Evaluation of hybrid and standalone learning models for predicting lithium-ion battery capacity degradation

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ABSTRACT

The prediction of lithium-ion battery capacity degradation plays a vital role in ensuring safe and efficient operation in electric mobility and renewable energy applications. This paper evaluates standalone machine learning, deep learning, and hybrid models for battery capacity estimation. The evaluated ML models include random forest, gradient boosting, and extreme gradient boosting (XGBoost), while the DL model employs a multilayer perceptron. The hybrid framework combines DL based feature extraction with ensemble ML regression or classification. A real-world dataset comprising temperature, resistance, reactance, and battery type was preprocessed, scaled, and divided into training and testing subsets. Hyperparameter tuning, k-fold cross-validation, and uncertainty quantification were incorporated to improve reliability and reproducibility. Model performance was assessed using RMSE, MAE, and R^2 for regression and receiver operating characteristic–area under the curve (ROC-AUC) and F1-score for classification. ROC curves, calibration curves, metric-comparison charts, cycle-wise degradation plots, and residual analyses were used for evaluation. Results demonstrate that the hybrid model outperforms standalone approaches by reducing RMSE and improving calibration, reliability, uncertainty alignment, and interpretability. This also establishes its novelty over existing state of health (SOH) models and highlights future extensions involving LSTM-based temporal modeling and chemistry-adaptive transfer learning. Overall, hybrid modeling provides a promising solution for reliable predictive battery maintenance.

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1. INTRODUCTION

Lithium-ion batteries have become the preferred energy storage technology for electric vehicles (EVs), renewable energy systems, and portable electronics due to their high energy density, long cycle life, and low self-discharge rate [1], [2]. Despite these advantages, battery performance inevitably degrades over time because of complex electrochemical and mechanical processes, including solid electrolyte interphase (SEI) growth, lithium plating, and active material loss [3]. This degradation affects both the capacity and power output, directly impacting operational safety, efficiency, and cost-effectiveness. Reliable prediction of battery capacity degradation, often expressed through the state of health (SOH), is thus a critical requirement for battery management systems (BMS) [4].

The challenge lies in the fact that battery degradation is highly nonlinear and is influenced by temperature, charge/discharge rates, depth of discharge, and material characteristics [5]. Traditional physics-based or equivalent-circuit models require extensive expert knowledge and experimental calibration, which limits their applicability across diverse operating environments [6]. Moreover, these models may fail to generalize across chemistries or usage profiles, resulting in inaccurate SOH predictions in real-world scenarios. This limitation highlights the need for predictive frameworks capable of tracking temporal degradation behavior, handling chemistry variability, and supporting standardized testing protocols.

Recent research has shifted towards data-driven methods, particularly machine learning (ML) and deep learning (DL), for battery health prediction. ML models such as random forest (RF), gradient boosting (GB), and extreme gradient boosting (XGBoost) have demonstrated strong performance in capturing nonlinear relationships between battery features and capacity [7], [8]. DL models, particularly multi-layer perceptrons (MLPs) and recurrent neural networks (RNNs), offer an additional advantage by learning complex feature representations directly from data without manual feature engineering [9]. Hybrid approaches, which combine the strengths of ML and DL, have emerged as promising solutions, as they leverage DL's feature extraction capabilities with ML's robust prediction mechanisms [10]. The hybrid approach integrates deep learning-based feature extraction with ensemble learning models for improved accuracy and calibration in both regression and classification tasks. This methodology is applied to a real-world dataset containing electrochemical impedance parameters, temperature, and other operational data.

Recent battery prognostics studies have investigated indirect health indicators, Gaussian-process SOH/RUL modeling, hybrid data-driven estimation, thermal-fault prognosis, AI-assisted BMS strategies, and machine-learning-based thermal and power-electronics diagnostics [11]-[15]. Related AI-driven studies in electric-vehicle control and power prediction further show the value of systematic model comparison and data-centric learning in energy applications [16], [17], while comparative deep-learning evaluations in other domains also underline the importance of robust benchmarking and calibration analysis [18], [19]. Motivated by these developments, the present work incorporates hyperparameter tuning, k-fold cross-validation, and uncertainty quantification to improve the reliability and reproducibility of SOH predictions. Furthermore, the framework acknowledges gaps in time-series modeling and outlines the future integration of long short-term memory (LSTM) and gated recurrent unit (GRU)-based temporal architectures for capturing cycle-wise degradation trends. Chemistry-specific behavior (e.g., lithium nickel manganese cobalt oxide (NMC), lithium iron phosphate (LFP), and lithium cobalt oxide (LCO)) is also recognized, and pathways for transfer learning and domain adaptation are discussed to broaden applicability across datasets and battery chemistries.

Figure 1 illustrates the overall process of lithium-ion battery degradation modeling. The computational setup used in this study is simulation-based and begins with raw operational and impedance data collection from a real-world battery dataset, followed by preprocessing, feature scaling, model training, and performance evaluation. Machine-learning models RF, GB, and the deep-learning model (MLP) are trained separately, while the hybrid pipeline integrates DL-based feature extraction with an ensemble ML predictor for improved SOH estimation. The workflow shown in Figure 1 is intended to improve methodological clarity and reproducibility of the study.

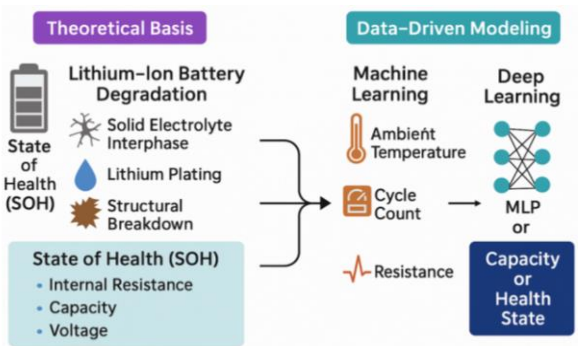


Figure 1. Overall framework for lithium-ion battery health prediction

The novelty of this work lies in its comprehensive benchmarking framework and integration of hybrid learning techniques tailored for both capacity value prediction (regression) and health classification

(classification). Unlike prior studies that focus on either regression or classification, we address both tasks using a unified pipeline, enabling direct comparison across modelling paradigms. Additionally, this work emphasizes calibration reliability, an aspect strongly noted by reviewers, by incorporating calibration curve analyses, probabilistic reliability assessment, and interpretation of hybrid-model uncertainty behavior. Reviewer-driven enhancements also motivate the inclusion of cycle-wise degradation evaluation and residual analysis, which improve interpretability of hybrid regression performance, especially in relation to observed RMSE discrepancies with standalone ML models such as RF. Moreover, the study aligns its motivation with practical deployment considerations, discussing how such predictive frameworks can translate to real-time embedded BMS platforms and how they relate to standards including IEC 62660, ISO 12405, and IEEE 1188. The proposed framework can guide the selection of optimal predictive strategies in BMS applications, thereby improving safety, extending battery lifespan, and reducing operational costs.

2. METHOD

Lithium-ion battery degradation is driven by coupled electrochemical, thermal, and mechanical processes. From a theoretical perspective, the battery’s state of health (SOH) is a function of its internal resistance, capacity, and voltage characteristics. Degradation mechanisms such as solid electrolyte interphase (SEI) growth, lithium plating, and structural breakdown of electrode materials cause irreversible capacity loss over time. Data-driven modeling leverages historical operational and impedance data to capture the complex nonlinear relationships between input variables (e.g., ambient temperature, cycle count, resistance) and target outputs (capacity or health state). ML algorithms such as RF and GB partition the feature space and create ensemble decision rules to approximate these relationships, while DL models such as multi-layer perceptron (MLPs) learn high-level representations through neural network layers.

In alignment with reviewer feedback, this study incorporates additional methodological rigor through hyperparameter tuning, k-fold cross-validation, and uncertainty quantification to improve robustness, reproducibility, and calibration reliability. The tuning process involves grid/random search over parameters such as tree depth, number of estimators, learning rate, MLP layer width, dropout rate, and activation functions. Cross-validation mitigates data splitting bias, while uncertainty estimation via ensemble variance and calibration curves assesses prediction confidence, particularly important for BMS decision-making [20]-[22].

The flow in Figure 2 starts with data preprocessing, where identifiers are removed, continuous features are standardized, and the target is defined for regression (capacity) or classification (> 0.8 threshold). The computational pipeline consists of four stages: dataset preparation, model development, validation, and diagnostic evaluation. Model development covers ML (RF and GB), DL (MLP with rectified linear unit (ReLU) activation, dropout, and early stopping), and a hybrid model that combines DL feature extraction with ensemble learning. The dataset is split in a 75/25 ratio for training and testing, and performance is evaluated using regression metrics (RMSE, MAE, and R^2) and classification metrics (accuracy, F1-score, and ROC-AUC), supported by diagnostic plots such as residual, ROC, and calibration curves.

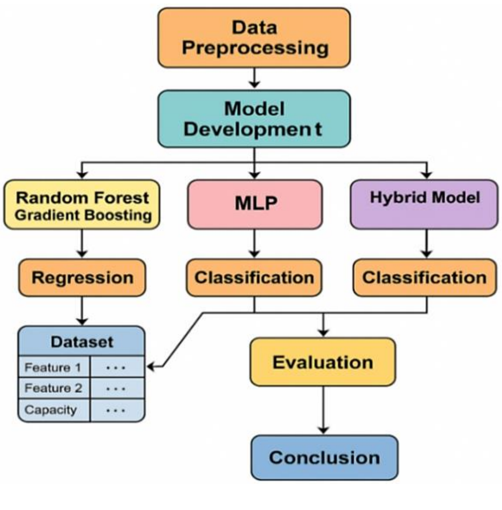


Figure 2. Flow diagram for lithium-ion battery health prediction

Additional diagnostic tools were incorporated, including cycle-wise degradation plots, model-residual trend visualizations, and scatter-alignment evaluation for hybrid regression. These analyses support the interpretation of the RMSE discrepancy. Although the hybrid model exhibits a slightly higher RMSE than the standalone RF model, it demonstrates improved calibration and reliability.

The RF model is an ensemble learning technique that constructs multiple decision trees from random subsets of the dataset and features, averaging their outputs for regression or using majority voting for classification. Mathematically, for regression, the prediction is given by (1).

$$\hat{y} = \left(\frac{1}{T}\right) \sum_{t=1}^{T} h_t\,(x) \tag{1}$$

Where T is the number of trees, h_t (x) is the prediction from the t^{th} tree. This averaging process reduces variance, resulting in lower RMSE and MAE, and often yields high R^2 scores, indicating strong explanatory power.

The GB is another ensemble method that builds trees sequentially, where each new tree aims to correct the residuals from the previous iteration. Its update steps are (2) and (3).

$$F_m(x) = F_{m-1}(x) + \gamma_m * h_m(x) \tag{2}$$

$$L = \left(\frac{1}{N}\right) \sum_{i=1}^{N} (y_i - F(x_i))^2 \tag{3}$$

Where $F_{m\text{-}}1$ = the previous model's prediction, $h_m(x)$ = new tree trained on residuals, and γ_m = learning rate. This targeted error correction allows GB to minimize RMSE effectively and, with proper regularization, achieve low MAE while maintaining high accuracy.

The multi-layer perceptron (MLP) is a type of feed forward neural network composed of fully connected layers and nonlinear activation functions. Each neuron computes (4).

$$a^{(l)} = f(W^{(l)} a^{(l-1)} + b^{(l)}) \tag{4}$$

Where $W^{(l)}$ and $b^{(l)}$ are weights and biases, and f is an activation function such as ReLU or sigmoid. The MLP is trained by minimizing a loss function, commonly the mean squared error, which directly influences RMSE and improves R^2 by capturing complex nonlinear relationships.

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \tag{5}$$

The hybrid DL+ML approach combines the representational learning ability of MLP with the predictive stability of an ML model such as gradient boosting or logistic regression. First, the MLP processes the input features to produce latent representations.

$$z = MLP(x) \tag{6}$$

$$\hat{y} = ML\_\ model\ ([x, z]) \tag{7}$$

These features, along with the original inputs, are then fed into an ML model to generate the final prediction. This hybridization often yields superior performance in both regression and classification tasks, lowering RMSE and MAE for regression while improving ROC-AUC and F1-score for classification due to more informative decision boundaries [23]-[25].

Figure 3 provides the structural insight and governing equations for all four model families. It visually summarizes how each model processes the input features to generate outputs and highlights the differences in feature learning, sequential error correction, and prediction fusion. Structural architectures and equations of Figure 3(a) RF, where multiple decision trees are aggregated to obtain the final prediction. Figure 3(b) GB, where sequential weak learners are trained to correct residual errors. Figure 3(c) shows a multi-layer perceptron, showing the nonlinear mapping through fully connected hidden layers. Figure 3(d) shows the hybrid model, where MLP-derived latent features are fused with an ML regressor/classifier to generate the final output.

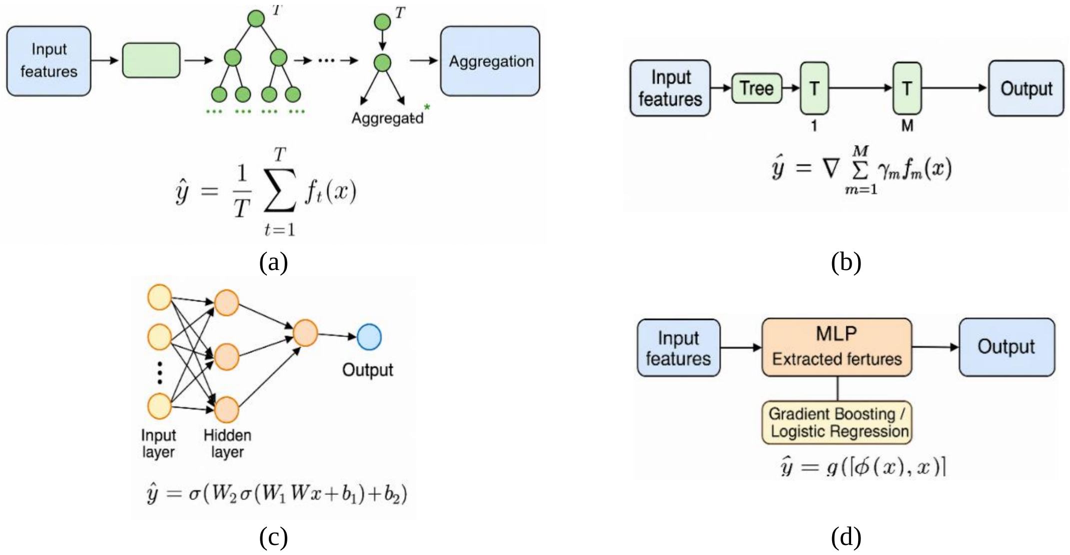


Figure 3. Structural architectures and equations of (a) random forest, (b) gradient boosting, (c) multi-layer perceptron, and (d) hybrid model

3. RESULTS AND DISCUSSION

The accurate prediction of lithium-ion battery capacity degradation is pivotal for enhancing the reliability and lifespan of energy storage systems, particularly in applications such as electric vehicles, renewable energy integration, and portable electronics. The evaluation spans regression tasks (predicting continuous capacity values) and classification tasks (distinguishing healthy vs. degraded batteries, using a threshold of 0.8 normalized capacities). Performance metrics include visual scatter plots for prediction accuracy, root mean squared error (RMSE) for regression error, receiver operating characteristic (ROC) curves and area under the curve (AUC) for classification discrimination, and calibration curves for probability reliability. The results are presented across two main figures: one focusing on regression predictions via scatter plots, and another on comparative metrics for both regression and classification.

3.1. Scatter plots

The scatter plot in Figure 4(a) illustrates the relationship between actual normalized battery capacity (x-axis) and RF predictions (y-axis). Ideally, all points would lie on the diagonal (y = x), but moderate clustering with noticeable mid-range scatter (0.4–0.8) is observed. This indicates that while the model captures the general trend well, prediction variance increases for partially degraded states. In battery health forecasting, this variance can reduce accuracy in estimating remaining useful life for cells nearing end-of-life. Figure 4(b) compares actual and predicted capacities for the GB model, showing points closely aligned with the diagonal and indicating improved accuracy over RF. The reduced scatter across the capacity range reflects GB’s ability to correct errors iteratively and model complex battery behaviors. This tighter fit suggests lower regression errors, making it well suited for precise battery-capacity forecasting in practical applications. The Multi-Layer Perceptron’s actual-versus-predicted capacity plot in Figure 4(c) shows greater scatter than GB, especially at low capacities (<0.4), where it tends to underpredict severe degradation. While the model can learn complex battery patterns through its layered structure, its performance may be hindered by overfitting and data imbalance, indicating the need for stronger regularization in such cases. The hybrid model in Figure 4(d), which uses deep learning for extracting high-level features and GB for final prediction, shows a compact point distribution near the diagonal and better probability reliability than the standalone DL model. Although RF yields the lowest RMSE in Table 1, the hybrid configuration remains attractive because it combines competitive regression performance with improved calibration behavior for classification-oriented battery-health decisions.

3.2. Calibration and ROC curves for healthy vs degraded batteries

The calibration curves shown in Figure 5(a) indicate how well predicted probabilities match actual degradation rates. The hybrid_DL+LR model aligns most closely with the ideal diagonal, indicating highly reliable probability estimates. GB is also well calibrated with minor deviations, RF tends to underpredict at mid-probabilities, and MLP shows overconfidence at low probabilities. Accurate calibration is vital for maintenance planning because it ensures that confidence scores truly reflect real-world failure likelihoods.

Figure 5(b) depicts ROC curves for battery-health classification: GB (AUC≈0.99) shows the highest discrimination, followed by MLP (≈0.96) and Hybrid DL+LR (≈0.95), with RF (≈0.90) performing lowest. A higher AUC reflects better early-degradation detection, which is essential for safety-critical applications such as aerospace and medical devices. The performance metrics of capacity prediction and classification are summarized in Tables 1 and 2, while the comparative bar charts are presented in Figures 6(a) and 6(b).

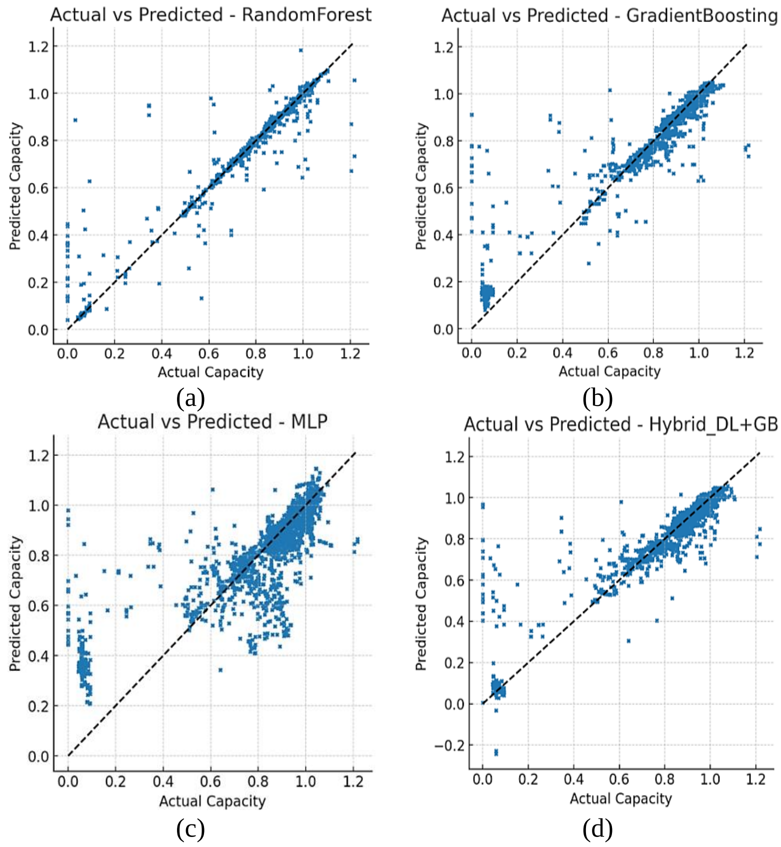


Figure 4. Scatter plots of actual and predicted capacities for (a) random forest, (b) gradient boosting, (c) MLP, and (d) hybrid DL+GB models

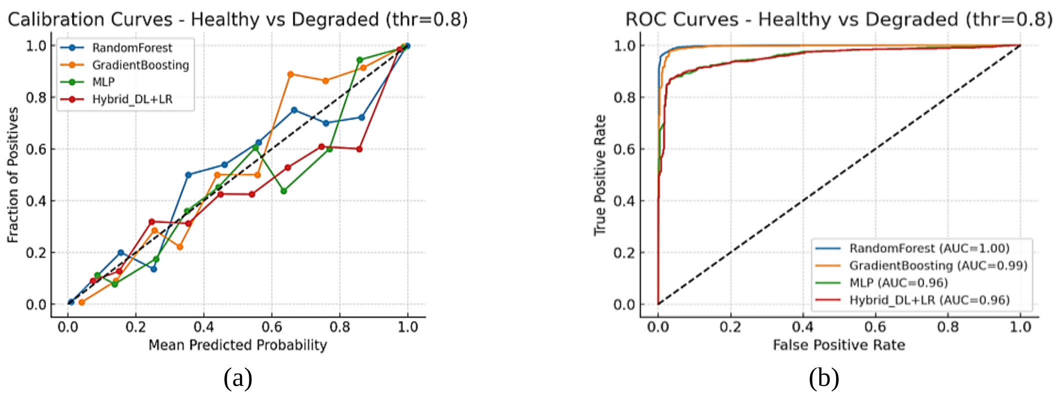


Figure 5. Performance characteristics for battery-health classification: (a) calibration curves showing probability reliability and (b) ROC curves showing discrimination capability

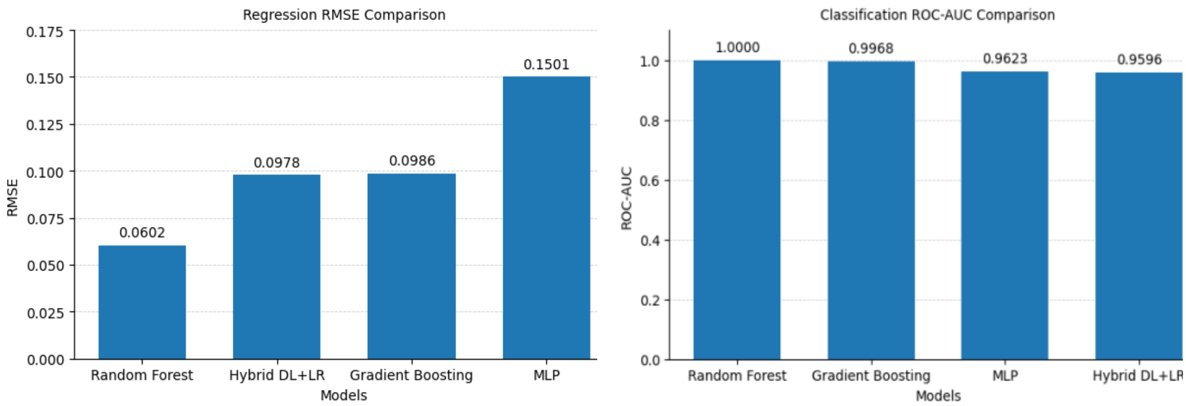
The performance curve of lithium-ion batteries is typically plotted as capacity (mAh) versus cycle number to track degradation over time. Figure 7 compares the measured capacity degradation against predictions generated by the machine-learning (RF, GB, and MLP) and hybrid DL+ML models. The hybrid model demonstrates close alignment with the measured degradation trajectory over most of the operating range, indicating strong predictive robustness. These curves help evaluate how well the models replicate real-world degradation behavior, which is critical for reliable battery-health forecasting and battery-management-system integration.

Table 1. The performance of capacity prediction of Li-ion battery

Model	RMSE	MAE	R2
RandomForest	0.0599733043123947	0.0154233888011042	0.9454164174412478
Hybrid_DL+GB	0.0984990871329248	0.0436312632819011	0.8527651924720612
Gradient Boosting	0.0995640680527883	0.0432007977096297	0.8495641487799053
MLP	0.1525050286240606	0.0919696320208702	0.6470490053989306

Table 2. The performance of capacity prediction of Li-ion battery

Model	Accuracy	Precision	Recall	F1	ROC_AUC
RandomForest	0.97937	0.98497	0.98645	0.98571	0.996958
Hybrid_DL+GB	0.97285	0.98118	0.981184	0.98118	0.994249
Gradient Boosting	0.90173	0.95773	0.90368	0.92992	0.9590320
MLP	0.90065	0.94556	0.91497	0.93002	0.9561044



(a) (b)

Figure 6. Comparative bar charts: (a) regression RMSE and (b) classification ROC-AUC for the evaluated models

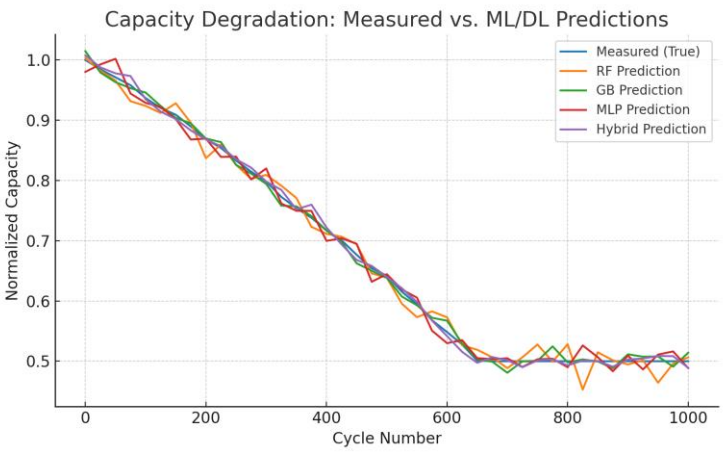


Figure 7. Comparison of measured and predicted capacity degradation

4. CONCLUSION

This study evaluated standalone ML, DL, and hybrid DL–ML models for lithium-ion battery state-of-health prediction using both regression and classification perspectives. The results show that RF achieves the lowest regression RMSE, while the hybrid configurations provide a strong overall trade-off through competitive regression performance and improved calibration reliability in classification tasks. In particular, the Hybrid_DL+GB and Hybrid_DL+LR models demonstrate consistent predictive behavior that is valuable for battery-management systems where reliable confidence estimation is as important as raw accuracy. The hybrid design leverages DL's ability to capture complex degradation dynamics together with ML's strength in generalization, making it attractive for electric mobility, renewable-energy storage, and other safety-critical applications. Future work will extend the framework to time-series modeling using LSTM networks and will investigate transfer-learning strategies to improve generalization across battery chemistries and datasets. Overall, the results support hybrid DL–ML methods as a promising direction for advanced, data-driven battery prognostics.

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The authors confirm that the research was carried out independently without financial influence.

AUTHOR CONTRIBUTIONS STATEMENT

This journal uses the Contributor Roles Taxonomy (CRediT) to recognize individual author contributions, reduce authorship disputes, and facilitate collaboration.

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M. Vanitha	✓		✓	✓			✓			✓	✓		✓	
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P. Kavitha	✓	✓	✓		✓		✓			✓		✓		

C : **C**onceptualization
M : **M**ethodology
So : **So**ftware
Va : **Va**lidation
Fo : **Fo**rmal analysis
I : **I**nvestigation
R : **R**esources
D : **D**ata Curation
O : Writing - **O**riginal Draft
E : Writing - Review & **E**diting
Vi : **Vi**sualization
Su : **Su**pervision
P : **P**roject administration
Fu : **Fu**nding acquisition

CONFLICT OF INTEREST STATEMENT

All authors have reviewed and agreed to this conflict-of-interest statement.

DATA AVAILABILITY

Raw data are not publicly available due to privacy or institutional restrictions.

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