Quantum Autoencoder in Particle Physics

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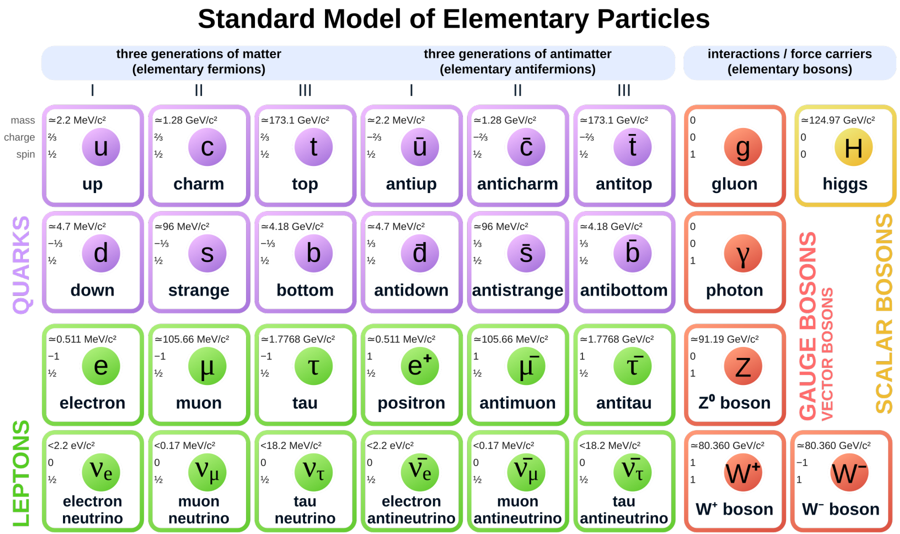
What is the Standard Model?



Limitations of the Standard Model & Need for New Physics

- **Dark Matter:** The Standard Model lacks a candidate particle for dark matter, which constitutes about 27% of the universe's energy.
- **Neutrino Masses:** Neutrinos have mass, contrary to the Standard Model's original prediction of massless neutrinos.
- **Matter-Antimatter Asymmetry:** The observed imbalance between matter and antimatter is not fully explained by current theories.
- **Gravity:** The Standard Model does not incorporate gravity, leaving a gap in our understanding of quantum and gravitational interactions.
- **Other Anomalies:** Various experimental and theoretical puzzles suggest phenomena that lie beyond the Standard Model.

These limitations motivate the exploration of Beyond Standard Model (BSM) theories for a more complete understanding of the universe.

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Definition of BSM and Its Significance

- **Definition:**
  - BSM (Beyond Standard Model) refers to theories and phenomena that extend the Standard Model of particle physics.
  - It encompasses new particles, forces, or interactions not accounted for in the current model.
- **Significance:**
  - Addresses fundamental issues such as dark matter, neutrino masses, and the matter-antimatter asymmetry.
  - Aims to provide a more complete and unified description of all known forces, including gravity.
  - Offers explanations for experimental anomalies that the Standard Model cannot fully describe.

Examples of BSM Phenomena

- **Heavy Higgs:**
  - Extensions of the Standard Model predict additional Higgs bosons.
  - Heavy Higgs particles would have different mass and decay patterns compared to the observed Higgs.
- **Gravitons:**
  - Hypothetical quantum particles that mediate the gravitational force.
  - Their discovery would provide evidence for a quantum theory of gravity.
- **Scalar Bosons:**
  - Particles with zero spin that may arise in various BSM models.
  - They can offer insights into phenomena like mass generation or symmetry breaking beyond the Standard Model.

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Intuition behind Autoencoders

Compress data from high dimension to **low dimension**
The lower dimension will capture the features in a more **compact way**
The lower dimension feature vector can be used to reconstruct the data

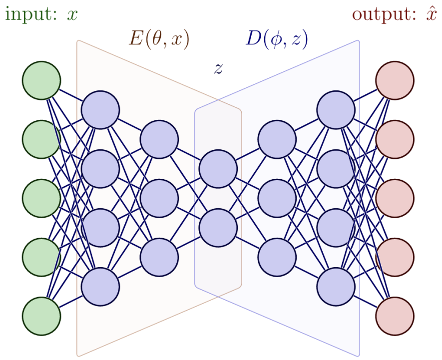

FIG. 1: An autoencoder neural network architecture consisting of five input features and a latent space of two. The encoder and decoder each consist of three hidden layers comprising of [4, 3, 2] neurons.

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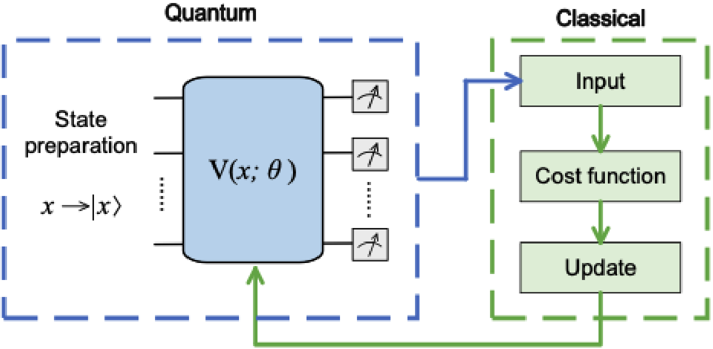
Anomaly Detection with Autoencoders

- Autoencoders are trained on normal data to minimize **reconstruction error.**
- **Anomalies**, being different from the norm, yield higher reconstruction errors.
- A preset **error threshold** is used: data points above this threshold are flagged as anomalies.

Variational Quantum Circuits



2

[2] Runqiu Shu et al. (2023). "Variational Quantum Circuits Enhanced Generative Adversarial Network". In: *arXiv preprint arXiv:2308.11062*.

Quantum Data Encoding

There are 3 Encoding Methods to encode classical data points into quantum data[3]

- **Basic Encoding :** Each binary string x_m is mapped to a computational basis state of N qubits. For instance, the binary string (1, 0, 1) would be mapped to the quantum state $|101\rangle$
- **Angle Encoding :**
  - Different from basis encoding, which is limited to binary data. Angle encoding can be used to encode real, floating-point numbers.
  - Data points are then used to rotate the state of a qubit around a specific axis on the Bloch sphere by an angle corresponding to the data. This is done by using rotation gates like Rx, Ry, and Rz, which rotate the qubit state around the X, Y, and Z axes, respectively.
- **Amplitude Encoding :** Represent classical data as quantum states by encoding the classical data into the amplitudes of those quantum states.

[3] Smaldone et al. 2024.

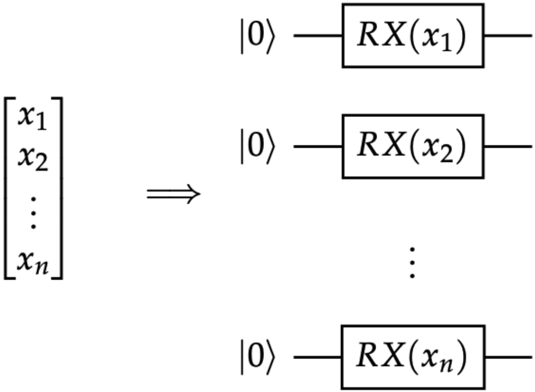


Figure: An example of quantum encoding. Individual elements of an input classical vector is used as the rotation angles of rotation Pauli X (RX) gates, creating a quantum state

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[4] Ju-Young Ryu, Eyuel Elala, and June-Koo Kevin Rhee (2023). "Quantum Graph Neural Network Models for Materials Search". In: *arXiv preprint arXiv:2308.11759*.

Quantum Auto Encoder

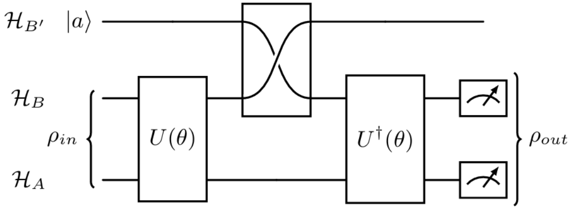

FIG. 2: A general schematic of the quantum autoencoder. Input states, ρ_{in}, are derived from a feature map and then processed by the unitary ansatze $U(\theta)$, $U^\dagger(\theta)$. The Hilbert spaces $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H}_{B'}$ are the latent space, the trash space, and the reference space, respectively.

[5]

[5] Callum Duffy et al. (2024). "Unsupervised Beyond-Standard-Model Event Discovery at the LHC with a Novel Quantum Autoencoder". In: Preprint, dated July 12, 2024. arXiv: 2407.07961v1 [quant-ph].

Different Circuits

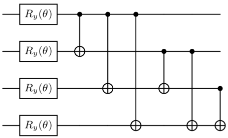

FIG. 4: The all-to-all entangling ansatz, which contains parameterised Pauli-Y rotation gates followed by CNOT gates that entangle all pairs of qubits to one another.

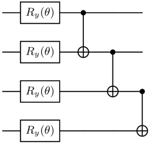

FIG. 5: The HEA, which contains parameterised Pauli-Y rotation gates followed by CNOT gates that entangle neighbouring pairs of qubits to respect the qubit connectivity of real quantum devices.

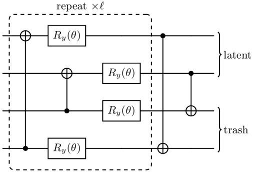

FIG. 6: The newly proposed ansatz. Initially CNOT gates link every qubit in the trash space to those in the latent space, follow by parameterised arbitrary Pauli-Y rotation gates. From here a second set of CNOT gates which act on every qubit in the latent space with target bits lying in the trash space. This ansatz is aware of which qubits belong to $\mathcal{H}_A$ and which to $\mathcal{H}_B$, adapting where CNOT gates act accordingly.

[6]

[6] Callum Duffy et al. (2024). "Unsupervised Beyond-Standard-Model Event Discovery at the LHC with a Novel Quantum Autoencoder". In: Preprint, dated July 12, 2024. arXiv: 2407.07961v1 [quant-ph].

Circuit Properties

- **Entanglement:**
  - Measured via the Meyer-Wallach entanglement metric.
  - Training the circuit reduces the overall (global) entanglement.
  - Lower entanglement suggests an optimal balance, enough to capture correlations but not so high as to scramble information.
- **Magic:**
  - Quantified using the 2-Rényi stabilizer entropy.
  - Indicates how “non-classical” a state is and its resistance to classical simulation.
  - Trained circuits show lower magic, implying they use quantum resources efficiently.

[7]

[7] Callum Duffy et al. (2024). “Unsupervised Beyond-Standard-Model Event Discovery at the LHC with a Novel Quantum Autoencoder”. In: Preprint, dated July 12, 2024. arXiv: 2407.07961v1 [quant-ph].

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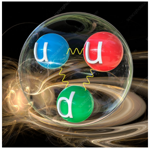

Figure: Proton

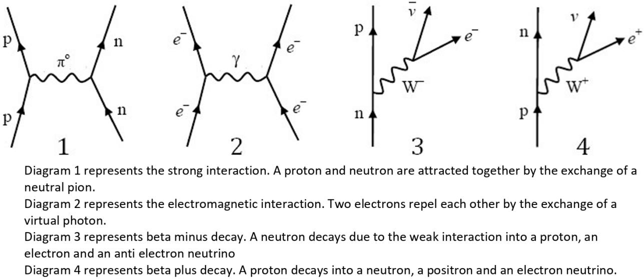

Figure: Feynman Collision Diagrams

Heavy Higgs Dataset: Feature Descriptions

- **Transverse Energy (E_T):** Energy measured perpendicular to the beam direction. It helps identify events with significant energy deposition away from the beam axis a common signature in high-energy collisions.
- **Lepton Transverse Momenta (p_{l1T} and p_{l2T}):** Momenta of the first and second leptons (e.g., electrons or muons) in the transverse plane. Leptons yield clean signals, crucial for reconstructing decay chains.
- **Angle Between Two Leptons (θ_l):** The angular separation between the two leptons, providing insight into the spatial distribution of the decay products.

Heavy Higgs Dataset: Feature Descriptions

- **Bottom Jet Transverse Momenta (p_{b1T} and p_{b2T}):** These capture the momenta of jets formed by bottom quarks from top quark decays in heavy Higgs events, essential for identifying decay products.
- **Angle Between Bottom Jets (θ_b):** Measures the spatial separation between jets from bottom quarks, aiding in differentiating signal events from background.
- **Lepton Angular Separation (ΔR_{l1}):** Defined using differences in azimuthal angle and rapidity, this feature indicates how isolated a lepton is from other nearby particles, helping to separate genuine signals from background noise.

Heavy Higgs Dataset feature map

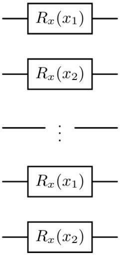

FIG. 7: A feature map for the Heavy Higgs dataset consisting solely of R_x rotation gates to embed features x.

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[8] Callum Duffy et al. (2024). "Unsupervised Beyond-Standard-Model Event Discovery at the LHC with a Novel Quantum Autoencoder". In: Preprint, dated July 12, 2024. arXiv: 2407.07961v1 [quant-ph].

Graviton/ZZZ Scalar Boson Dataset feature map

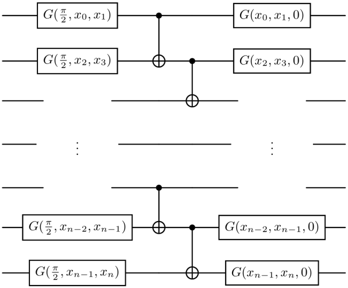

FIG. 8: A feature map for the graviton and scalar boson dataset consisting solely $G(\phi, \theta, \omega)$ rotation gates ($G(\phi, \theta, \omega) = R_z(\omega) R_y(\theta) R_z(\phi)$) and nearest neighbour entangling gates.

[9]

[9] Callum Duffy et al. (2024). "Unsupervised Beyond-Standard-Model Event Discovery at the LHC with a Novel Quantum Autoencoder". In: Preprint, dated July 12, 2024. arXiv: 2407.07961v1 [quant-ph].

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- **Data Preparation:**
  - Two main datasets: Heavy Higgs events and Graviton/ZZZ Scalar Boson events.
  - Kinematic features extracted from simulated proton-proton collisions.
  - QCD events serve as the in-distribution background; BSM events are the signals of interest.
- **Model Architectures:**
  - Classical Autoencoders (CAEs) and Quantum Autoencoders (QAEs) are implemented.
  - QAEs utilize a novel ansatz with fewer parameters compared to traditional CAE.

[10]

[10] Callum Duffy et al. (2024). "Unsupervised Beyond-Standard-Model Event Discovery at the LHC with a Novel Quantum Autoencoder". In: Preprint, dated July 12, 2024. arXiv: 2407.07961v1 [quant-ph].

Experimental Setup and Methodology

- **Training Procedure:**
  - Models are trained using the Adam optimizer.
  - A randomized grid search is employed for hyperparameter tuning.
  - Different input feature sets (e.g., 4, 6, and 8 features) are evaluated.
- **Benchmarking and Analysis:**
  - Performance is compared using ROC curves and AUC scores.
  - Analysis includes measuring circuit properties such as entanglement and magic.

[11]

[11] Callum Duffy et al. (2024). "Unsupervised Beyond-Standard-Model Event Discovery at the LHC with a Novel Quantum Autoencoder". In: Preprint, dated July 12, 2024. arXiv: 2407.07961v1 [quant-ph].

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Results

- **Superior Detection:**
  - QAEs outperform Classical Autoencoders in distinguishing BSM signals from QCD background.
  - Higher ROC/AUC scores, particularly as the number of input features increases.
- **Parameter Efficiency:**
  - New QAE ansatz achieves comparable or better performance with significantly fewer parameters than CAE.
- **Robust Performance Across Datasets:**
  - Consistent improvements observed for both the Heavy Higgs and Graviton/ZZZ Scalar Boson datasets.
- **Optimized Circuit Properties:**
  - Training reduces global entanglement and magic, leading to more efficient quantum circuits.

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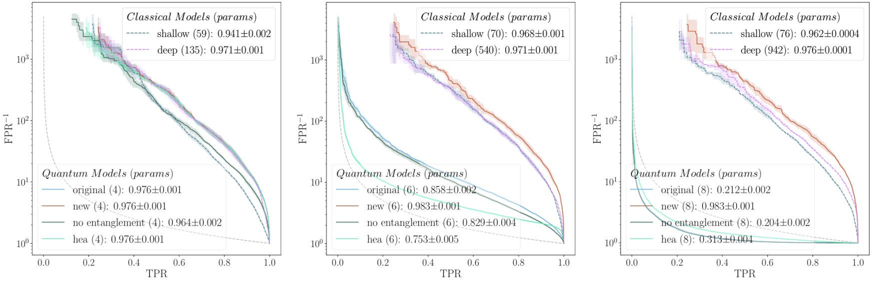
[12] Callum Duffy et al. (2024). "Unsupervised Beyond-Standard-Model Event Discovery at the LHC with a Novel Quantum Autoencoder". In: Preprint, dated July 12, 2024. arXiv: 2407.07961v1 [quant-ph].

Heavy Higgs



(a) 4 features (b) 6 features (c) 8 features

FIG. 9: Each subplot depicts the ROC curve for a collection of quantum and classical autoencoders on test data for a given set of input features. The grey dashed line represents a model performing random guessing. Panel (a) four input features with kinematic variables $\{E_T, p_T^{b_1}, p_T^{l_1}, p_T^{l_1}\}$ with five folds of test data. Panel (b) six input features with kinematic variables $\{E_T, p_T^{b_1}, p_T^{l_1}, p_T^{l_1}, \theta_l, p_T^{b_1}\}$, with 3 folds of test data. Panel (c) eight input features with kinematic variables $\{E_T, p_T^{b_1}, p_T^{l_1}, p_T^{l_1}, \theta_l, p_T^{b_1}, \theta_b, dR_{l1}\}$, with 3 folds of test data.

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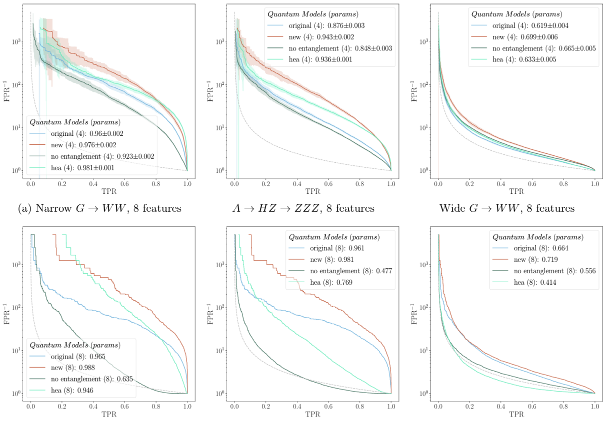
[13] Duffy et al. 2024.

Randall-Sundrum Gravitons and ZZZ Scalar Bosons



(a) Narrow $G \to WW$, 8 features

$A \to HZ \to ZZZ$, 8 features

Wide $G \to WW$, 8 features

(b) Narrow $G \to WW$, 16 features

$A \to HZ \to ZZZ$, 16 features

Wide $G \to WW$, 16 features

FIG. 10: Each subplot depicts the ROC curve for a collection of QAEs for various numbers of input features and BSM signals. Each column corresponds to identifying a different BSM signal, going from left to right we have the narrow graviton, scalar ZZZ boson and wide graviton respectively. The QAEs depicted here each contain the same feature map seen in Figure 8 but differing ansatz design. Row (a) eight input features with five folds of test data. Row (b) 16 input features with one fold of test data.

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[14] Duffy et al. 2024.

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Quantum Optimizers ?

- **Quantum Annealing :** non convex optimization

[15] Richard P Feynman (1982). "Simulating physics with computers". In: *International Journal of Theoretical Physics* 21.6/7, pp. 467–488.

Quantum Optimizers ?

- **Quantum Annealing :** non convex optimization

Can Quantum Computers really perform better when it comes to tasks related to natural sciences ?[15]

- **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.

[15] Richard P Feynman (1982). "Simulating physics with computers". In: *International Journal of Theoretical Physics* 21.6/7, pp. 467–488.

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