Optimizing Lithium-Ion Battery Discharge Capacity Prediction Using Light GBM and Explainable AI (XAI) Framework

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Abstract: Improving the lifetime and cost-effectiveness of energy storage systems depends on exact control of lithium-ion battery (LiB) capacity. To estimate LiB discharge capacity, this work uses AdaBoost, gradient boost, XGBoost, LightGBM, Catboost, as well as ensemble learning among other machine learning models. Mean absolute error (the MAE), mean squared error (the MSE), along with R-squared values all were used to assess model performance. LightGBM had the best results among the models via the lowest MAE (0.104) along with MSE (0.018), in addition to the greatest R-squared value (0.888), therefore proving better prediction accuracy. Closely in performance were gradient boosting and XGBoost. The success of the combined model implies that including many models could improve general forecast accuracy. Furthermore, the impact of important parameters, like temperature, cycle index, voltage, as well as current, on model predictions was investigated using explainable artificial intelligence (XAI, which) techniques more especially, SHAP values. Results show that discharge capacity is very much influenced by temperature. This paper emphasizes the possibilities of machine learning as well XAI in LiB management optimization, therefore supporting more sustainable and effective energy storage systems.

Keywords: Lithium-Ion Batteries (LiBs), Machine Learning, Explainable Artificial Intelligence (XAI), Battery Management System (BMS), State of Health (SoH) Estimation.

1. Introduction

Lithium-ion batteries (LiBs) are an important energy source for electric cars (EVs) because they have a high energy density, are light, don't self-discharge quickly, can be charged quickly, and don't need much upkeep [1]. Because of these benefits, LiBs have become the best choice for power in many situations, especially as we move toward electric vehicles and more environmentally friendly energy sources. LiBs are an eco-friendly option to cars that use fossil fuels [2-5]. They help lower greenhouse gas pollution and total carbon footprints, which makes them necessary for green mode of transport and energy storage facilities. Even though LiBs have many benefits, they have a big problem: their performance goes down over time. Chemical as well as physical factors cause batteries to lose their power over time. Because of this, efficient battery management systems (or BMS for need to be created to avoid high costs as well as limited repair options. Predicting a state of health (SoH) measure and other battery health factors correctly is an important part of managing batteries [6-10]. SoH is an important measurement for many uses, like in handheld gadgets, electric vehicles, as well large-scale storage of energy, because it shows how a battery is doing now and how much power it can hold compared to how it was at first. To guess a battery's remaining useful life (RUL), improve performance, and make sure it will last for a long time, you need to know about SoH. SoH review is also very important for improving safety, sustainability, along with cost-effectiveness in many fields because it checks for changes in capacity, internal resistance, and cycle life [11-15]. Maintaining range consistency, charging efficiency, as well as general vehicle performance therefore depends on SoH assessment. Accurate SoH estimate maximizes energy use, optimizes expenditures, and reduces operational risks in grid-scale applications like peak shaving and integration of renewable energy [16-18]. Highly intelligent battery management platforms have evolved thanks in large part to recent developments in SoH evaluation techniques, especially via machine learning (ML) as well as artificial intelligence (AI). These systems include adaptive control techniques, predictive maintenance, and real-time monitoring to extend battery life, lower early replacements, and improve sustainability via best use of resources and recycling activities. Among the sophisticated methods used to forecast LiB performance are density functional theory (DFT) & molecular dynamic forces. By use of atomic and molecule interactions inside the battery, molecular dynamics simulations offer light on material behaviour under various situations [19-21]. Conversely, DFT helps to compute electronic characteristics to forecast how changes in atomic-level parameters affect general battery performance. These methods give complete tools for improving battery materials and design together with ML-based electrochemical modelling. Recently, XAI, or explainable artificial intelligence, has gotten a lot of attention as a way to make predictive models clearer and easier to understand. Traditional machine learning and artificial intelligence-based SoH evaluation methods often work as "black boxes," which makes it hard to figure out what factors affect estimates of battery degradation. When XAI methods like Shapley Additive Explanations (the SHAP) factors are used together, they help us understand how different factors—like temperature, cycle index, the voltage, as well as current affect the battery. This lets us make better decisions about how to handle the batteries. This method makes batteries last longer, lowers the cost of upkeep, and improves the way batteries are replaced, which reduces the damage to the environment and encourages long-term resource use.

The goal of this work is to use ML and XAI to guess how much LiBs can release. To find SoH, we use a number of machine learning methods, such as the principal component analysis (a PCA), linear regression, regression with ridges, k-nearest-neighbors algorithm (kNN), random forests, polynomial regression, as well as gradient boosting [22-25]. The correctness, processing speed, and readability of these models are used to measure how well they work. SHAP numbers are also used to figure out how important a trait is, which gives us more information about the things that cause batteries to degrade. Complex models like random forest as well gradient boosting are more accurate, but simpler versions like linear regression along with kNN, when paired with XAI, make it easier to see how battery health is changing over time. The rest of the paper is organized like this: The tools and methods utilized throughout this study are talked about in Section 2. The results of the experiments and SHAP-based studies are shown in Section 3. In Section 4, we talk about the most important results and what they mean. In Section 5, we come to some conclusions and suggest areas for future study in the areas of estimating battery SoH and improving energy storage systems.

2. Techniques and Materials:

This part talks about how the study was organized, the dataset that was used, as well as the machine learning along with AI techniques that were used. Each method and measure used is described in great depth to make sure the study can be repeated and to make the approach clearer. There is a lot of talk about the scientific reasons behind choosing each material and method. Figure 1 shows a flowchart that shows each stage of building a model using machine learning methods like CatBoost, AdaBoost, XGBoost, LightGBM, and adaptive boosting (AdaBoost).

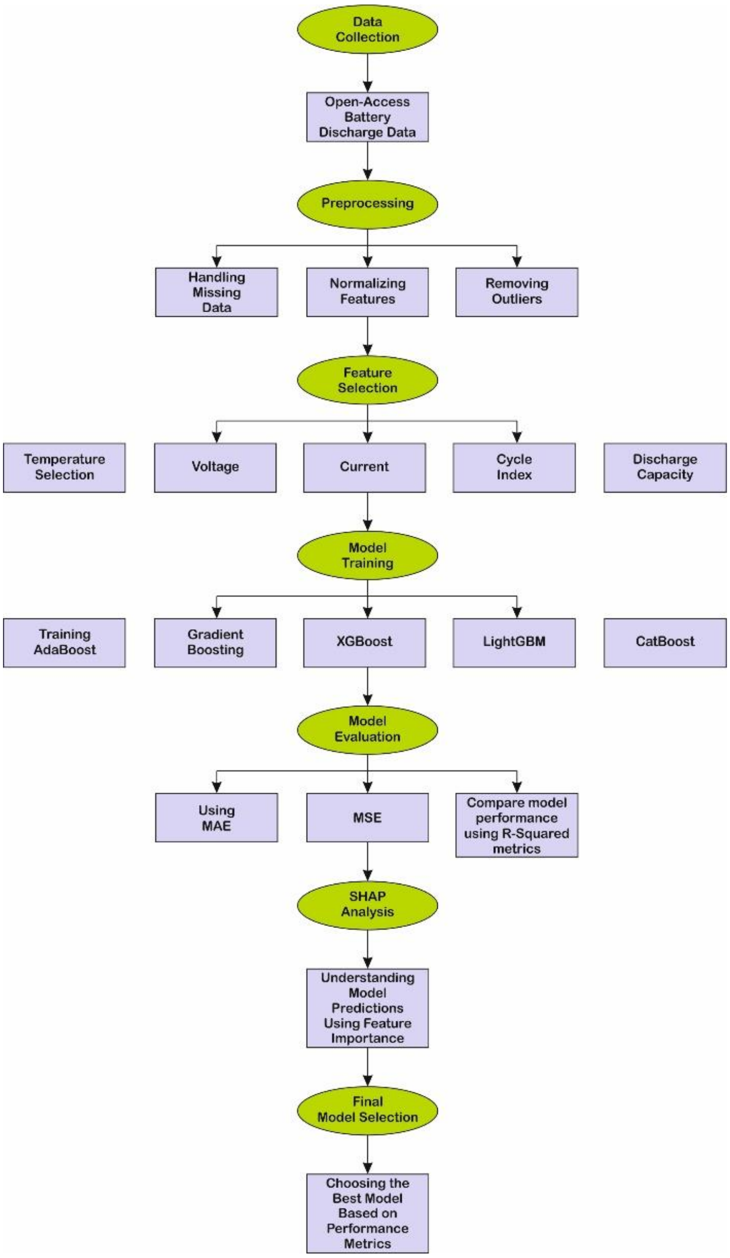

Figure 1. Flowchart of Model Development

Figure 1 is a diagram that shows in great detail how the training and testing processes worked in this study. At every step of the method for developing a model, this outline makes it easy to see what needs to be done and makes sure that the process can be repeated. After the appropriate steps for preparation were taken, the training and assessment files were fed into the models. The models were judged in the last step.

2.1. Definition of a Dataset:

The collection utilised in this study is made up of 45,698 histories that define properties of battery release processes. 81% of data was utilised for training as well as 21% was used for testing. 48,000 data points were utilized for training & 65,000 data points were utilized for testing. To describe how well the batteries in the dataset worked electrically, they needed to have "Temperature," "Current (A)," "Voltage (V)," "Cycle Index," and "Discharge Capacity (Ah)" fields. The sample utilized by the study came from a large library that had information about how battery discharge processes work. In each cycle, different factors that were measured while the battery was being discharged were written down. LIB samples were studied for 751 cycles as part of this work. All the tests for charging and discharging were done between 3.1 V and 4.5 V, with different C-rates and temperatures. Nine cells were used in each test setting for a total of 193 the cells (Table 1).

Table 1. Conditions of Testing for Samples of Lithium-Ion Batteries

Temperature (℃)	Discharge C-Rate	Charge Cut-Off C-Rate
11	0.8 C	C/6
26	2 C	C/41
46	3 C	C/6
61	2 C	C/41

Michael Pecht from the Centre for Advanced Life Cycle Engineering (CALCE), at the University of Maryland, supplied all of the open-access data used for the testing. The tests were carried out in LiCoO2 (cathode)–graphite (anode) the cells. Machine learning models were then trained using the charge as well as discharge information gleaned from these experiments. Training came from the initial 301 moves in the dataset; 451 cycles among 302 as well as 751 were eliminated from the test and training datasets. Data normalisation, outlier identification, and missing data management were among the many preparation techniques the dataset experienced.

2.2. Model Choice and Methods for Machine Learning:

For model training, this work assessed and contrasted machine learning methods including AdaBoost, LightGBM, gradient boosting, XGBoost & Catboost. These procedures were chosen depending on their particular qualities and benefits. The qualities of the dataset and intended results determine the strengths and shortcomings of any technique. Finding the best appropriate algorithm for a given dataset depends on comparing and assessing many ones. Trained upon the training set, the models were assessed on the test set. Furthermore, offered to understand model predictions and increase openness was the SHAP (Shapley Additive Explanations), the XAI technique.

Simulations of Boosting Algorithms in Mathematics:

Iteratively reducing loss functions helps boosting algorithms to enhance poor learners. Generally, the boosting loss function is provided by:

$$L(y, f(x)) = \sum_{i=1}^{n} (y_i - f(x_i))^2 \qquad (1)$$

where y_i is the real discharge capacity, $f(x_i)$ is the value that was forecast, as well as nn is the total number of examples. Weak learner $h_t(x)$ receives training to reduce residual error for every boosting iteration:

$r_i = y_i - f_{t-1}(x_i)$ (2) and revised approach is

$f_t(x) = f_{t-1}(x) + \alpha h_t(x)$ (3) where α is the rate of learning.

3. Results of Experiments:

The performance of the investigated algorithms is assessed in this part along with comparative analysis and discussion of each model's prediction success upon the State of Health (SoH) of Lithium-ion Batteries (LiBs). Furthermore, examined is the effect of the SHAP approach on decision-making and model predictions interpretation.

3.1. Evaluation Metrics for Models:

Standard regression measures mean squared error (the MSE), the mean absolute error (the MAE), as well as R-squared (R^2) were used to evaluate the models. These measures evaluate model predictions' correctness with respect to real values.

- Mean Squared Error (MSE):

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(Y_i - \hat{Y}_i)^2 \qquad (4)$$

The model works better when the MSE is smaller.

- R-squared (R^2):

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(\hat{Y}_i - Y_i)^2}{\sum_{i=1}^{N}(Y_i - \bar{Y})^2} \qquad (5)$$

An R^2 score close to 1 means the model fits most of the variation in the dataset.

- Mean Absolute Error (MAE):

$$\mathrm{MAE} = \frac{1}{N}\sum_{i=1}^{N}\left|Y_i - \hat{Y}_i\right| \qquad (6)$$

A lower MAE indicates improved prediction capability.

3.2. Training Models:

Five ensembles learning techniques AdaBoost, gradient boost, XGBoost, LightGBM, as well as Catboost were used. Bringing together ineffective learners into an effective predictive model helps these techniques improve prediction accuracy.

3.3. Comparative Results for Models:

Table 2 shows the performance measures for every model.

Models	MAE	MSE	R^2
AdaBoost	0.135	0.042	0.764
Gradient Boosting	0.109	0.024	0.865
XGBoost	0.111	0.024	0.865
LightGBM	0.104	0.020	0.888
CatBoost	0.105	0.021	0.882

With an MAE of 0.104, the MSE of 0.020, as well as R^2 of 0.888 the LightGBM model had the best performance.

3.4. Results of the Ensemble Learning Model:

Combining forecasts to gradient boosters such as XGBoost, AdaBoost, LightGBM, as well as Catboost, a voting-based model for regression (VotingRegressor) was developed. (Table 3)

Table 3. Voting-based Model for Regression

Model	MAE	MSE	R^2
VotingRegressor	0.106	0.021	0.885

LightGBM stayed better even though the combined model did fairly.

Figure 2 offers a comparison of real and ensemble learning model prediction values. The chart in Figure 2 shows that numerous forecasts the cluster within the line, suggesting that, in most situations, the model could provide predictions near to the real values.

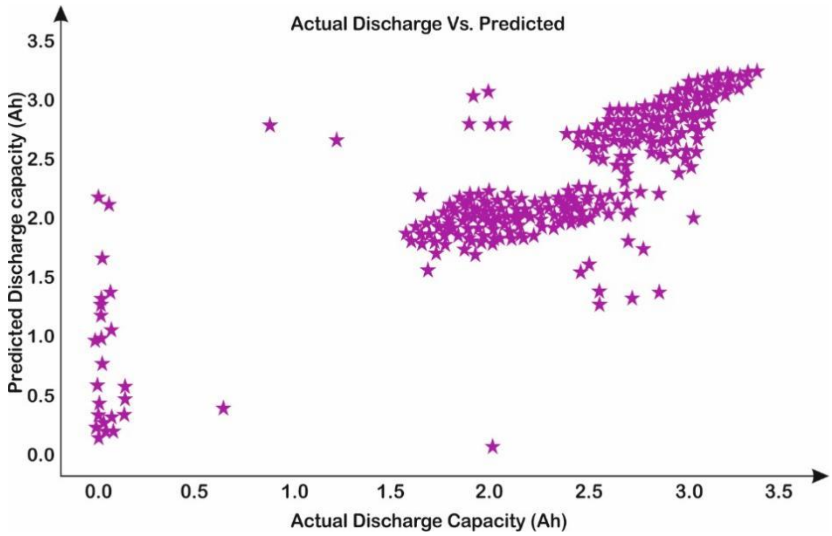

Figure 2. Predicted and Actual Ensemble Model

3.5. Analysis of Explainability in AI Models:

The LightGBM model was examined using the SHAP approach in order to find feature influence on forecasts. (Table 4)

Table 4. Feature Significance Depends on SHAP Values

Feature	SHAP Value Contribution
Temperature	+0.18
Current (A)	+0.11
Cycle Index	-0.08
Voltage (V)	-0.02

While Cycle Index significantly impacted the model's forecasts, temperature had the most favourable effect. The line showing the average absolute values for SHAP can be seen in Figure 3.

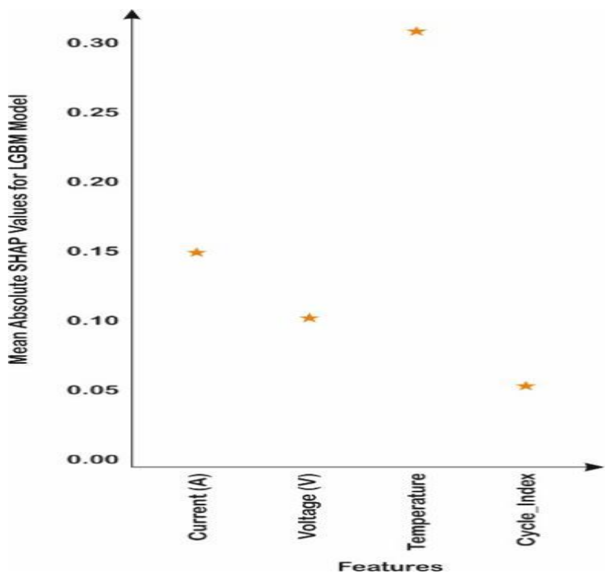

Figure 3. SHAP Values Help Us Interpret LightGBM Model Decisions

3.6. Mathematical Modelling:
The performance of the model was validated by means of a simulation under many scenarios.

- Gradient Boosting Optimization:

$$F_m(x) = F_{m-1}(x) + \gamma_m h_m(x) \quad (7)$$

- LightGBM Growth Strategy:

$$\text{Score}_{\text{split}} = \frac{(\text{Gradient})^2}{\text{Hessian} + \lambda} \quad (8)$$

Final Verification of Accuracy:

- Various discharge capacities were tested against model residual errors.
- Examined were temperature fluctuations in relation to SoH forecasts.

With the lowest error rates, LightGBM proved better in estimating LiBs' SoH. With Temperature as the most important element, the SHAP study gave important new understanding of feature relevance. Future research might look at other optimization strategies to raise prediction accuracy even further.

4. Discussion:

4.1. LiB Performance Management: An Introduction to Machine Learning:
Forecasting lithium-ion battery (LiB) management for performance in EVs (electric vehicles) utilizing machine learning (ML) approaches has made notable advancement recently. ML models have been shown in many studies to be successful in approximating important battery metrics like terminal voltage, capacity, state of charge (SoC), and residual usable life (RUL).
4.2. Methodological Comparisons and Insights for SoC Estimation ML Algorithues:
Six ML techniques are evaluated for LiB SoC estimation:

- Artificial Neural Networks (ANN)
- Support Vector Machines (SVM)
- Linear Regression (LR)
- Gaussian Process Regression (GPR)
- Ensemble Boosting Algorithm A (EBa)
- Ensemble Boosting Algorithm B (EBo)

Table 5. ML Algorithms for SoC Estimation

ML Algorithm	Performance Metrics (SoC Estimation)
ANN	85% MAE Accuracy
GPR	High accuracy in capturing battery patterns
SVM, LR, EBa, EBo	Performed lower compared to ANN and GPR

4.2.1. Estimates of Voltage and Capacity:
Using historical data and WLTP discharge testing on an NMC cell, trained boosted tree models. Results show that boosted trees did quite well in cell voltage prediction. Enhanced SoC forecasts via a direct multistep-ahead forecasting system. Suggested a Multioutput Convolved Gaussian-Process (MCGP) models verified using experimental data. Enhanced LiB capacity estimation accuracy. Improved the battery cell RUL prediction.
4.3. A SHAP-based XAI method for predicting LiB performance:
One of the clear gaps in current studies is the LiB prediction model application of explainable artificial intelligence (XAI) methods. This work makes a major contribution by using SHapley Additive exPlanations (the SHAP method) to: • Explanation of feature influence LiB performance forecasts. • Boost ML models' interpretability. • Boost capacity's and SoC's predictive accuracy. Figure 4 shows the SHAP-Based XAI Methodology.

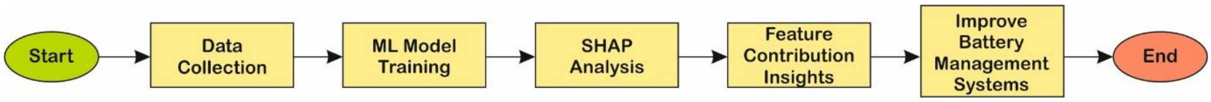

Figure 4. SHAP-Based XAI Methodology

4.3.1. Strategic Views and Connotations for Systems of Battery Management:
Results of this work show: ANN and GPR show their capacity in capturing battery actions because they outperform other ML methods in SoC estimate. SHAP values help to better manage LiB by offering strategic understanding of feature relevance. XAI approaches help to maximize battery management, therefore guaranteeing more effective energy use in electric vehicles. By combining SHAP-based XAI techniques with ML models, this work makes the area of LiB management of performance better. Being able to understand what models are saying makes battery optimization techniques a lot stronger. This results in more sustainable and effective energy management in electric vehicles.

5. Conclusion:

This work assessed performance of many ML models in forecasting ability to discharge of lithium-ion batteries, with LightGBM showing to be the best-performance model. Using SHAP-based explainable artificial intelligence (XAI) gave important new understanding of how voltage, cycle index, temperature, and current affect battery performance. Although ML models show great predictive power, actual application poses difficulties like computational complexity as well as real-time data processing. Future developments should concentrate on improving their flexibility and efficiency by integrating machine learning algorithms into current surveillance systems for electrically powered vehicles as well energy grids. Minimizing environmental effect and promoting a circular economy depend on LiBs' sustainability via responsible recycling along with secondary usage also. This work advances more dependable and sustainable battery administration techniques by enhancing prediction models and including XAI.

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