Simulating Quenched Quantum Feature Maps

Dataset and Target. In order to be able to simulate the protocol from the Kipu paper on Quenched Quantum Feature Maps [1], we used the reduced molecular toxicity dataset with 13 features ("Toxicity-13F.csv") from the UCI repository.[1] The binary label was mapped as `NonToxic`$\to 1$ and `Toxic`$\to 0$. Let $X \in \mathbb{R}^{N\times 13}$ denote features and $y \in \{0,1\}^N$ the labels.

Classical preprocessing. For each train/test split:

1. Imputes missing values in X_{train} with feature-wise median, then applies the same imputer to X_{test}.
2. Standardizes features with a *StandardScaler* (zero mean, unit variance) fit on X_{train} and applied to X_{test}.

This yields $(X^{\text{std}}_{\text{train}}, X^{\text{std}}_{\text{test}})$ used by both classical and quantum-enhanced pipelines.

Problem and driver Hamiltonians. With $n = 13$ qubits, the driver (transverse field) and problem (Ising) Hamiltonians are

$$H_D \;=\; -\sum_{i=1}^{n} \sigma_i^x, \qquad H_P(x) \;=\; \sum_{i=1}^{n} h_i \sigma_i^z + \sum_{1\le i<j\le n} J_{ij}\, \sigma_i^z \sigma_j^z.$$

For each sample $x \in \mathbb{R}^{13}$ from *standardized* data, local fields are set to the feature values, $h_i = x_i$. Couplings are the (training-set) Pearson correlations,

$$J_{ij} \;=\; \rho_{ij}, \quad \rho \;=\; \text{corrcoef}\big(X^{\text{std}}_{\text{train}}\big), \quad \text{diag}(\rho) = 0,$$

and *all* pairs (i, j) are included (no thresholding).

Quench schedule and analog evolution. The time-dependent Hamiltonian is

$$H(t) \;=\; A(t)\, H_D \;+\; B(t)\, H_P(x), \qquad t \in [0, \tau].$$

The notebook uses a fast "coherent" regime with total time $\tau = 30\,\text{ns}$ and mid-point integration. The scalar schedules are implemented as

$$s(t) \;=\; \sin^2\!\big(\tfrac{\pi}{2}\,\sin^2\!\big(\tfrac{\pi t}{2\tau}\big)\big), \qquad A(t) = A_0\,(1 - s(t)), \;\; B(t) = B_0\, s(t),$$

with amplitudes $A_0 = 2\pi \times 15\,\text{GHz}$ and $B_0 = 2\pi \times 11\,\text{GHz}$ (units carried as rad/s). The initial state is $|+\rangle^{\otimes n}$.

Digital simulation (Qiskit). The continuous evolution $U = \mathcal{T}\exp\{-i\int_0^\tau H(t)\,dt\}$ is approximated by first-order time slicing and second-order Suzuki–Trotter synthesis per slice:

- Number of time slices $m = \lceil 2000/\text{reps}\rceil$, with `reps`$= 64 \Rightarrow m = 32$ slices, step $\Delta t = \tau/m$.
- At each slice k, the Hamiltonian is frozen at the mid-point $t_{k+\frac{1}{2}} = (k + \frac{1}{2})\Delta t$; a `PauliEvolutionGate` with `SuzukiTrotter(order=2, reps=64)` is appended for time Δt.

Circuits are transpiled with preset pass manager (optimization level 0). Expectation values are obtained with Qiskit `EstimatorV2` on `AerSimulator(method="statevector")`, using the transpiled layout for observable remapping.

Quantum feature extraction. After evolution, the notebook measures *single-qubit* longitudinal observables (weight-1 Z operators):

$$\tilde{x}_i \;=\; \langle\psi_f(x)|\sigma_i^z|\psi_f(x)\rangle, \qquad i = 1, \ldots, n,$$

[1] `https://archive-beta.ics.uci.edu/dataset/728/toxicity-2/files?path=Toxicity-13F.csv`

i.e., $k_{\max} = 1$; higher-order Z-correlators are implemented but not used in this run. The quantum feature vector is $\tilde{x} \in \mathbb{R}^{13}$. For train/test matrices, the map is applied row-wise to $X^{\text{std}}_{\text{train}}$ and $X^{\text{std}}_{\text{test}}$.

Feature augmentation and classifier. Classical and quantum features are concatenated with unit scaling $\gamma_q = 1$:

$$X^{\text{aug}}_{\text{train}} = \left[X^{\text{std}}_{\text{train}} \mid \tilde{X}_{\text{train}}\right], \qquad X^{\text{aug}}_{\text{test}} = \left[X^{\text{std}}_{\text{test}} \mid \tilde{X}_{\text{test}}\right].$$

A `GradientBoostingClassifier` (scikit-learn, default hyperparameters, `random_state=42`) is trained on $X^{\text{aug}}_{\text{train}}$ and evaluated on $X^{\text{aug}}_{\text{test}}$. For the classical baseline, the same model is trained on standardized features only.

Cross-validation and metrics. We used `StratifiedKFold` with 5 splits, shuffling and `random_state=42`. For each fold it was reported AUC, overall F1, balanced accuracy, and per-class precision/recall. Aggregation is done by median over the 5 folds (printed at the end).

Summary of choices. $n = 13$ qubits; $h_i = x_i$ (standardized); $J_{ij} = \rho_{ij}$ from the training fold; fast quench with mid-point rule; $A_0 = 2\pi \times 15\,\text{GHz}$, $B_0 = 2\pi \times 11\,\text{GHz}$; $\tau = 30\,\text{ns}$; $m = 32$ slices; second-order Suzuki–Trotter with `reps`= 64 per slice; observables: weight-1 Z only; classifier: Gradient Boosting; CV: 5-fold stratified.

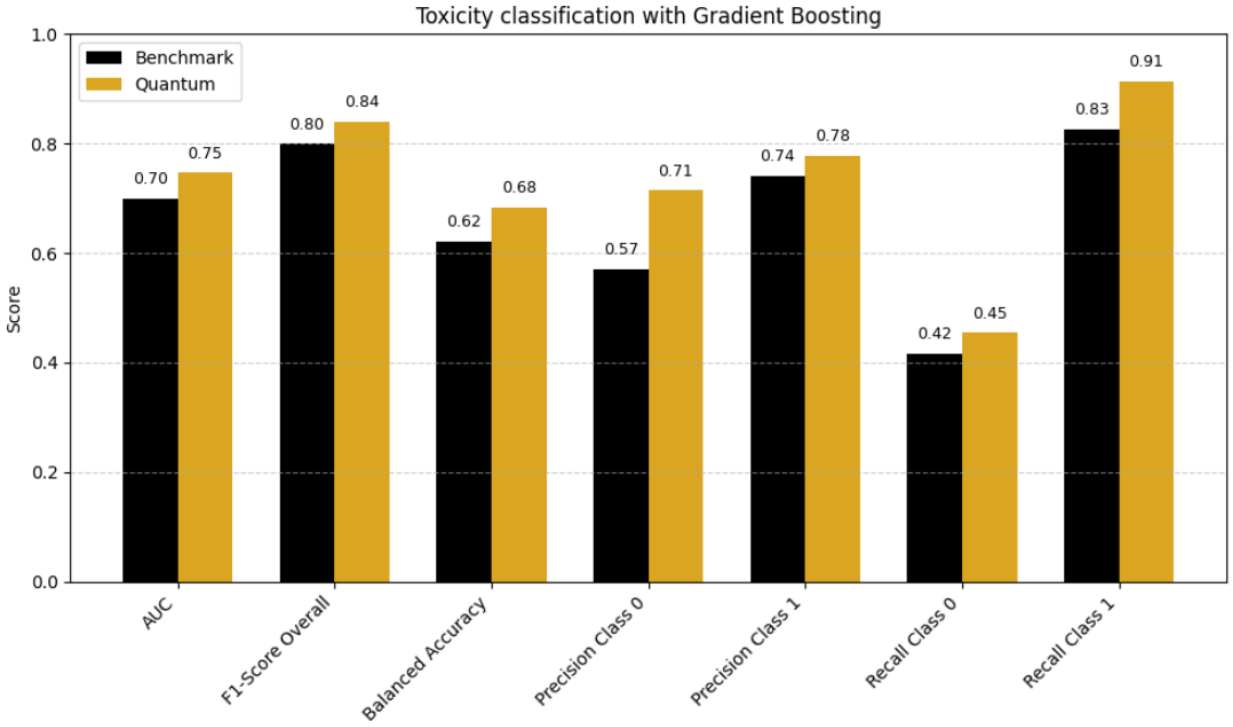

Figure 1: Toxicity classification with Gradient Boosting: benchmark vs. quantum-augmented features (5-fold mean).

References

[1] A. Simen, C. Flores-Garrigos, M. H. De Oliveira, G. D. Alvarado Barrios, J. F. R. Hernández, Q. Zhang, A. Gomez Cadavid, Y. Vives-Gilabert, J. D. Martín-Guerrero, E. Solano, N. N. Hegade, and A. Dalal, "Quenched Quantum Feature Maps," *arXiv:2508.20975*, 2025. Available at `https://arxiv.org/abs/2508.20975`.