Optimizing Battery Charge Prediction Accuracy Utilizing Machine Learning Methods

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Abstract: Energy storage systems are more cost-effective when they correctly manage the capacity for lithium-ion batteries (LiBs), especially when they are used on a big scale. The design saves money, in the long run, to repair or fix LiBs less often. To determine the amount that LiBs were capable of holding, adaptive boosting (AdaBoost), extreme gradient boosting (XGBoost), gradient boosting, light gradient boosting machine (LightGBM), category boosting (CatBoost), as well as ensemble learning models are utilized. Employing the mean absolute error (MAE), and the mean squared error (MSE) along R2 numbers, the researcher compared the accuracy with which each model could predict future outcomes. For example, the LightGBM model had the least MAE (0.102) as well as MSE (0.018) values, as well as the greatest R-squared (0.886) value, which means that its predictions were most closely related to reality. It was about the same in terms of speed among the gradient boosting as well as XGBoost models, which came next to LightGBM. The ensemble model's efficiency suggests that integrating many models might result in an overall increase in performance. In addition, the research uses Shapley additive explanations (SHAP) values to analyze important aspects influencing model predictions within the context of explainable artificial intelligence (XAI). This study found that discharge capacity is strongly influenced by temperature, cycle index, voltage, and power. This study demonstrates that Machine Learning (ML) methods can improve energy storage systems and regulate LiB in XAI.

Keywords: Machine Learning, Explainable Artificial Intelligence, Shapley Additive Explanations, Lithium-Ion Batteries, Energy Storage Systems.

1. Introduction

The substantial energy density, low discharge rates, lightweight setting up, rapid charging speed, and minimal maintenance needs of LiBs make them an essential power of electric vehicles (EVs) [1]. LiBs' qualities have made them the preferred power source of EVs in several applications. With electrification reducing overall carbon footprints and greenhouse emissions compared to traditional fossil fuel automobiles, LiBs have become more appealing as alternative sources of energy [2–5].

The state of health (SoH) parameter serves as a crucial element to estimate the efficacy of LiB. This acts as a significant factor in several domains, including personal electronics, electric vehicles, and grid-scale power storage [6-8]. SoH indicates the current performance of a battery and its power capacity relative to its starting condition. It assists in estimating the length of efficacy & total efficiency [9-14]. It includes essential factors like capacity depletion, internal resistance disparities, durability of cycle & security issues. It is a crucial factor to improve corporate security, sustainability of the environment & cost efficiency [15-18].

Advanced SoH assessment methodology, including ML algorithms and diagnostic technologies, is enabling more advanced battery management systems comprising continuous monitoring, predictive maintenance, and adaptive control [19]. This proactive technique extends battery life and enhances maintainable practices by avoiding early substitutions & increasing resource usage as well as reprocessing. Molecular dynamics simulations & density functional theory are two advanced methodologies for evaluating lithium-ion battery performance [20,21]. Molecular dynamics simulations of battery atomic and molecular interactions may help researchers understand material behaviour [22].

Employing explainable artificial intelligence (XAI) methods is important for LiB as it simplifies prediction models. This facilitates control and comprehension of how well battery's function and maintain their optimum condition. What distinguishes this study is that XAI approaches are used in place of the conventional methods for assessing SoH for LiBs [23]. deteriorating and breakdown processes that impact battery performance may be promptly identified by the modern battery management systems.

The proposed XAI-based method uses ML & AI techniques that work together for making battery life signal estimation with high accuracy. Accordingly, model characteristics may optimize lifespan while reducing maintenance expenses to a minimum [24]. By maximizing the intervals among battery replacements, this strategy also seeks to reduce its negative effects on the environment and create more sustainable use of resources [25]. Thus, the research presents a key improvement in battery technology, particularly with XAI, that offers improved sustainability and dependability.

PCA, LR, RR, k-nearest neighbours (k-NN), RF, polynomial regression and gradient boosting were used for estimating Li-ion battery SoH in this research. Each model was assessed for accuracy, computational effectiveness, and interpretability. Utilizing SHAP, the researcher examined each model's explainability and how each attribute affected the model's predictions. Complex algorithms like random forest & gradient boosting are more accurate, while simpler models like linear regression & k-NN, along with XAI approaches, reveal battery degradation aspects more clearly.

The suggested models work for both Li-ion and Na-ion cells, too. Combining ML as well as XAI methods, this study attempts to determine how much lithium-ion batteries can be discharged. This paper has three parts. The second part goes into detail about the materials and methods used. The third part shows the results of the experiments and the conclusions based on SHAP studies. It examines the results in the fourth segment. Finally, it sums up the study's findings, including the conclusion, in the fifth and last part.

2. Materials and Methods

This section discusses regarding the way the study was organized, the dataset that was utilized, and the ML as well as AI techniques that were evaluated. Large amounts of information are given about every technique and the factors that were used to make the study repeatable and the approach clearer. Researchers carefully talked about the scientific reasons behind their choices of each material and method. According to the study, ML algorithms like AdaBoost, gradient boosting, LightGBM, XGBoost as well as CatBoost were used to build a model. Figure 1 shows an illustration that shows the steps that were taken to make the model.

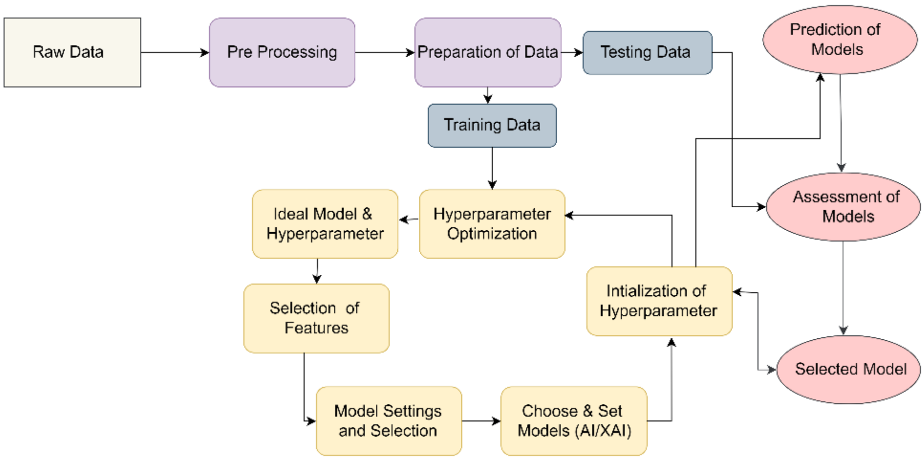

Figure 1 Model's Flowprocess.

Figure 1's flowchart provides additional details on the work's training and testing methods. This flowchart ensures transparency and consistency by explicitly illustrating the actions taken at each stage of the model creation process. Following the application of the required preprocessing procedures to the raw data, the models are applied to the training and testing datasets. The model was assessed at the last stage.

2.1. Description of Dataset

For this analysis, researchers combed through 45,698 records detailing various aspects of battery exhaustion cycles. The researcher trained on 80% of the dataset and tested on 20%. Training and testing made use of a combined total of 38,844 and 6854 data points, respectively. To define the electrical efficiency of the batteries in the dataset, features like "Temperature," "Current (A)," "Voltage (V)," "Cycle Index," and "Discharge Capacity (Ah)" were important. This study's dataset was taken from an extensive database detailing the features of battery exhaustion cycles. With every cycle, researchers tracked the number of metrics related to the battery-exhausting procedure.

The research examined LIB samples for 750 cycles. C-rates and temperatures were varied for all charge/discharge experiments within the 3.0 to 4.3 V voltage range. Every test condition had 7 cells, totalling 191. In each condition, 7 cells were tested at various temperature ranges (10, 25, 45 & 60), discharge rates (0.6C, 1C and 2C), and charge cut-off rates (C/5 and C/40) in the CV procedure. These investigations used $LiCoO2$ (cathode)-graphite (anode) cells. ML models were trained using the discharge and charge datasets from these experiments. ML models were then trained using the charge & discharge statistics gathered from these experiments. In the preprocessing stage, the dataset's first 300 cycles were utilized for training. Accordingly, 450 cycles from 301 to 750 were eliminated from the test and training datasets. To improve its suitability for direct usage, the dataset underwent several preparation procedures. The dataset was discovered to have no missing values when one of these procedures was used to correct missing data. It was assured that outliers would be identified and corrected. The model was given a stable technique all over the training & evaluation stages thanks to this process. The dataset's initial 300 cycles were used for training and testing.

2.2. Selection of a Model

This study compared AdaBoost, CatBoost, LightGBM, XGBoost, & gradient boosting to train models. Due to their unique merits, these algorithms were picked. The most effective strategy depends on the dataset as well as the results. Contrasting and estimating methods help determine the most effective one for a dataset. The algorithms were trained on the training subset of the dataset, and their performance was evaluated on the subset of the test. A summary of SHAP is provided along with the outcomes and the data from the LightGBM model.

The way AdaBoost speeds processes up is by making a lot of useless algorithms that fix mistakes in classification. Most of the time, AdaBoost is known for being able to handle noise and mistakes well. Overfitting is more likely when the data structures are complicated, but it works well when the datasets are small and simple.

The technique called LightGBM can analyze big datasets while using minimal memory. The benefits of LightGBM become increasingly apparent as the dataset's size and feature count increases. It builds datasets in a leaf-wise fashion by using a leaf-wise method. The model can learn more quickly because of its leaf-wise structure. CatBoost has been specifically designed to handle categorical variables. By automatically converting category characteristics, this approach may lessen the requirement for feature engineering. In general, CatBoost has a strong structure that lowers the possibility of overfitting. For optimal outcomes, repeated parameter adjustment could still be necessary.

Gradient boosting improves weak learners via error correction to create a model. New trees eliminate mistakes from the earlier ones. Customizability makes gradient boosting advantageous. Model-tuning parameter optimization takes time. Scalability, as well as efficiency, are improved via XGBoost for gradient boosting. It excels in efficiently processing huge datasets and using regularization features to improve the accuracy of the models. Missing data and cross-validation are supported by XGBoost.

The selection of these methods was greatly impacted by the size and variety of the dataset. The ability of each method to adjust to the quantity and complexity of the dataset was the basis for evaluation. CatBoost was specially chosen for the dataset because of its capacity to analyze categorical data and the effectiveness of the XGBoost & LightGBM algorithms in handling huge datasets. SHAP provides insight into the factors that impact model predictions. In mission-critical applications, such as LiB lifetime prediction, it improves decision-making and shows where the model may be enhanced. In this work, the model's efficiency is improved & the scientific rate is increased by the system's choices through the combination of boosted tree-based technique with the SHAP approach.

3. Experimental Outcomes

The performance ratings of the algorithms as well as how well each model predicted the SoH of LiBs are provided in this section. The SHAP technique benefits in understanding technique prediction & making choices are additionally examined.

3.1. Evaluation Criteria for Models

Standard regression measures, like MSE, MAE, and R2 (R-squared), were used to evaluate the extent to which the models worked. These metrics check the accuracy of the models' predicted values that were seen along with how well they were able to adapt to the task.

MSE values quantify the variation among each model's predicted and actual values. Better model performance is indicated by less MSE.

$$\mathrm{MSE} = \frac{1}{\mathrm{N}}\sum_{\mathrm{i}}^{\mathrm{N}}\left[\Upsilon_{\mathrm{i}} - \Upsilon_{\mathrm{prediction\ (i)}}\right]^{2} \qquad (1)$$

The R2 number tells you the extent to which the model describes the differences among the dependent & independent factors. If the R^2 number is near to 1, indicates the model fits well and describes most of the data.

$$R^2 = 1 - \frac{\sum_i^N [\Upsilon_i - \Upsilon_{prediction\ (i)}]^2}{\sum_i^N [\Upsilon_i - \Upsilon_{mean}]^2} \quad (2)$$

To figure out where each model is, the researcher may look at their MAE values. Model performance is improved with a lower MAE:

$$MAE \frac{1}{N} \sum_{i=1}^{N} |\Upsilon_i - \Upsilon_{prediction}| \quad (3)$$

3.2. Training of Models

For model training, 5 learning algorithms were employed: AdaBoost, CatBoost, XGBoost, LightGBM, and gradient boosting. These algorithms use ensemble learning techniques to combine many weak learners to produce a robust model. To produce a more robust model, these techniques combine predictions from many separate models made using various algorithms or variations of the same methodology. By mitigating the shortcomings of a single system, ensemble learning improves the performance of estimation. Utilizing several model advantages to make up for the mistakes, this method greatly improves the precision of model estimates. There are, however, differences in the manner in which this method works, and testing them on specific datasets is the only way to be sure they'll work for a given job. The study's dataset and the significance of ensemble learning modelling help to make accurate and reliable predictions, especially when it comes to estimating the SoH of LiBs, which single models might not be able to accomplish. Therefore, the model gives better and more accurate outcomes in real-life situations. Figure 2 shows complete information about the hyperparameters for the models utilized in the research.

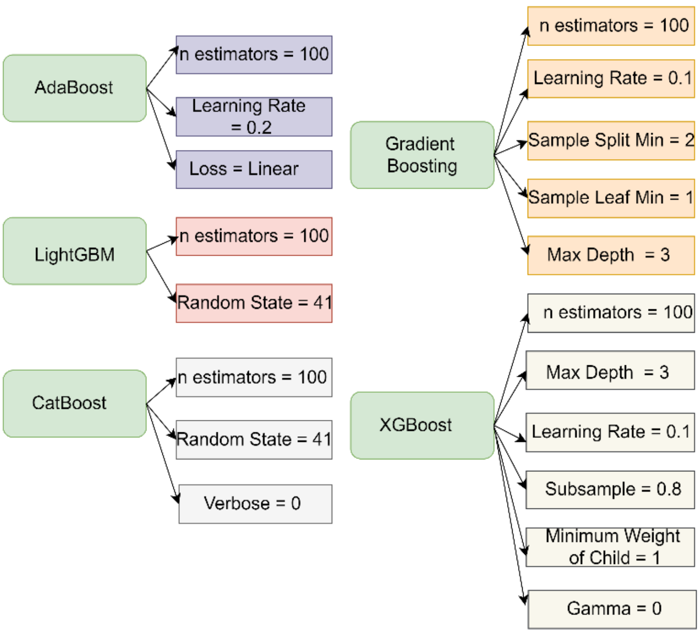

Figure 2 Proposed Model's Hyperparameters.

Hyperparameters for AdaBoost, XGBoost, LightGBM gradient boosting as well as CatBoost models are identified in Figure 2. The iteration number ("n_estimators") had been scheduled to hundred for each model, with customized learning rates and parameters to improve data fit and learning speed. To assure repeatability, AdaBoost used a "linear" loss function, gradient boosting used branching criteria, XGBoost used sampling and splitting criteria, and LightGBM and CatBoost used "random_state" parameters. By controlling the extent to which deep learning algorithms do in the data at training and how fast they change, these factors have a big impact on how well the models do. As a last step, the "random_state" setting was changed to 41 and the "verbose" level was altered to 0. There is a big difference between these hyperparameters and the general success of the model because they determine the depth to which each model learns during training, how quickly it adapts, and how effectively it fits the data.

3.3. Model Contrasts Outcomes

Figure 3 shows the performance measures we got when we used different boosting methods for ensemble learning on the dataset. The model's results are judged by the extent to which each indicator correlates.

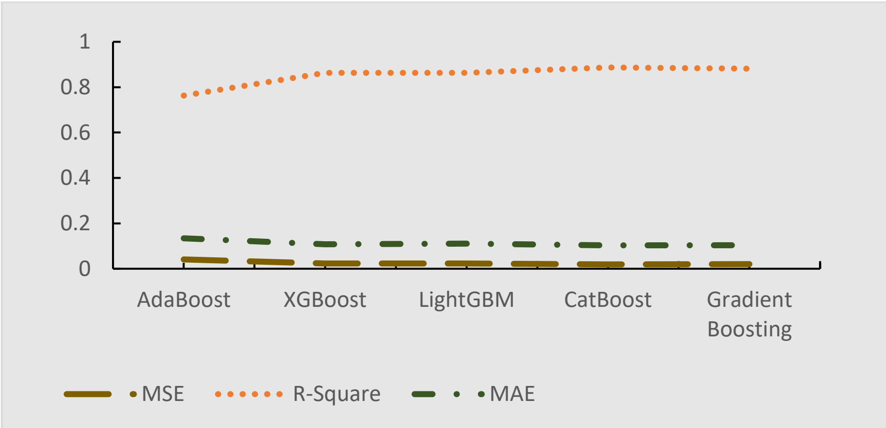

Figure 3 Comparison of Model Outcomes.

The effectiveness of five distinct models in predicting the SoH of LiBs is shown in Figure 3. The LightGBM model performed most effectively among these models, with a 0.886 R-squared, 0.018 MSE, and 0.104 MAE.

Performance is enhanced in LightGBM (boosting algorithm). Innovative techniques like histogram-dependent training & leaf dependent tree development provide efficient processing of significant, HD information. These qualities form LightGBM a popular technique for large-scale ML tasks. Instead of level-wise tree growth, LightGBM utilizes leaf-wise development, unlike other boosting algorithms like XGBoost. Starting with the leaf with the largest mistake rate, trees deepen leaf-wise. This creates more complicated decision boundaries with stronger generalization power than same-depth trees. Figure 4 shows several estimations clustered near the line, suggesting the model may match real values in most situations. However, low & high capacity values are different. These ranges may affect model accuracy. Further, the model operates better at 1.5 Ah & 2.5 Ah, as estimated by clustering.

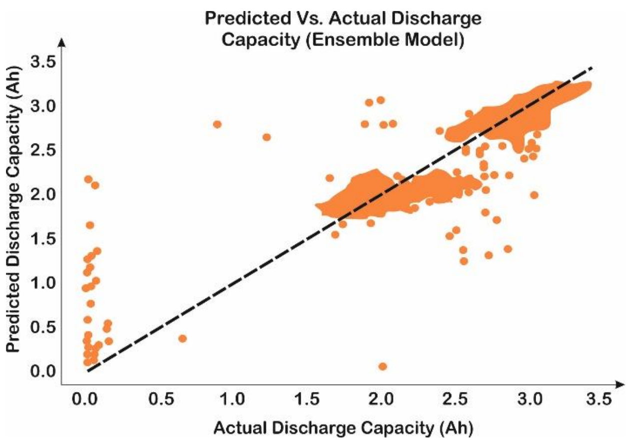

Figure 4 Estimation of Ensemble Model.

3.4. Ensemble Learning Model Output

Voting Regressor, a voting-based regression model, was created as part of the project. Many regression models' results are added together to make a combined model by Voting Regressor. Five regression methods make up this model: XGBoost, AdaBoost, LightGBM, gradient boosting & CatBoost.

Every submodel must be able to generate estimations and have had prior training for the overall model to succeed. The Voting Regressor sums together all of these models' forecasts by calculating their average. This may increase the overall accuracy of forecasts by using the best features of several models and compensating for their shortcomings. The ensemble model used in the research produced consistent findings among models, with an R-squared of 0.883, an MAE of 0.104, and an MSE of 0.019.

The LightGBM model outperformed the ensemble system, of LightGBM's efficiency in dealing with dataset complexity and its capacity to adapt to dataset features via its leaf-wise growth strategy. However, it's possible that the ensemble model's fundamental average of predictions from multiple models doesn't always capture the unique characteristics and strengths of each model. Proper data preprocessing and model parameterization are crucial, as shown by LightGBM's higher performance compared to other models.

3.5. Analyzing the Explainability of AI Models

SHAP explainability analysis was performed on the LightGBM method, which predicted LiB discharge capabilities successfully. SHAP uses game theory-derived Shapley values to quantify the influence of attributes on model predictions. This research revealed the biggest and weakest effects on predictions, helping clarify the way the model worked and the dynamics behind estimations. This study graphically illustrates which factors the model provides greater importance to as well as how these features affect the results of predictions. Figure 5 uses the SHAP model to describe the effects of the four primary characteristics that the LightGBM model uses to estimate LiB discharge capacity. The SHAP approach is used to analyze the LightGBM algorithm's choices, which provide the greatest efficiency and outcomes, once all dataset characteristics and predictions have been established. The influence ratios of the feature names "Temperature," "Current," "Voltage," and "Cycle Index" in defining the resultant characteristic "Discharge Capacity" are assessed when interpreting using the SHAP approach.

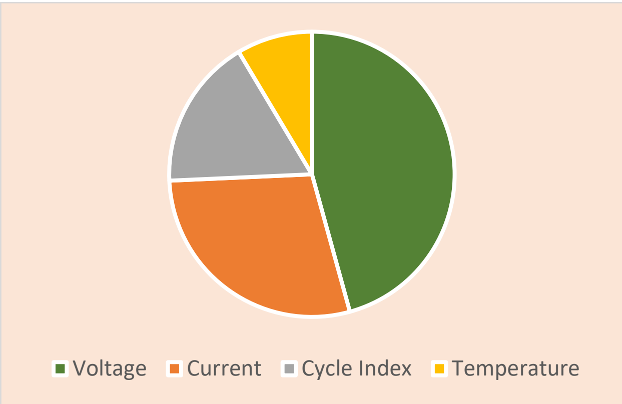

Figure 5 LGBM Model SHAP Value.

Positive SHAP values for "Temperature" and "Current (A)" in Figure 5 indicate that these characteristics improve model predictions. The largest positive influence (+0.16) comes from "Temperature" implying that increasing temperature improves discharge capacity estimation. Predictions benefit less from "Current (A)" (+0.1). In contrast, "Cycle_Index" and "Voltage(V)" have negative SHAP values, lowering model predictions. The most important thing that changes model estimates is "Cycle_Index" (-0.06). "Voltage (V)" has a smaller effect (-0.01). The final model estimate for f(X) is 3.062, with an E[f(X)] value of 2.872. This can be obtained through incorporating the SHAP numbers. This makes it very clear how the sum of the effects of traits leads to modifications in model results. The graph of the mean absolute SHAP values can be seen in Figure 6.

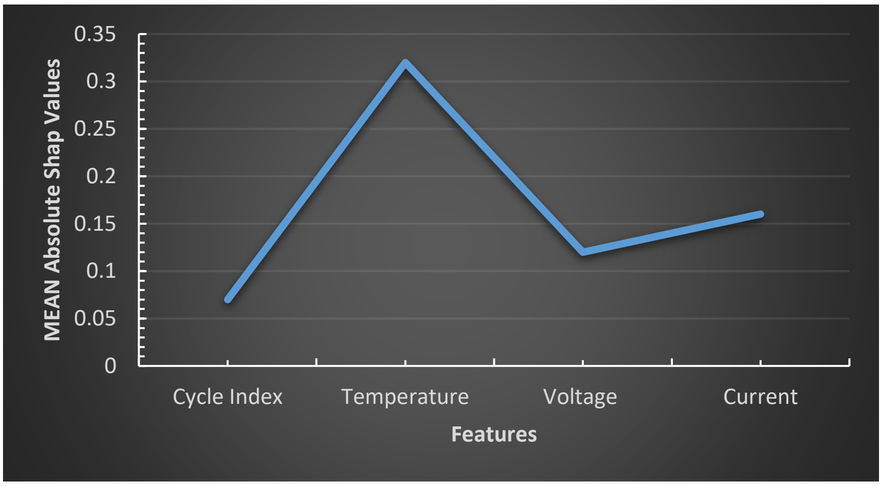

Figure 6 Explainability of LightGBM Model Parameters with SHAP Values.

The "Temperature" characteristic includes the most influence on "Discharge Capacity (Ah)" predictions, according to the data shown in Figure 5, & SHAP values often fall between -1.4 & 0.4. The majority of "Current" attributes's SHAP values fall inside the positive range, which spans from -0.4 to 0.2. The "Cycle_Index" feature's SHAP values mostly show negative impacts, ranging between -0.2 and -0.1, while the "Voltage" feature's SHAP values range between -0.4 and 0.1.

Discharge capacity decreases with low temperature and increases with high temperature. One of the five models, the LightGBM model, has the smallest MSE as well as MAE and the greatest R-squared value, suggesting the strongest connection between predicted and actual outcomes. XGBoost and gradient boosting function identical to LightGBM.

It's possible that integrating these models may result in a model that performs well generally because the ensemble model does well. SHAP figures out the extent to which every case is affected by a model along with the changes as a result. According to these numbers, the traits that help the model make predictions are more or less important. Different values show how important a certain trait is to the change in predictions.

4. Discussion

Predictive precision on LiB capacities has been the subject of several research; nevertheless, there are very few instances of XAI approaches being used in this domain. As a result, the present work, which makes use of SHAP, makes a substantial contribution to the body of literature. To determine which characteristics and to what degree they affect a model's predictions, SHAP values are used. In particular, factors influencing lithium-ion battery performance and their role in forecasting have been thoroughly examined. The current work improved the dependability of the models utilized for predicting the state and ability of LiBs by facilitating an improved comprehension of those models.

Existing ML methods used to estimate the state and ability of LiBs are compared with the results discussed in the chapter on testing results. This study must give important strategic information for improving and creating battery management systems, especially by using SHAP-based XAI methods. These results indicate that SHAP values are very important for figuring out which traits affect model predictions and how much. By learning more about battery technologies, this method makes their applications broader.

It is important to note that ANN and GPR models can capture battery activity more accurately compared to other ML methods when it comes to predicting SoC. Consequently, this research allows for the creation of management systems that may enhance battery usage efficiency and strengthen models employed for predicting LiB performance.
This strategy may yield critical information for the improvement and advancement of battery managing schemes, facilitating high effectual battery utilisation. Consequently, the SHAP-dependent XAI research enhances the understanding of battery technologies as well as widens the applicability.

5. Conclusion

This research looked at whether the different ML models could predict the charging capacity of LiBs. It specifically looked at AdaBoost, XGBoost, LightGBM, CatBoost, gradient boosting as well as an ensemble learning system. The results showed that the LightGBM did more effectively than other models. It had the smallest MAE as well as MSE values and also a higher R-squared value, which means that expected and real values were strongly related. Gradient boosting and also XGBoost both worked about the same, but they were somewhat behind LightGBM.
By highlighting the ease with which many models may be combined to create a strong prediction framework, the ensemble model of learning demonstrated competitive performance. The importance of several characteristics including temperatures, cycle index, voltage & current in impacting predictions was underlined by the use of SHAP values to explain the most effective model, LightGBM. Temperature in particular turned out to be a crucial factor. High temperatures hurt discharge capacity, according to XAI investigations, which is consistent with physical predictions for battery performance.
Study findings show ML models effectively forecast LiB status and capability. Applications of these techniques in real-time applications face real obstacles over the algorithm tolerability, including the model's complexity, computational specifications & capacity of real-time information processing, that might hinder their incorporation into industrial applications. ML models in electric car battery management systems may use real-time information like traffic jams, driving style & weather to improve battery life and range. These models can predict the extent to which energy will be needed in smart grids that employ green energy. This makes the grids more energy efficient and lowers the costs of running them. In plants, ML models may figure out when battery-powered equipment needs repair so that they can predict when it will break down. These real-time uses show how useful the model is in the real world and how well it can be used in commercial settings. Using smarter BMS systems that use AI and ML can assist with keeping a check on and taking care of battery longevity, making sure that the right number of charging and discharge processes are used to extend battery life.
To further improve prediction accuracy, future research can investigate more intricate ensemble techniques that use more varied or recent machine learning models. Adding these techniques to real-time tracking models for EVs might give estimations that are dynamic and may modify to changing conditions. This would help make the most effective use of batteries and increase their life. More thorough insights will be obtained from a closer examination of other characteristics that could influence battery life, such as environmental influences or material deterioration. Prediction-based models may become more applicable and have a greater influence on various energy systems if they are extended to other battery & storage technologies.
It's important to keep working on XAI models because understanding model predictions could have significant impacts on design and operation decisions. It's especially important for sensitive uses like electric cars. As more important apps use ML models, it becomes more important to create rules and guidelines that make sure they are safe and reliable. Through the use of XAI, transparency is ensured and useful insights are obtained that may impact future

advancements in battery technology. As the demand for alternative sources of energy expands, it will be necessary to define the physical characteristics of LiBs as well as the relationships between the estimation algorithms to develop more accurate models for prediction and interpret them using XAI approaches.
If Li-ion batteries drop their power, it's important to get rid of them properly and recycle them. Also, repairing used batteries so they can be used in less demanding situations again could make them last longer and support the cycle economy. Effective and long-lasting ways to handle used lithium-ion batteries are needed to protect the environment and meet the increasing demand for battery materials.

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