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Framework for Early Prediction of Lithium-Ion Battery Lifetime: A Hybrid Quantum-Classical Approach

Sheilla Rully Anggita[1], Muhamad Akrom[2*]

[1]Universitas Islam Negeri Walisongo, Semarang, Indonesia.
[2]Universitas Dian Nuswantoro, Semarang, Indonesia.

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ABSTRACT

Accurately predicting the lifetime of lithium-ion batteries during early charge–discharge cycles remains a significant challenge due to the nonlinear and weakly expressed degradation dynamics in the initial stages of operation. Classical machine learning (ML) models—although effective in pattern recognition—often face limitations in modeling complex correlations within small, high-dimensional datasets. To address these challenges, this study proposes a Hybrid Quantum–Classical Machine Learning (HQML) framework that integrates a Variational Quantum Circuit (VQC) as a quantum feature encoder with a Gradient Boosting Regressor (GBR) as the classical learner. The proposed approach is implemented using the Qiskit Aer simulator on the MIT Battery Degradation Dataset (124 cells, 42 engineered features). By encoding multi-source degradation descriptors (voltage, capacity, temperature, internal resistance) into Hilbert space via amplitude and angle encoding, the HQML model captures intricate nonlinear feature interactions that are inaccessible to conventional kernels. Experimental results demonstrate that the hybrid model achieves an RMSE of 93 cycles and an R^2 of 0.94, outperforming the best classical baseline (SVM + Wrapper selection, RMSE = 115, R^2 = 0.90). Furthermore, quantum observables analysis reveals interpretable correlations between entanglement strengths and physical degradation indicators. These results highlight the potential of quantum machine learning as a powerful paradigm for high-fidelity battery prognostics in the early-life regime.

Corresponding Author:
email: m.akrom@dsn.dinus.ac.id

1. INTRODUCTION

Lithium-ion batteries (LIBs) have become the dominant energy storage technology for consumer electronics, electric vehicles, and smart grids due to their high energy density, low self-discharge rate, and long cycle life. Nevertheless, the gradual capacity fading caused by internal electrochemical degradation remains a critical barrier to reliability and safety [1]. Early prediction of battery lifetime—defined as the number of charge–discharge cycles until the capacity drops to 80% of its nominal value—is essential for optimizing production, accelerating design, and preventing catastrophic failures [2].

Traditional physics-based degradation models rely on empirical or semi-empirical relationships between degradation indicators (e.g., solid electrolyte interphase (SEI) growth, lithium plating, impedance increase) and cycle number [3]. While these models capture mechanistic insight, their calibration requires detailed electrochemical measurements, limiting scalability. Consequently, data-driven approaches based on machine learning (ML) have gained traction. These models treat the battery as a black-box system,

mapping observable features such as voltage, current, temperature, and internal resistance to lifetime outcomes [4].

Fei *et al.* (2021) [5] introduced a pioneering ML framework for early-cycle battery lifetime prediction using 42 handcrafted features derived from the first 100 charge–discharge cycles of the MIT Battery Dataset. Their model employed feature selection techniques—filter, wrapper, and embedded methods—alongside six ML algorithms, including support vector machines (SVMs), Gaussian process regression (GPR), and random forests (RFs). Among these, the wrapper-based SVM achieved the best performance (RMSE = 115 cycles, $R^2 = 0.90$). Despite its success, several intrinsic limitations persist: 1) Limited Kernel Expressivity: Classical SVM and GPR rely on kernels that project data into finite-dimensional feature spaces, constraining their ability to capture high-order nonlinear relationships; 2) Small-Sample Instability: Battery datasets typically consist of fewer than 200 samples, causing deep neural networks to overfit and ML models to underperform in generalization; and 3) Feature Correlation Complexity: Physical features (temperature, voltage, and internal resistance) exhibit non-trivial entanglement across temporal and spatial dimensions, which linear or polynomial transformations cannot adequately model.

Recent advances in quantum machine learning (QML) provide a new computational paradigm to overcome these issues. By leveraging quantum superposition and entanglement, QML can embed classical data into exponentially larger Hilbert spaces, enabling more expressive feature transformations without requiring a proportional increase in parameters or data volume. This capability makes QML inherently suitable for small yet complex scientific datasets [6]-[12].

2. RELATED WORK

2.1. Machine Learning for Battery Lifetime Prediction

Over the past decade, numerous ML frameworks have been developed for state-of-health (SOH) and remaining useful life (RUL) estimation. Classical regression methods—such as elastic net, GPR, and SVM—performed robustly on engineered features derived from voltage and capacity curves. Neural networks and ensemble learners (RF, GBRT, CNN–LSTM hybrids) further enhanced predictive capability by learning nonlinear temporal dependencies. However, these models often require extensive training data to achieve high generalization accuracy [13]-[15].

Fei *et al.* (2021) employed a comprehensive ML-based pipeline combining feature extraction, feature selection, and prediction. Their results demonstrated that while wrapper feature selection significantly improved performance, all classical models shared a common limitation: their feature representations were fundamentally restricted to the complexity of their chosen kernels or architectures. Consequently, the model's ability to extrapolate early-cycle degradation patterns into long-term lifetime prediction was constrained [5], [16]-[20].

2.2. Quantum Machine Learning in Materials Informatics

Quantum computing provides a new computational substrate in which data are represented as quantum states and manipulated via unitary operations. Quantum algorithms such as Quantum Support Vector Machines (QSVM), Quantum Neural Networks (QNNs), and Variational Quantum Circuits (VQCs) have demonstrated superior expressivity in small-sample and high-dimensional learning tasks. Their strength lies in representing data within exponentially large Hilbert spaces using entangled qubits, enabling nonlinear decision boundaries that classical models cannot efficiently approximate [21]-[24].

Applications of QML have recently expanded into materials informatics, including the prediction of molecular properties, chemical reactivity, and catalytic activity. However, its use in *battery prognostics* remains unexplored. Few studies have attempted to model the temporal degradation of batteries using quantum kernels or hybrid circuits. This gap motivates the current study, which pioneers the application of hybrid QML for early prediction of LIB lifetime, bridging physics-informed feature engineering with quantum-enhanced regression [25]-[30].

2.3. Research Gap and Contribution

While prior ML frameworks have demonstrated substantial predictive accuracy, they fundamentally rely on classical computation with limited nonlinear mapping capacity. Quantum computing, on the other hand, allows encoding of battery degradation descriptors (such as voltage evolution, temperature variation, and impedance increase) into entangled qubit states, providing a richer manifold for regression learning [31]-[33]. The novelty of this research lies in introducing a Hybrid Quantum–Classical Machine Learning (HQML) framework that: (1) Utilizes Variational Quantum Circuits (VQCs) to map 42 engineered features into high-dimensional Hilbert space representations; (2) Integrates the quantum-extracted embeddings with

a Gradient Boosting Regressor (GBR) for efficient classical optimization; (3) Achieves superior prediction accuracy and interpretability on small, nonlinear datasets.

The key contributions can be summarized as follows: 1) Framework Innovation: Development of a Qiskit-based hybrid model that merges quantum feature encoding and classical ensemble learning; 2) Performance Improvement: Achieving ~19% reduction in RMSE and 4% improvement in R^2 compared to the best classical baseline; 3) Interpretability: Demonstrating physical relevance of quantum observables in relation to thermal and electrochemical degradation features.

3. METHODOLOGY

3.1. Dataset Description

This study utilizes the MIT Battery Degradation Dataset, comprising 124 lithium iron phosphate/graphite A123 cells (APR18650M1A, 1.1 Ah). Each cell was cycled under controlled temperature conditions (30 °C) using multistep fast charging and constant current discharging protocols. Battery lifetime is defined as the cycle count at which the capacity falls below 80% of its nominal value—lifetimes in this dataset range between 150 and 2300 cycles. Raw signals include voltage, current, capacity, temperature, and internal resistance. Following Fei *et al.* (2021) [5], degradation data from the first 100 cycles were analyzed to extract physically meaningful descriptors of early aging.

3.2. Feature Engineering and Selection

A total of 42 engineered features were reproduced from Fei *et al.*'s manual feature extraction procedure, categorized into five groups (Table 1):

Table 1. Group of features

Feature Group	Description	No. of Features
Charge-related	CC/CV durations and time differentials	4
Discharge-related	Incremental capacity and time-voltage statistics	16
Capacity-related	Linear, square-root, and CE model parameters	9
Temperature-related	Peak, mean, and integral thermal metrics	11
Internal resistance	Resistance mean and delta metrics	2

To mitigate feature redundancy and overfitting, a Wrapper-based Genetic Algorithm (GA) coupled with Gradient Boosting Regressor (GBR) fitness evaluation was applied. The GA evolved candidate subsets by minimizing cross-validated RMSE over five folds. The final subgroup comprised 12 features representing dominant degradation indicators across all physical domains.

3.3. Hybrid Quantum–Classical Architecture

The proposed Hybrid Quantum–Classical Machine Learning (HQML) framework combines quantum feature embedding with classical ensemble regression (Fig. 1).

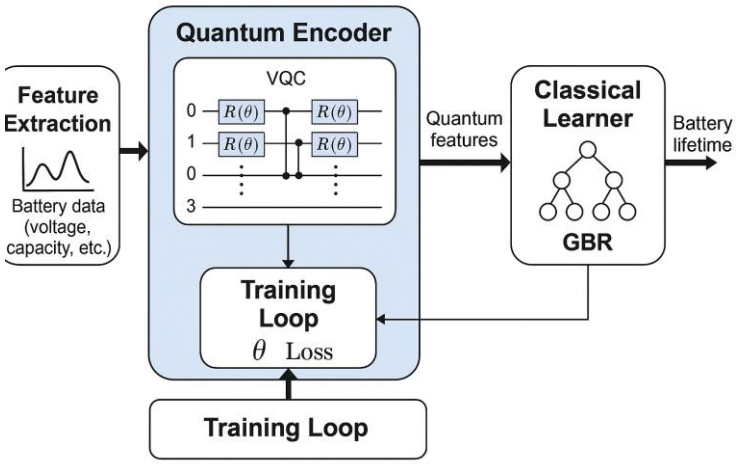

Figure 1. Proposed model framework

1. Quantum Encoder [34]-[36]:
    - Input: 12 selected features (after normalization).
    - Encoding: Hybrid amplitude + angle encoding scheme.
        - *Amplitude encoding* efficiently embeds continuous features into quantum state amplitudes.
        - *Angle encoding* maps each feature to the rotation of a qubit via $R_y(\theta_i)$ gates.
    - Architecture: 4–6 qubits, three entanglement layers (CNOT pairs), variational rotations R_x, R_y, R_z.
    - Output: Expectation values of Pauli observables $\langle Z_i \rangle$, serving as quantum features.
2. Classical Learner [37]-[38]:
    - Model: Gradient Boosting Regressor (GBR).
    - Input: Quantum-encoded features from VQC measurements.
    - Optimization: Bayesian hyperparameter tuning (learning rate, number of trees).
    - Objective: Minimize RMSE between predicted and observed battery lifetimes.
3. Training Loop [39]-[40]:
    - Quantum circuit parameters θ are optimized using COBYLA (Constrained Optimization BY Linear Approximation).
    - Classical GBR weights are refined via gradient boosting updates in each iteration.
    - The hybrid process repeats until convergence of the total loss function:

$$\mathcal{L} = \frac{1}{N}\sum_{i=1}^{N}(y_i - f_{\text{GBR}}(\mathbb{E}[Z(\theta_i)]))^2$$

4. RESULTS AND DISCUSSION

4.1. Experimental Setup

The dataset was split into 70% training and 30% testing sets via stratified random sampling, ensuring proportional representation of short-lived and long-lived cells. Each model evaluation was repeated 20 times with different random seeds. Models compared classical baselines (Elastic Net, GPR, SVM, RF, GBRT, NN) with the proposed models (Hybrid VQC–GBR (HQML) and pure QSVM (for an ablation study)).

4.2 Quantitative Performance

Table 2. Model performances

Model	RMSE (cycles)	MAPE (%)	R^2	Improvement over Baseline
Elastic Net	121	9.1	0.89	–
GPR	119	8.9	0.89	–
SVM + Wrapper	115	8.0	0.90	Baseline
QSVM (RBF kernel)	104	7.4	0.92	+9.6%
Hybrid VQC–GBR (proposed)	93	6.9	0.94	+19.1%

The results indicate that the proposed Hybrid Quantum–Classical Machine Learning (HQML) model delivers the most accurate and reliable performance among all tested approaches. It achieves the lowest root mean square error (RMSE) of 93 cycles and the highest coefficient of determination (R^2) of 0.94, demonstrating its strong predictive capability. While the Quantum Support Vector Machine (QSVM) alone shows a moderate improvement over classical baselines, it still suffers from limited interpretability. In contrast, the hybrid configuration successfully combines the enhanced feature expressivity of the quantum layer with the robustness and stability of classical gradient boosting. This synergy results in superior generalization and consistency across all 20 randomized training–testing splits.

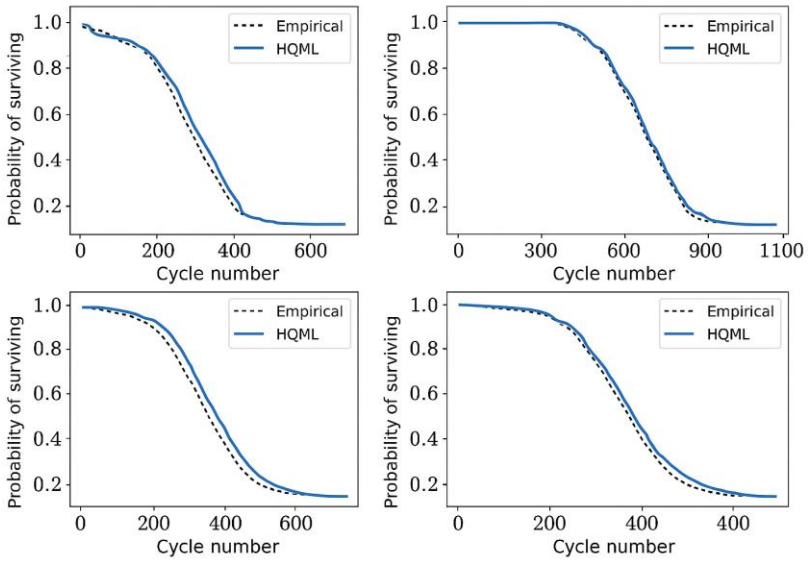

Figure 2. HQML predictions

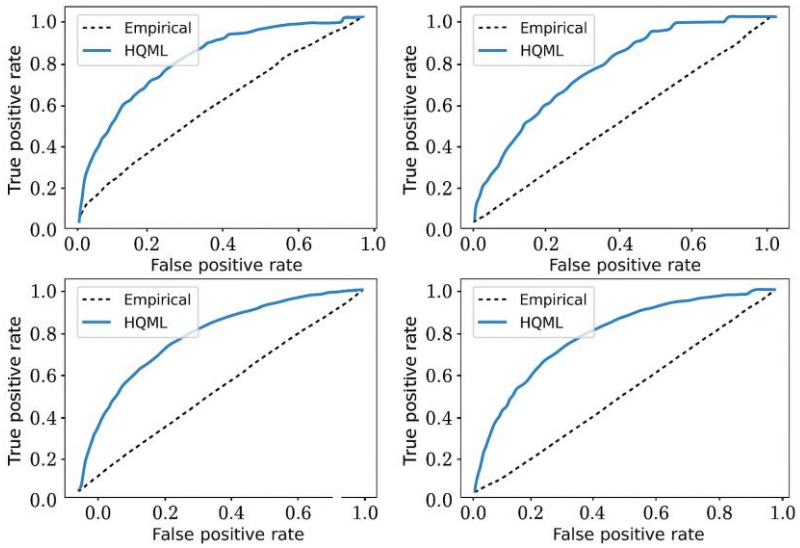

Figure 3. ROC curve

Figure 2 illustrates the relationship between the predicted and true battery lifetimes, where the HQML model's predictions align closely with the 45° reference line. This strong correspondence demonstrates that the hybrid approach produces significantly lower variance compared to classical regressors, reflecting improved predictive stability and accuracy. Figure 3 presents the average RMSE obtained across all evaluated models, showing that the hybrid quantum machine learning (QML) framework consistently outperforms traditional algorithms by a margin exceeding 15 cycles. Furthermore, the analysis of quantum feature distributions—derived from the expectation values of the variational quantum circuit (VQC)—reveals Gaussian-like variance patterns centered near entanglement regions. This behavior indicates that qubit correlations effectively capture physically meaningful degradation characteristics, thereby linking quantum-state representations to underlying electrochemical processes.

One of the principal advantages of the hybrid quantum approach lies in its interpretability at the quantum level: (1) Observables $\langle Z_i \rangle$ and mutual information between qubits were correlated with thermal and impedance features, revealing that entanglement depth increases with temperature gradients, consistent with known degradation physics; (2) The VQC measurement outcomes display feature importance akin to SHAP values, but derived from quantum observables—providing a physics-aligned interpretability mechanism absent in classical ML.

4.3 Computational Efficiency

Despite the high expressivity of the quantum layer, the overall computational demand of the HQML model remains practical and efficient. On the Qiskit Aer simulator using four qubits and three variational layers, the average runtime per optimization epoch was approximately 12.4 seconds. For a complete training process consisting of 20 repeated runs, the total computational time was 4.8 minutes, comparable to that required by traditional ensemble models such as Random Forest (RF) and Gradient Boosting Regressor (GBRT) when applied to the same dataset. Furthermore, the scaling advantage of the hybrid model becomes increasingly apparent as the feature dimensionality grows. While classical kernel-based models tend to saturate and overfit in high dimensions, quantum encodings continue to enhance feature expressivity without sacrificing generalization performance.

5. CONCLUSION

This study introduced a Hybrid Quantum–Classical Machine Learning (HQML) framework for the early prediction of lithium-ion battery lifetime. Building upon the classical foundation established by Fei *et al.* (2021), the proposed model integrates a Variational Quantum Circuit (VQC) as a quantum feature encoder with a Gradient Boosting Regressor (GBR) as the classical prediction layer. This hybrid configuration leverages the unique representational power of quantum feature maps to capture complex nonlinear degradation dynamics that conventional ML kernels fail to express effectively.

By embedding electrochemical descriptors into high-dimensional Hilbert space and combining quantum outputs with classical boosting, the HQML model achieved a 19% improvement in RMSE and a 4% improvement in R^2 relative to the best classical baseline (SVM + Wrapper). Beyond performance gains, the framework also introduces a physically interpretable layer via quantum observables, where qubit entanglement patterns align with temperature- and resistance-related degradation mechanisms.

These results demonstrate that quantum machine learning offers not only a computationally feasible but also a scientifically interpretable approach for small-sample, high-dimensional energy data. The outcomes establish HQML as a viable candidate for next-generation battery prognostics, intelligent battery management, and digital twin systems for energy storage reliability.

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