Quantum Machine Learning (QML) Classifiers

Submitted by
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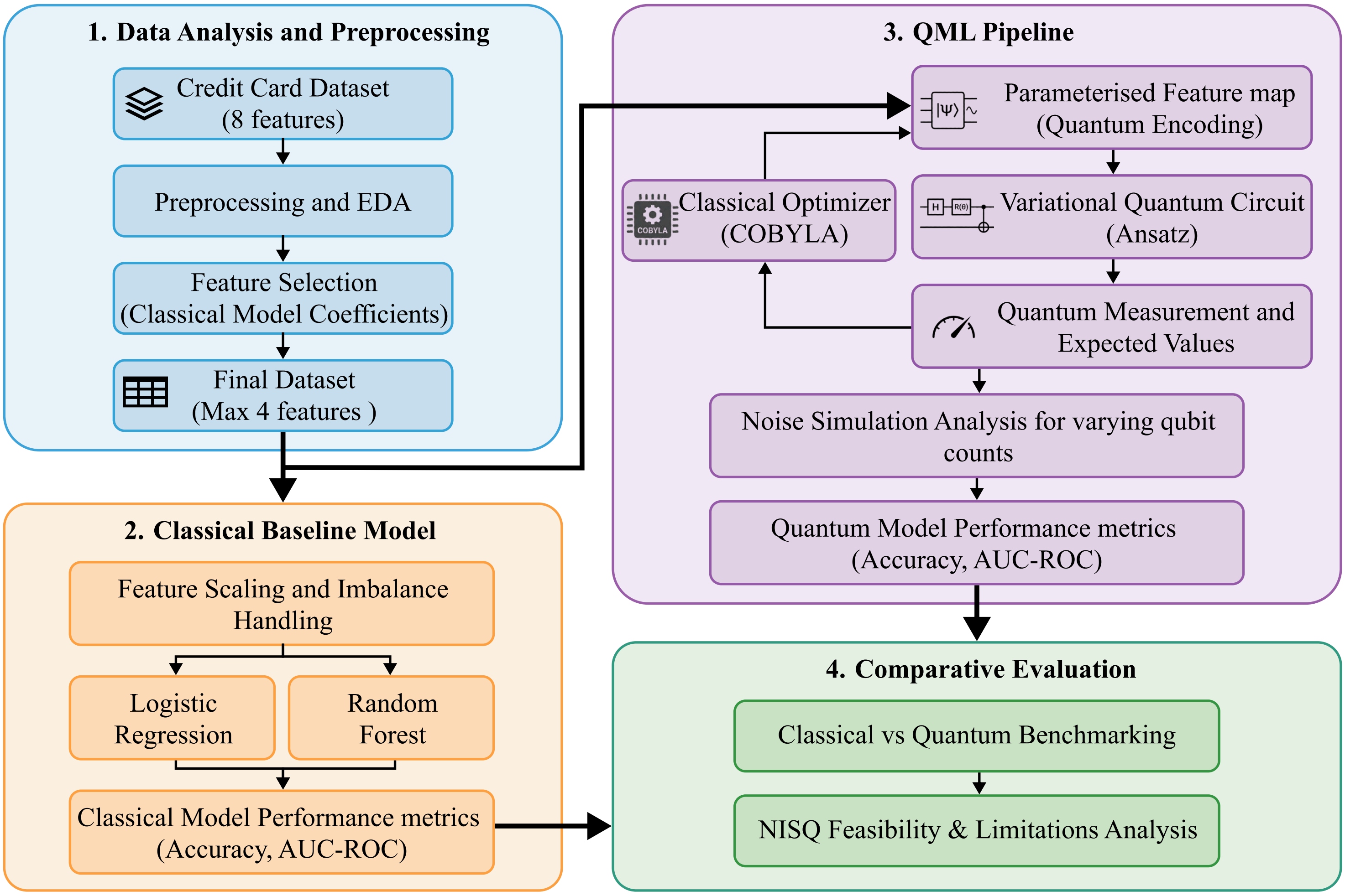
1. Objective

To design and benchmark a hybrid Quantum Machine Learning classifier for credit card fraud detection, evaluate its performance against classical models under realistic hardware constraints, and assess the practicality and limitations of QML on noisy, real-world data.

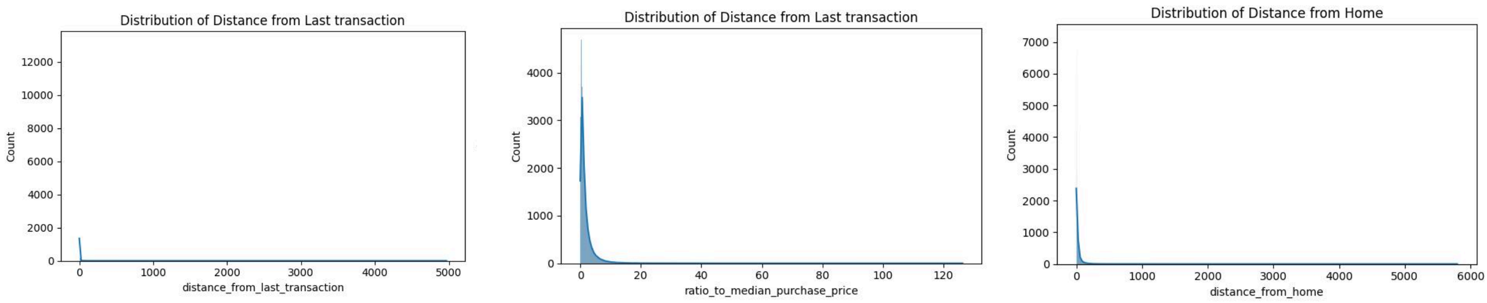
2. Overview



3. Data Analysis and Preprocessing

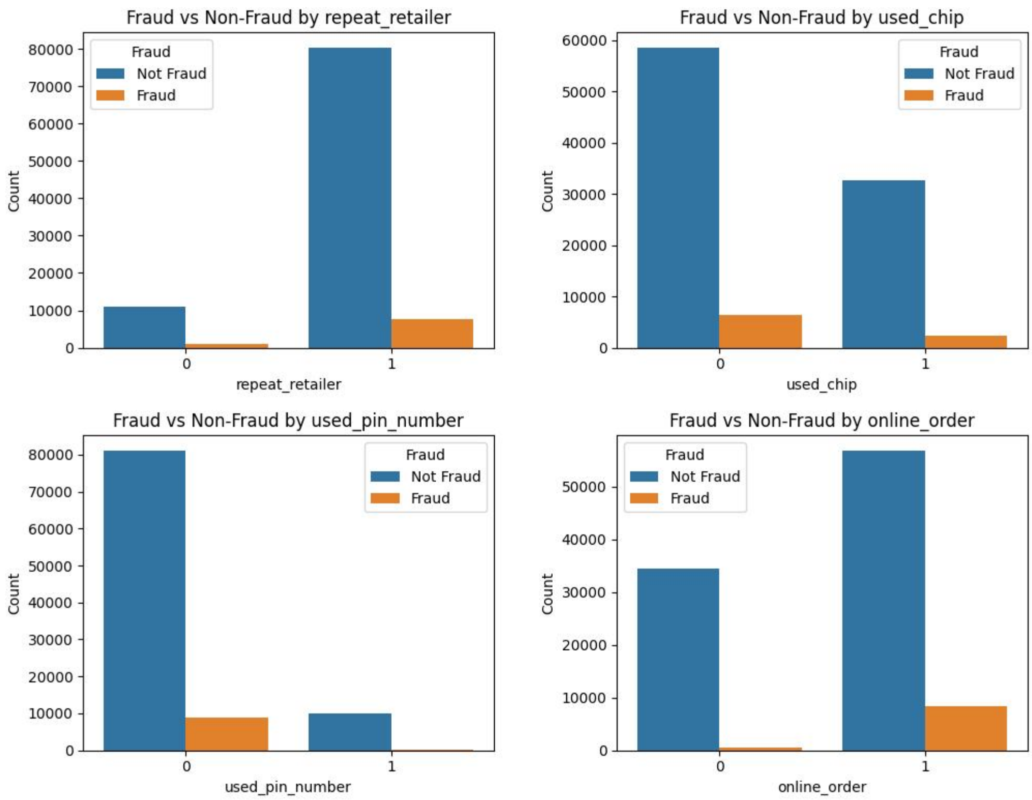
1. Dataset Overview

- The dataset consists of 100,000 credit card transaction records with 8 input features, representing a mix of transactional and behavioral attributes.
- The dataset contains no missing values, ensuring consistency and eliminating the need for imputation during preprocessing.
- The target variable is fraud, a binary label indicating whether a transaction is fraudulent (1) or legitimate (0).
- Continuous Features:
  distance_from_home, distance_from_last_transaction, ratio_to_median_purchase_price
  Binary / Categorical Features:
  repeat_retailer, used_chip, used_pin_number, online_order
- The dataset exhibits strong class imbalance, which is characteristic of real-world fraud detection scenarios.



2. Distribution of continuous variables

- Right-Skewed: All continuous features—distance_from_home, distance_from_last_transaction, and ratio_to_median_purchase_price—exhibited strong right-skewness with heavy tails and numerous extreme outliers. These characteristics indicate non-Gaussian behavior and the presence of anomalous transaction patterns commonly associated with fraud.
- Log Transformation: To address skewness and mitigate the influence of extreme values, log transformations were applied to all continuous features. This reduced distributional skew, compressed outliers, improved numerical stability, and enhanced class separability, making the features more suitable for both classical machine learning models and quantum classifiers.



3. Binary Feature vs Target Variable

- Repeat retailer behavior provides useful contextual information and contributes to distinguishing fraudulent from legitimate transactions.
- The absence of chip usage is a strong indicator of increased fraud risk, making this feature highly informative for classification.
- PIN usage is a strong negative indicator of fraud, and this feature plays a critical role in separating fraudulent and non-fraudulent transactions.
- Online transaction status is a strong behavioral signal and contributes meaningfully to fraud detection.

4. Feature Importance Analysis (Weight-Based Selection)

- Feature selection is critical in this project due to qubit limitations in near-term quantum hardware, making it infeasible to encode all original features.
- A Random Forest–based feature importance approach was chosen because it provides a model-driven, quantitative measure of feature relevance while capturing nonlinear and non-convex fraud patterns.
- Correlation analysis confirmed minimal redundancy among the top-ranked features, ensuring each selected feature contributes unique information rather than correlated noise.
- Based on the importance ranking, three reduced datasets were extracted using the top 2, top 3, and top 4 features, enabling controlled experimentation under varying feature dimensionality.

4. Quantum Circuit Design

1. Qubit Allocation and Input Mapping

- Each selected classical feature is mapped to one qubit, ensuring a direct and interpretable feature–qubit correspondence suitable for NISQ-era hardware.
- Quantum circuits with 2, 3, and 4 qubits were constructed using the top-2, top-3, and top-4 features, enabling controlled analysis of performance scaling with increasing feature dimensionality.
- This one-to-one mapping avoids complex encoding schemes, keeps circuit depth low, and supports stable training under limited quantum resources.

2. Feature Map (Classical-to-Quantum Encoding)

- Angle encoding is used to embed classical features into quantum states, where each normalized feature value directly controls the rotation angles of single-qubit RY and RZ gates.
- A rotation-only feature map is employed to keep the encoding stage shallow and noise-resilient, ensuring stable training on NISQ-era quantum devices.
- Feature interactions are not introduced during encoding and are instead learned later through the variational circuit, improving interpretability and trainability.

3. Variational Quantum Circuit (Ansatz)

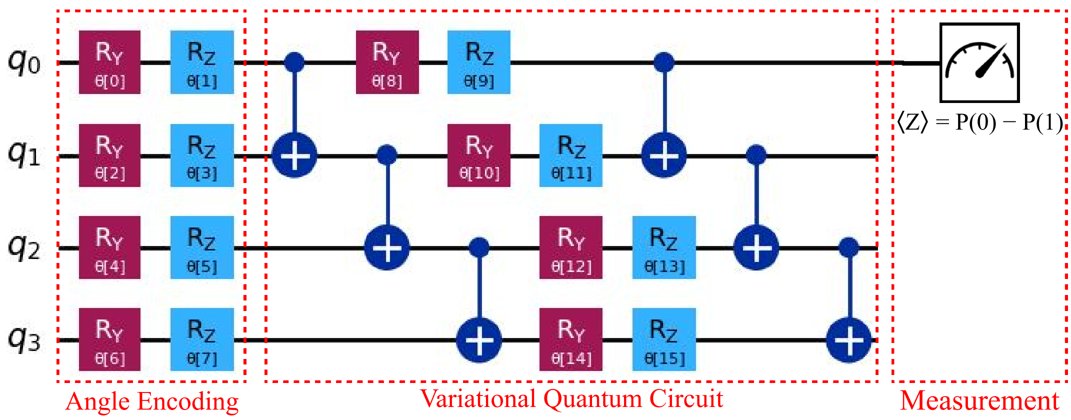
- A hardware-efficient variational ansatz is used, consisting of alternating layers of parameterized single-qubit rotation gates (RY and RZ) and entanglement gates (CNOT) applied across qubits.
- The rotation gates introduce trainable parameters, allowing the circuit to adapt during optimization, while the CNOT gates create entanglement, enabling the model to learn interactions between features.
- The circuit depth is intentionally kept shallow (1–2 layers) to balance expressive power with stable optimization and to remain compatible with Noisy Intermediate-Scale Quantum (NISQ) hardware.

4. Measurement and Label Extraction

- Only one designated output qubit is measured because entanglement in the variational circuit ensures that information from all input features and their interactions is encoded into the global quantum state and reflected in this qubit.
- The output qubit is measured over multiple circuit executions (shots) to estimate measurement probabilities, which are used to compute a stable expectation value rather than relying on a single noisy measurement.
- Measurement is performed using the Pauli-Z observable, which distinguishes between $|0\rangle$ and $|1\rangle$ states and produces a continuous output given by $\langle Z\rangle = P(0) - P(1)$, with values in the range $[-1, +1]$.
- A fixed decision threshold is applied during classical post-processing to convert this continuous output into a binary label:
  $\langle Z\rangle \geq 0 \rightarrow$ Class 0 (non-fraud),
  $\langle Z\rangle < 0 \rightarrow$ Class 1 (fraud).

5. Optimization

- A hybrid quantum–classical optimization loop is used, where the quantum circuit produces model outputs and a classical optimizer updates the trainable circuit parameters.
- The COBYLA optimizer is employed to minimize the loss computed from the Pauli-Z expectation value by iteratively adjusting the variational circuit parameters.
- COBYLA is chosen because it is gradient-free, robust to noise, and effective for low-dimensional parameter spaces, making it suitable for NISQ-era quantum models.
- The combination of a shallow variational circuit and COBYLA optimization ensures stable convergence and helps mitigate training issues such as barren plateaus under limited quantum resources.



5. Training Pipeline

1. **Classical Baseline Model Training**
- Prior to training classical models, all numerical features were scaled using StandardScaler to ensure consistent feature ranges and stable model training.
- Model-based feature importance (weight-based selection) was used to identify the most informative features. In particular, feature importance scores from the Random Forest classifier were leveraged to extract the top-ranked features for subsequent experiments.
- Two classical models were trained:
  - Logistic Regression, serving as a linear baseline model
  - Random Forest, capable of capturing non-linear and non-convex patterns
- Both models were trained and evaluated using the same train–test split and evaluation metrics as the quantum models to ensure fair benchmarking.
- Empirical results showed that Random Forest consistently outperformed Logistic Regression, indicating the presence of strong non-linear relationships in the dataset and motivating the use of expressive quantum models for comparison.

2. **Quantum Circuit Model Training**
- The quantum model was trained using three reduced datasets containing the top 2, top 3, and top 4 features, corresponding to 2-, 3-, and 4-qubit circuits, respectively.
- For quantum model training, a reduced subset of the training data was used to manage simulation cost, while classical models were trained on the full training set.
- For each dataset configuration:
  - Classical features were encoded into quantum states using angle encoding.
  - A Variational Quantum Classifier (VQC) was trained using a hybrid quantum–classical loop.
  - Circuit parameters were optimized using the COBYLA optimizer until convergence.
- This staged training enables analysis of model performance as a function of feature dimensionality and qubit count.

3. **Noise Simulation Analysis**
- After training the quantum model on an ideal (noise-free) simulator, the learned circuit parameters were reused without retraining and evaluated under noisy quantum simulations. This isolates the effect of noise from the learning process itself.
- Realistic noise models were introduced to emulate NISQ hardware behavior, including gate imperfections and measurement errors. This allows the quantum classifier to be tested under conditions closer to real quantum devices.
- The impact of noise was analyzed across different qubit configurations (2, 3, and 4 qubits) to study how increasing circuit size affects robustness. As the number of qubits grows, circuits become more susceptible to accumulated noise.
- Model performance under noisy settings was compared with ideal results to quantify performance degradation, providing insights into the trade-off between circuit expressivity and noise sensitivity.
- This analysis helps determine whether the proposed quantum model remains practically usable under realistic hardware constraints rather than only performing well in ideal simulations.

6. Comparative Analysis

1. **Classical vs Quantum Model Performance**
- Across all qubit configurations (2, 3, and 4 qubits), classical models consistently outperform QML models in both accuracy and AUC-ROC.
- Classical classifiers achieve high accuracy (above 0.90) across all feature settings, with AUC-ROC values reaching up to 0.96, demonstrating strong performance on structured tabular data.
- Ideal QML models show lower performance, with accuracy values in the range of 0.49–0.55 and AUC-ROC values around 0.52–0.55.
- This performance gap is influenced by NISQ hardware constraints, such as gate errors, short coherence times, shallow circuits, and increasing optimization difficulty as circuit size grows.
- Additionally, quantum models were trained on a reduced subset of the training data, limiting exposure to data variability and further contributing to lower predictive performance compared to classical models..

Number of Qubits	Model	Accuracy	AUC_ROC
2 Qubits	Classical	0.9020	0.9057
	QML(Ideal VQC)	0.5407	0.5267
	QML(Noisy VQC)	0.4667	0.4911
3 Qubits	Classical	0.9398	0.9372
	QML(Ideal VQC)	0.5492	0.5492
	QML(Noisy VQC)	0.5000	0.8482
4 Qubits	Classical	0.9543	0.9605
	QML(Ideal VQC)	0.4978	0.5099
	QML(Noisy VQC)	0.4333	0.6071

2. Effect of Increasing Qubit Count on QML Performance

Increasing the number of qubits from 2 to 3 leads to a modest improvement in QML accuracy and AUC, suggesting that adding informative features increases the expressive capacity of the quantum model. However, moving from 3 to 4 qubits does not result in further gains, instead, a slight performance drop is observed.
This behavior reflects a fundamental trade-off in near-term QML systems:

- Additional qubits increase the representational space,
- But also introduce more parameters, greater sensitivity to noise, and higher optimization difficulty.

As a result, 3 qubits appear to offer the best balance between expressivity and trainability in the ideal simulation setting.

3. Impact of Noise on Quantum Model Performance

- Noise simulation leads to a consistent drop in accuracy across all qubit configurations, indicating that quantum classifiers are highly sensitive to hardware noise.
- The degradation in accuracy becomes more severe as the number of qubits increases, due to accumulated gate errors, decoherence, and longer effective circuit depth.
- Under noisy conditions, AUC-ROC does not always decrease in the same proportion as accuracy.
- In the 3- and 4-qubit configurations, the noisy QML models show higher AUC values compared to ideal QML, even though overall accuracy is lower.
- This behavior suggests that noise affects absolute class predictions more strongly than relative ranking of samples, which AUC-ROC measures.
- As a result, AUC-ROC remains informative under noise, while accuracy is more sensitive to prediction instability.

4. Noise Robustness Across Qubit Configurations

Among the tested configurations:

- 2-qubit models show the least expressive power and moderate sensitivity to noise.
- 3-qubit models demonstrate the highest robustness, achieving the best noisy AUC while maintaining stable accuracy.
- 4-qubit models suffer the most from noise, reflecting increased circuit complexity and error accumulation.

These observations indicate that moderate qubit counts may be more practical for near-term quantum devices, as they offer a better balance between information capacity and noise resilience.

Quantum Neural Network

1. Overview of Quantum Neural Networks

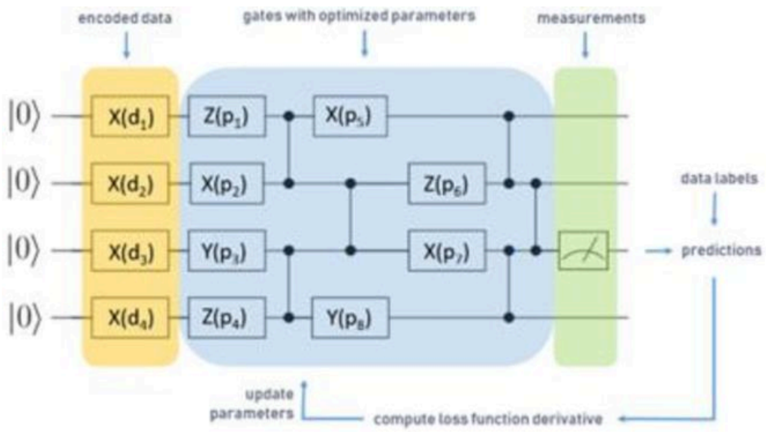
- Quantum Neural Networks (QNNs) are a class of hybrid quantum–classical models that extend the concept of classical neural networks into the quantum domain. Similar to neural networks, QNNs consist of trainable parameters, but these parameters are embedded within quantum circuits rather than classical weight matrices. Learning in QNNs is achieved by optimizing parameterized quantum gates using classical optimization algorithms.
- Unlike classical neural networks that rely on matrix multiplications and activation functions, QNNs exploit quantum superposition, entanglement, and interference to represent and process information in a high-dimensional Hilbert space. This makes QNNs particularly suitable for modeling non-linear and non-convex decision boundaries, which are common in real-world classification problems.

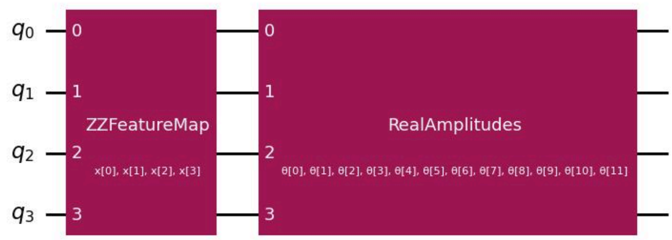
2. QNN Architecture

In this project, a Quantum Neural Network was implemented using a parameterized quantum circuit trained in a supervised learning setting. The QNN architecture consists of:

- Input Encoding Layer
  Classical features are embedded into quantum states using angle encoding, where normalized input values control single-qubit rotation gates.
- Trainable Quantum Layers
  Multiple layers of parameterized rotation gates and entangling gates (CNOT) are used. These layers act as the quantum analogue of hidden layers in classical neural networks.
- Measurement and Output Layer
  The output of the QNN is obtained by measuring the Pauli-Z expectation value of a designated output qubit. This continuous value is mapped to a class label using thresholding.

The QNN parameters are optimized using a classical optimizer, forming a hybrid training loop similar to classical neural network training.





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3. Dataset and Training Procedure

To demonstrate the working of the QNN, the same credit card fraud classification dataset used for earlier QML experiments was employed. This ensures consistency and enables direct comparison.

- The dataset was preprocessed using feature scaling and dimensionality reduction, ensuring compatibility with limited qubit resources.
- The QNN was trained using a noise-free quantum simulator to learn optimal circuit parameters.
- Training followed a supervised learning approach, minimizing a classical loss function computed from quantum measurement outputs.

4. Results

Number of qubits	Accuracy	AUC-ROC
4 qubits	0.05535	0.5405
3 qubits	0.05755	0.5420
2 qubits	0.06250	0.5167

1. Quantum Neural Network (QNN) Results and Analysis
  - The QNN achieves very low classification accuracy across all qubit configurations, indicating difficulty in producing reliable hard class predictions for the fraud detection task.
  - Despite low accuracy, the AUC values remain slightly above 0.5, suggesting that the QNN captures weak discriminative patterns and is able to rank fraudulent and non-fraudulent transactions better than random guessing.
  - Increasing the number of qubits from 2 to 4 does not significantly improve performance, as higher-dimensional QNNs introduce more complex optimization landscapes and are more susceptible to barren plateaus under limited training iterations.
  - The strong class imbalance in the dataset further impacts QNN performance, as the model optimizes a continuous expectation value rather than a class-specific loss, leading to poor threshold-based classification.
  - Overall, the results indicate that while QNNs demonstrate theoretical expressive power, their trainability and robustness remain limited for practical classification tasks on NISQ-era hardware.
2. Comparison Between VQC and QNN
  - The VQC consistently outperforms the QNN in both accuracy and AUC, demonstrating more effective learning of class boundaries in the fraud detection task.
  - Unlike the QNN, which outputs a single expectation value, the VQC is explicitly designed for classification, enabling more stable decision boundary learning and better translation of quantum measurements into class predictions.
  - The simpler and more structured architecture of the VQC makes it easier to optimize using gradient-free methods such as COBYLA, whereas the QNN's deeper parameterization increases sensitivity to optimization instability.
  - VQC performance is strongest with fewer qubits, indicating that compact variational models generalize better under NISQ constraints, while QNN performance degrades or stagnates as circuit complexity increases.
  - These results highlight that, under current hardware and simulation limitations, VQC models are more practical and robust than QNNs, while QNNs remain primarily exploratory models for future fault-tolerant quantum systems.

7. Conclusion

- A complete hybrid quantum–classical benchmarking pipeline was implemented, covering data preprocessing, feature selection, classical baselines, Variational Quantum Classifiers (VQC), Quantum Neural Networks (QNN), and noise-aware evaluation.
- Classical models, particularly Random Forest, consistently outperformed both VQC and QNN models across all feature and qubit configurations, reflecting the maturity and robustness of classical machine learning for structured fraud detection data.
- The VQC models demonstrated stable learning behavior but showed limited expressive capacity under NISQ constraints, especially as circuit size increased.
- The Quantum Neural Network (QNN) implementation successfully learned meaningful patterns and exhibited performance comparable to VQC, validating its ability to function as a quantum analogue of classical neural networks.
- Increasing the number of qubits did not guarantee performance improvement for either VQC or QNN models, highlighting the trade-off between expressivity, optimization difficulty, and noise sensitivity.
- Noise simulation analysis revealed significant performance degradation in quantum models, with deeper and wider circuits being more vulnerable to accumulated hardware noise.
- Despite lower accuracy, quantum models sometimes retained useful ranking information, as reflected by relatively stable AUC-ROC values under noisy conditions.
- Overall, the results indicate that current QML and QNN approaches are not yet competitive with strong classical baselines, but they provide valuable insights into model design, scalability, and robustness.