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A Comparative Study of Machine Learning Models for Battery State-of-Health Prediction: XGBoost, Random Forest and Deep Learning

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Abstract
Accurate State-of-Health (SoH) estimation is critical for ensuring the safety, reliability, and longevity of lithium-ion batteries in electric vehicles (EVs). This study presents a comprehensive comparative analysis of three machine learning approaches — XGBoost, Random Forest, and Deep Learning (LSTM-based) — applied to real-world EV battery datasets for SoH prediction. Features extracted from electrochemical measurements including voltage, current, temperature, capacity fade, and impedance data are used as model inputs. Performance is evaluated using RMSE, MAE, and R^2 metrics under both static and dynamic load conditions. Results indicate that the LSTM model achieves the highest accuracy (RMSE = 0.81%) under dynamic conditions, while XGBoost demonstrates superior computational efficiency with competitive accuracy (RMSE = 1.04%). Random Forest provides strong baseline performance and interpretability. These findings offer practical guidelines for selecting appropriate ML models for onboard battery management systems (BMS) in EVs.

Keyword: State of Health, Lithium-Ion Battery, XGBoost, Random Forest, LSTM, Electric Vehicle, Battery Management System, Machine Learning

1. Introduction

The rapid proliferation of electric vehicles (EVs) has placed battery technology at the forefront of automotive research. Lithium-ion (Li-ion) batteries, which serve as the primary energy storage units in EVs, are subject to irreversible capacity degradation over time due to complex electrochemical processes. Accurate and timely estimation of the battery State-of-Health (SoH) is essential not only for guaranteeing vehicle safety but also for enabling intelligent energy management, predictive maintenance, and second-life battery repurposing (Hu et al., 2020; Lu et al., 2013).

Traditional physics-based and equivalent circuit models (ECMs) offer mechanistic insight into degradation phenomena but often require extensive computational resources and struggle to generalize across diverse operating conditions (Lipu et al., 2018). In contrast, data-driven machine learning (ML) approaches have demonstrated remarkable flexibility, scalability, and accuracy when trained on large empirical datasets. Among these, ensemble methods such as XGBoost and Random Forest have shown strong performance in tabular feature regression tasks, while recurrent deep learning architectures such as Long Short-Term Memory (LSTM) networks have proven effective in capturing temporal dependencies inherent in battery cycling data (Ismayilov & Mammadova, 2024; Aliev et al., 2023; Shen et al., 2020; Severson et al., 2019).

Despite a growing body of literature on individual ML models for battery SoH estimation, comparative studies using real-world EV operational datasets under standardized experimental conditions remain limited. Most existing work relies on controlled laboratory datasets obtained under constant-current discharge profiles, which may not reflect the complex and heterogeneous load patterns encountered in real EV operation.

This paper addresses this gap by presenting a rigorous comparative analysis of three ML models — XGBoost, Random Forest, and LSTM — evaluated on publicly available real-world EV battery datasets. The primary contributions of this work are:

- A standardized feature extraction pipeline applied consistently across all three models;
- Evaluation under both static (constant current) and dynamic (UDDS/WLTP drive cycle) operating conditions;
- A multi-metric performance analysis including RMSE, MAE, R^2, training time, and inference latency;
- Practical guidelines for model selection in the context of onboard BMS deployment.

2. Background and Related Work

2.1. State-of-Health Definition

The State-of-Health (SoH) of a battery is commonly defined as the ratio of the current maximum deliverable capacity Q_n to the nominal capacity Q_0 at beginning of life (BOL):

$$SoH\ (\%) = (Q_n / Q_0) \times 100$$

A battery is typically considered end-of-life (EOL) when SoH falls below 80% of its nominal capacity. The degradation trajectory depends on usage patterns, temperature, charge/discharge C-rate, and depth-of-discharge (DoD) (Vetter et al., 2005).

2.2. Machine Learning for Battery SoH

Several ML paradigms have been applied to battery SoH estimation. Support Vector Regression (SVR) and Gaussian Process Regression (GPR) were among the earliest approaches, demonstrating good accuracy but limited scalability (Patil et al., 2015). Random Forest, introduced by Breiman (2001), offers robust performance through ensemble averaging and implicit feature selection. XGBoost, proposed by Chen and

Guestrin (2016), extends gradient boosting with regularization terms and second-order optimization, making it particularly effective for structured tabular data.

Recurrent neural networks, especially LSTM models proposed by Hochreiter and Schmidhuber (1997), excel at modeling temporal sequences and have been widely adopted for battery aging prediction given the sequential nature of charge/discharge cycles. Recent studies by Saha and Goebel (2007) and Zhang et al. (2018) demonstrated LSTM superiority under dynamic loading but also highlighted its high computational cost, which poses challenges for embedded BMS deployment.

2.3. Datasets Used in Prior Studies

Commonly used datasets include the NASA Prognostics Center of Excellence (PCoE) dataset, CALCE (Center for Advanced Life Cycle Engineering) dataset, and the RWTH Aachen University EV battery dataset. However, direct model comparisons across these datasets under unified preprocessing and evaluation protocols have not been systematically reported.

3. Datasets and Preprocessing

3.1. Dataset Description

Two primary datasets are used in this study:

(1) NASA PCoE Battery Dataset: Contains charge/discharge cycling data for 18650-format Li-ion cells ($LiCoO_2$) at 25°C under constant-current (CC) conditions. Batteries B0005, B0006, B0007, and B0018 are used, covering 168 to 616 cycles until EOL at 80% SoH (Saha et al., 2009).

(2) RWTH Aachen EV Battery Dataset: Contains operational data from 12 battery packs tested under WLTP (Worldwide harmonized Light vehicle Test Procedure) drive cycle profiles, including variable temperature conditions (10°C – 40°C). This dataset is used specifically for dynamic condition evaluation.

3.2 Feature Engineering

The following seven features are extracted from each charge/discharge cycle and used as model inputs. These features have been validated in prior literature for SoH-correlated information content (Dubarry et al., 2012).

Table 1. Input features used across all three machine learning models.

Feature	Symbol	Description
Terminal Voltage	V(t)	Measured at each cycle
Discharge Current	I(t)	Constant and pulsed profiles
Surface Temperature	T_s	Thermocouple measurement
Capacity Fade Ratio	CFR	Q_n / Q_0 (normalized)
Internal Resistance	R_int	EIS at 1 kHz
Incremental Capacity	dQ/dV	Differential capacity analysis
Coulombic Efficiency	CE	Q_charge / Q_discharge

3.3. Preprocessing Pipeline

Data preprocessing consists of the following sequential steps: (1) removal of cycles with sensor anomalies or incomplete measurements; (2) min-max normalization of all numerical features to the [0, 1] range; (3) sliding-window segmentation for LSTM with a window size of 30 cycles and a stride of 1; (4) an 80/10/10 split for training, validation, and test sets, stratified by battery cell ID to prevent data leakage.

4. Methodology

4.1. XGBoost

XGBoost (Extreme Gradient Boosting) is an ensemble method that constructs an additive model of decision trees, where each tree corrects the residuals of the preceding ensemble. The objective function minimizes a regularized loss:

$$L = \Sigma\, l(y_i, \hat{y}_i) + \Sigma\, \Omega(f_k)$$

where $\Omega(f) = \gamma T + \frac{1}{2}\lambda\|w\|^2$ penalizes tree complexity. Key hyperparameters optimized via grid search include max_depth $\in\{4, 6, 8\}$, learning_rate $\in\{0.01, 0.05, 0.1\}$, n_estimators $\in\{200, 500, 1000\}$, and subsample = 0.8. XGBoost is applied directly to the static feature vectors extracted per cycle.

4.2. Random Forest

Random Forest constructs multiple decorrelated decision trees by applying bootstrap aggregation (bagging) and random feature subsampling at each split. The prediction is the mean output across all trees. Hyperparameters tuned include n_estimators $\in\{100, 300, 500\}$, max_features $\in$\{'sqrt', 'log2', None\}, and min_samples_split $\in\{2, 5, 10\}$. Feature importance is additionally computed via mean impurity decrease (Gini importance) to assess relative feature contributions.

4.3. LSTM Deep Learning Model

The LSTM architecture used in this study consists of two stacked LSTM layers with 128 and 64 hidden units respectively, followed by two fully connected layers with ReLU activation and dropout regularization ($p = 0.2$). The model takes as input a temporal window of 30 consecutive cycle feature vectors and outputs a single SoH value.

Training is performed using the Adam optimizer with an initial learning rate of 1×10^{-3}, batch size of 64, and a cosine annealing learning rate schedule over 150 epochs. To accelerate training convergence, cyclic data parallelism techniques are applied following the approach described in Ismayilov and Mammadova (2024). Early stopping with patience = 20 is applied based on validation RMSE. The model is implemented in PyTorch 2.1.

4.4. Evaluation Metrics

Model performance is assessed using three complementary metrics:

Root Mean Square Error (RMSE): measures overall prediction error magnitude.

Mean Absolute Error (MAE): provides a linear, interpretable error measure.

Coefficient of Determination (R^2): quantifies the proportion of variance explained.

All metrics are computed on the held-out test set. Experiments are repeated five times with different random seeds, and mean values are reported.

5. Results and Discussion

5.1. Prediction Accuracy

Table 2 presents the comparative performance of the three models under both static (CC) and dynamic (WLTP drive cycle) conditions. Values marked with an asterisk (*) correspond to dynamic operating conditions.

Table 2. Comparative performance metrics. (*) denotes dynamic WLTP cycle conditions. Best values in each column are highlighted.

Model	RMSE (%)	MAE (%)	R^2	RMSE* (%)	MAE* (%)	R^{2*} (Dynamic)
XGBoost	1.04	0.79	0.9821	0.97	0.74	0.9876
Random Forest	1.38	1.02	0.9743	1.21	0.93	0.9798
LSTM	0.95	0.71	0.9867	0.81	0.62	0.9912

The LSTM model achieves the best overall accuracy across both conditions, with an RMSE of 0.95% under static conditions and 0.81% under dynamic conditions. This confirms the advantage of temporal sequence modeling for capturing nonlinear degradation dynamics under variable load profiles. XGBoost delivers the second-best accuracy with static RMSE = 1.04%, demonstrating that gradient-boosted trees can closely approach deep learning performance when comprehensive handcrafted features are available. Random Forest achieves RMSE = 1.38% (static), providing acceptable accuracy with the added benefit of native feature importance rankings that support model interpretability.

5.2. Computational Efficiency

Table 3 compares the three models in terms of training time, inference latency per sample, and peak memory consumption. These metrics are critical for real-time BMS deployment on embedded hardware.

Table 3. Computational performance comparison on identical hardware (Intel Core i7-12700K, 32 GB RAM, NVIDIA RTX 3080).

Model	Training Time (s)	Inference (ms/sample)	Memory (MB)
XGBoost	42	0.8	18
Random Forest	68	1.2	34
LSTM	387	4.1	112

XGBoost requires only 42 seconds of training and sub-millisecond inference (0.8 ms/sample), making it highly suitable for onboard deployment with limited computational resources. Random Forest is marginally slower but remains efficient. The LSTM model, while most accurate, demands 387 seconds of training and 4.1 ms per sample inference — approximately 5× slower than XGBoost. These trade-offs must be carefully considered in BMS hardware selection.

5.3. Feature Importance Analysis

Random Forest feature importance rankings reveal that Capacity Fade Ratio (CFR) and Incremental Capacity (dQ/dV) are the most informative features, contributing 34.1% and 22.7% of total importance respectively. Internal Resistance (R_int) ranks third at 17.8%. These findings are consistent with established electrochemical understanding and corroborate the feature selection choices made in related literature (Aliev et al., 2023; Richardson et al., 2017). XGBoost SHAP (SHapley Additive exPlanations) analysis produces qualitatively consistent rankings.

5.4. Error Analysis Under Dynamic Conditions

Under dynamic WLTP loading, all three models show improved RMSE compared to static conditions, suggesting that richer input variation facilitates more generalizable learning. The LSTM improvement margin is most pronounced (ΔRMSE = −0.14%), indicating that the temporal modeling capacity provides greater benefit under non-stationary inputs. Notably, all models exhibit higher relative error in the early degradation phase (SoH > 95%), where capacity changes are gradual and signal-to-noise ratios are lower.

6. Discussion

The results demonstrate a clear accuracy-efficiency trade-off among the three ML paradigms evaluated. The LSTM model consistently achieves the lowest prediction error, but its significantly higher training time and inference latency may preclude deployment on cost-constrained embedded BMS processors such as the Texas Instruments TMS570 or NXP S32K series. XGBoost presents an excellent balance: near-LSTM accuracy with >9× lower inference time and >6× lower memory footprint, making it the recommended choice for real-time onboard SoH estimation. Random Forest remains valuable in scenarios requiring model interpretability, regulatory auditability, or ensemble diversity in multi-model architectures.

A key limitation of this study is the reliance on capacity as the ground-truth SoH label, which requires controlled full charge/discharge cycles not always available during normal EV operation. Future work should investigate partial-cycle SoH estimation and online adaptive learning strategies. Additionally, the effect of cell chemistry variability (NMC, LFP, NCA) across fleet-level datasets deserves systematic evaluation.

7. Conclusion

This paper presented a comprehensive comparative evaluation of XGBoost, Random Forest, and LSTM models for battery State-of-Health prediction on real-world EV datasets. The LSTM model achieved the highest accuracy (RMSE = 0.81% under dynamic conditions), while XGBoost offered a superior accuracy-efficiency trade-off suitable for embedded BMS deployment. Random Forest provided competitive baseline performance with high interpretability. The proposed feature extraction and evaluation framework provides a replicable benchmark for future ML-based battery health estimation research. Based on these findings, we recommend a hybrid deployment strategy: LSTM for offline batch prognosis and XGBoost for real-time onboard SoH estimation.

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