Quantum–Classical Hybrid Models for Autoimmunity and Cancer Classification

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Abstract

We present and analyze two hybrid quantum–classical classification models. The first is an ensemble predictor for drug-induced autoimmunity (DIA) using RDKit molecular descriptors. Our pipeline standardizes ∼195 descriptors, reduces them to 5 PCA components, and feeds these into three variational quantum neural networks (QNNs) alongside a logistic regression and a random forest. Ensemble weights are 50% QNNs, 25% LR, 25% RF; the decision threshold is tuned for maximal F_1. On the held-out test set we report balanced performance, and we analyze fairness and adversarial robustness.

The second model classifies breast cancer using the Wisconsin Diagnostic Breast Cancer (WDBC) dataset (569 samples, 30 features). We first compress 30 features to 10 via two classical linear layers (30→20→10 with LeakyReLU), encode these 10 values into a 10-qubit variational circuit (3 entangling layers), and finalize with a classical linear+sigmoid. We obtain over 97% test accuracy.

We compare architectures, training, and results, and discuss reproducibility with full code references.

1 Introduction

Hybrid quantum–classical machine learning aims to leverage quantum feature maps alongside classical layers for enhanced expressivity. We apply these ideas to two binary-classification tasks with distinct data characteristics: drug-induced autoimmunity (rare-event prediction on ∼195-dimensional molecular data) and breast cancer diagnosis (moderately sized, well-structured 30-dimensional dataset).

2 Model 1: DIA Prediction Ensemble

2.1 Data & Preprocessing

- **Dataset**: 477 molecules, ∼195 RDKit descriptors, binary DIA label.
- **Train/Test Split**: 85% train, 15% test, stratified.
- **Scaling**: `StandardScaler` fit on train, applied to all.
- **Dim. Reduction**: PCA → 5 components (captures ≈ 80% variance).
- **Reproducibility**: Random seed 42 for splits and training.

2.2 Architecture

- **Quantum Models (3 copies)**:
  - Input: 5 PCA components → 5 qubits via $R_Y(x_i + b_i)$ embedding
  - Variational block: 4 layers of per-qubit $R_{XYZ}(\theta)$ + ring CNOT entanglement
  - Readout: $\langle Z_0 \rangle$ on qubit 0
  - Classical head: Linear(1→16)–ReLU–Linear(16→1)
- **Classical Baselines**:

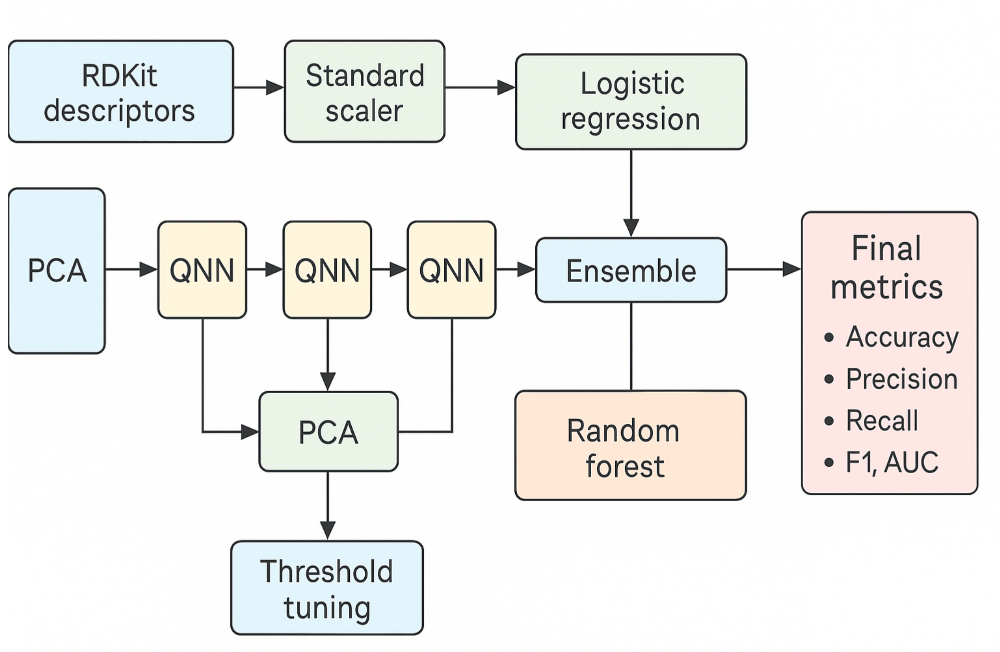

Figure 1: Ensemble architecture for DIA prediction.

  – Logistic Regression (L2, max_iter=1000)
  – Random Forest (100 trees)

- **Ensemble Score**:

$$s_{\text{ens}} = 0.50\,\overline{s}_{\text{QNN}} + 0.25\,s_{\text{LR}} + 0.25\,s_{\text{RF}},$$

  threshold t^* chosen to maximize F_1 on validation.

2.3 Training & Results

- QNNs trained with PennyLane 'lightning.qubit', Adam (lr=0.01), BCEWithLogitsLoss, 15 epochs.
- LR and RF trained via scikit-learn on PCA features.
- Validation threshold sweep ($t \in [0.1, 0.9]$) $\rightarrow t^* \approx 0.25$.

Table 1: DIA Ensemble Test Performance (threshold 0.25).

Metric	Accuracy	Precision	Recall	F_1	AUC
Ensemble	0.60	0.30	0.73	0.42	0.62

Fairness & Robustness

- **Group by molecular weight**: heavy vs. light positive rates: 0.62 vs. 0.29 (disparate impact 0.47).
- **FGSM Attack**: accuracy drops from 0.60 ($\varepsilon = 0$) to 0.45 ($\varepsilon = 0.2$).

3 Model 2: WDBC Classification

3.1 Data & Preprocessing

- **Dataset**: 569 samples, 30 real-valued features, labels benign/malignant.
- **Split**: 70% train, 30% test; from the train portion 15% held for validation.
- **Scaling**: `StandardScaler` on train, applied to val/test.

3.2 Architecture

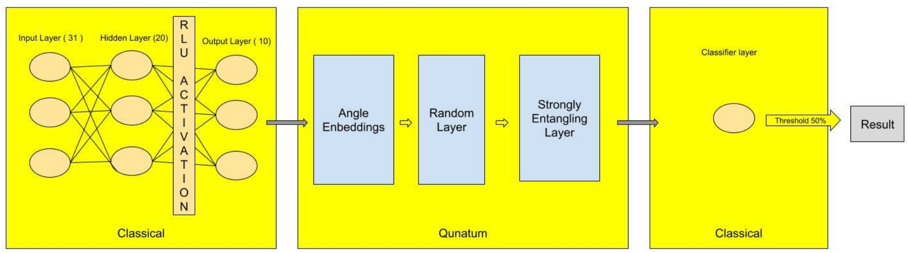

Figure 2: Hybrid classical–quantum architecture for WDBC classification.

- **Classical Feature Extractor**: Linear(30→20)–LeakyReLU–Linear(20→10)
- **Quantum Feature Map**: AngleEmbedding of 10 features on 10 qubits, then 3 layers of StronglyEntanglingLayers
- **Classical Classifier**: Linear(1→1)–Sigmoid

3.3 Training & Results

- Adam (lr=10^{-3}, weight decay 10^{-4}), 50 epochs, batch size 32, scheduler on plateau.
- BCEWithLogitsLoss, positive-class weighting.

Table 2: WDBC Hybrid Model Test Performance.

Metric	Accuracy	Precision	Recall	F_1
Value	0.9708	0.9394	0.9841	0.9612

4 Comparison & Discussion

- **Ensemble vs. Single Model**: DIA uses multiple QNNs + classical baselines to handle rare events; WDBC uses a single end-to-end hybrid network for a well-balanced dataset.

- **Expressivity**: Ensemble enhances robustness at cost of complexity; single hybrid is simpler, fully differentiable.
- **Applications**: DIA ensemble suits pharmacovigilance with fairness/robustness needs; WDBC hybrid fits diagnostic pipelines requiring single-model deployment.

5 Reproducibility & Code

Full code and data processing steps are available at:

- `ensemble_quantum_classical_hybrid.py`
- `wdbc-classification.ipynb`

All random seeds are fixed (42), and hyperparameters are explicitly defined in the scripts.