C(x)|x\rangle$$

QUBO cost function

$$C(x) = \sum_{i,j=1}^{n} x_i Q_{ij} x_j + \sum_{i=1}^{n} c_i x_i$$

$\longrightarrow$

Hamiltonian operator

$$H_C = \sum_{i,j=1}^{n} \frac{1}{4} Q_{ij} Z_i Z_j - \sum_{i=1}^{n} \frac{1}{2} \left(c_i + \sum_{j=1}^{n} Q_{ij} \right) Z_i + \left(\sum_{i,j=1}^{n} \frac{Q_{ij}}{4} + \sum_{i=1}^{n} \frac{c_i}{2} \right)$$

'https://www.youtube.com/watch?v=YpLzSQPrgSct=649s'

Time Evolution of Hamiltonians

Schrödinger Equation

Time evolution of a quantum system with Hamiltonian H

$$H|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle$$

For time-independent H: $$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle$$

Adiabatic Theorem

If the Hamiltonian of a quantum system in its ground state is perturbed slowly enough, the system remains in its ground state.

'https://www.youtube.com/watch?v=YpLzSQPrgSct=649s'

Quantum Annealing: Fundamentals

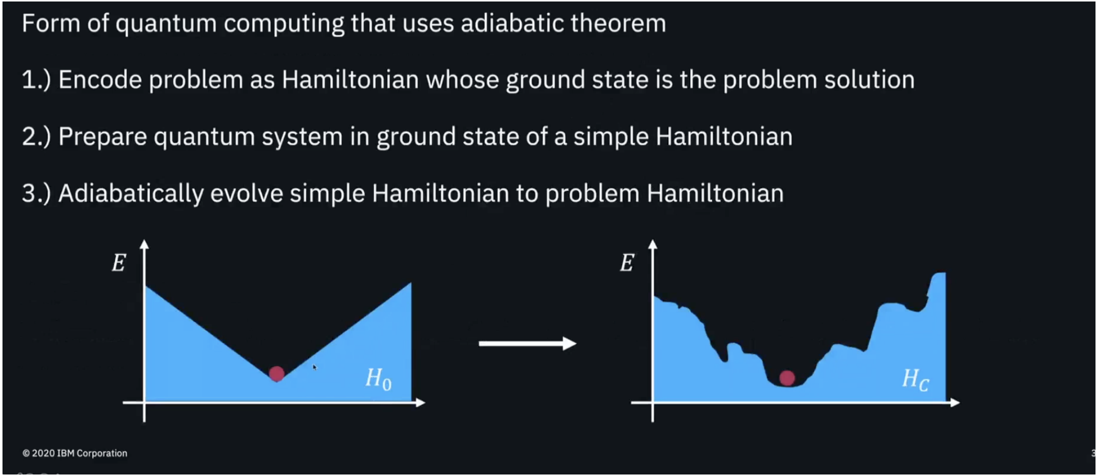
- **Definition**: Quantum Annealing (QA) is an optimization technique that utilizes quantum fluctuations to find the global minimum of a problem's energy landscape.
- **Process**:
  - Initialize the system in the ground state of a simple Hamiltonian H_0.
  - Slowly evolve to the problem Hamiltonian H_P:

$$H(t) = (1 - s(t))H_0 + s(t)H_P, \quad s(0) = 0, \quad s(T) = 1$$

  - Maintain adiabatic evolution to stay in the ground state.
- **Applications**: Suitable for solving combinatorial optimization problems like the traveling salesman problem, scheduling, and portfolio optimization.

[Rajak et al., 2022]

Adiabatic Quantum Computing



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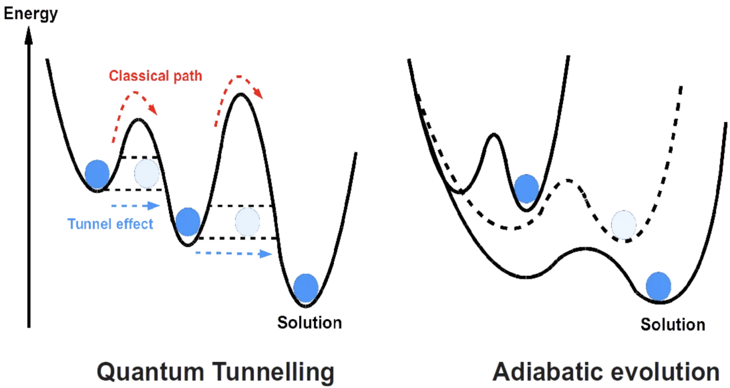
Challenges and Advancements in Quantum Annealing

- **Quantum Phase Transitions**:
  - Continuous transitions: Favorable for QA.
  - Discontinuous transitions: Can cause exponentially small energy gaps, hindering adiabatic evolution.
- **Kibble-Zurek Mechanism**:
  - Describes defect formation when crossing critical points at finite rates.
  - Important for understanding non-adiabatic effects in QA.
- **Environmental Coupling**:
  - Interaction with external environments can lead to decoherence.
  - Strategies include designing robust annealing schedules and incorporating error correction.
- **Speedup Strategies**:
  - Modify annealing paths to avoid problematic phase transitions.
  - Employ alternative driving Hamiltonians to maintain larger energy gaps.

[Rajak et al., 2022]



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Key Concepts in Quantum Annealing

Term	**Summary**
Quantum Tunneling	Mechanism: particles "teleport" through barriers
Quantum Annealing	Optimization strategy using tunneling and adiabatic evolution
Adiabatic Method	Slowly evolve the system so it stays in the ground state and finds the optimal solution

References I

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