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A standardized comparative framework for machine learning techniques in lithium-ion battery state of health estimation

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ABSTRACT

The accurate estimation of lithium-ion battery State of Health (SOH) is essential for enhancing performance, safety, and lifecycle management in modern energy systems. While numerous individual studies have explored machine learning approaches for SOH prediction, a systematic comparative analysis using consistent experimental protocols and rigorous cross-validation remains limited. This study addresses this gap by presenting the first comprehensive comparison of three advanced machine learning models—Extreme Gradient Boosting (XGBoost), Random Forest, and Support Vector Machine (SVM)—using a standardized experimental framework with NASA battery datasets. Our novel contribution lies in implementing a unified training-testing protocol using battery #5 for training and batteries #6, #7, and #18 for validation, combined with systematic hyperparameter optimization through grid search and k-fold cross-validation. Key improvements include: (1) first standardized one-to-many validation protocol ensuring cross-battery generalization assessment that eliminates the data splitting limitations of previous comparative studies, (2) unified hyperparameter optimization methodology applied identically across all algorithms, eliminating the confounding effects of inconsistent parameter tuning that have biased previous comparisons, and (3) establishment of quantitative performance benchmarks providing evidence-based model selection criteria for practical Battery Management System (BMS) applications. The XGBoost model achieved superior performance with MAE of 0.016 and MSE of 0.000347, establishing empirical benchmarks for model selection in battery health diagnostics through our systematic comparative methodology. This work provides the first standardized comparative framework for SOH estimation, offering evidence-based guidance for BMS implementations and advancing the field toward more rigorous and replicable research practices in battery prognostics.

1. Introduction

1.1. Introduction to energy storage and batteries

The global demand for energy is steadily increasing due to economic development and population growth. While traditional fossil fuel sources like oil, gas, and coal have historically been the primary energy sources, their availability is limited and is not sustainable in the long term. Renewable energy sources such as wind, solar, hydroelectricity, and geothermal energy are becoming increasingly accessible and cost-effective. Nonetheless, the continued reliance on fossil fuels contributes to environmental problems such as air pollution, water contamination, and greenhouse gas emissions, which exacerbate global warming and climate change [1,2]. Thus, there is an urgent need for new energy sources to meet the daily requirements of energy across the globe. A remarkable limitation of renewable energy sources is that that they are stochastic (thus not completely programmable) and highly fluctuating in daytime/night or season cycles. These matters of fact motivate the importance of doing research in the field of innovative energy storage technologies.

Among the various types of batteries, lithium-ion batteries stand out due to their high energy density, long lifetime, stable electrochemical properties, ability to store electrical energy with low loss, and absence of memory effect. These batteries are commonly used in various applications, including consumer electronics, electric vehicles, military systems, and maritime and space systems [3,4]. Compared to other battery types, lithium-ion batteries offer several advantages such as longer cycle lives, shorter recharge times, low self-discharge rates, and high-power densities [5].

Lithium-ion batteries are widely used in various applications, from

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portable electronic devices to electric vehicles and renewable energy systems [6]. However, these batteries have limitations in terms of performance and reliability, such as a decline in capacity, increased internal resistance, and shortened lifespan. To ensure safe and reliable operation, battery prognostics and diagnostics play a crucial role in predicting a battery's future health and remaining useful life, as well as identifying faults or anomalies in its operation [7].

1.2. Traditional methods and data-driven approaches

Traditional methods for battery prognostics and diagnostics rely on physical models and empirical methods, which may not accurately capture the complex electrochemical processes occurring in lithium-ion batteries. To overcome this, prognostics for lithium-ion batteries have emerged as a promising approach that leverages real-time data analysis from the battery system. However, as batteries age and deteriorate over time and usage, accurate estimation of their health status is essential to optimize maintenance and replacement strategies, prevent unexpected failures, and improve their economic and societal use [8]. With the ongoing demand for reliable and efficient energy storage solutions, accurate battery prognostics and diagnostics will continue to be a critical research area for enhancing the performance and safety of lithium-ion batteries in various applications.

With the ability to leverage the vast amounts of data generated by batteries during their operation, data-driven methods have emerged as a promising approach for battery prognostics and diagnostics [9]. A brief overview of recent advancements in data-driven methods for lithium-ion battery prognostics and diagnostics is presented here on.

Currently, there exists a multitude of studies that aim to evaluate the health status of lithium-ion batteries. These research approaches can be broadly classified into three types. The first method is the direct measurement method, which employs Coulomb counting or internal resistance measurement [10,11]. This method offers a simple and straightforward implementation, as the SOC of the battery is estimated through Coulomb counting by integrating the current during charging and discharging. Similarly, the internal resistance measurement method estimates the SOH of the battery by measuring its internal resistance through hybrid pulse power characterization. However, this method is susceptible to measurement noise due to the high precision requirements. The second method, called the physical failure method, estimates SOH by analyzing the physical characteristics of the battery, such as temperature, voltage, current, and electrolyte concentration. This method accounts for the effects of multiple dimensions and requires a considerable amount of computation, making it less efficient for SOH estimation at present. The third method is the data-driven method [11], which has gained prominence in recent years due to the increase in computing power. Data-driven methods have emerged as a highly promising approach for battery prognostics and diagnostics, as they have the ability to leverage the vast amounts of data generated by batteries during their operation. These methods utilize machine learning algorithms to extract patterns and relationships from the data, which can then be used to predict the battery's future health and diagnose faults [12]. Multiple studies have explored the application of data-driven methods for battery prognostics and diagnostics, yielding highly promising results.

Data-driven methods leverage test data of battery characteristics to study the relationship between the data and SOH, rather than researching the battery characteristics to find the best mathematical model for SOH estimation. Artificial neural networks (ANNs) have emerged as one of the most widely used data-driven methods for battery prognostics and diagnostics. For instance, a study conducted by Zhang et al. [13], implemented ANNs to predict the remaining useful life of lithium-ion batteries by analyzing their discharge capacity data. The results showed that ANNs could accurately predict the remaining useful life of the batteries, outperforming traditional physical models and empirical methods. Another study, conducted by Li et al. [14], proposed a spatial-temporal network model (OL-STRULF) that integrates a temporal attention mechanism and spatial LSTM to account for the capacity self-recovery effect in lithium-ion batteries. By extracting health factors from charging voltage and current data, the model achieved higher accuracy in predicting remaining useful life compared to existing methods, particularly under varying operating conditions. Yang et al. [15] developed a fractional-order model-based diagnostic approach to detect external short circuit (ESC) faults in lithium-ion batteries used in all-climate electric vehicles. By comparing fractional-order models with first-order RC models and employing a random forest classifier for electrolyte leakage detection, the proposed three-step framework efficiently diagnosed ESC faults and leakage conditions with high accuracy across various test scenarios

Li et al. [16] proposed a hybrid Elman-LSTM model for predicting the remaining useful life of lithium-ion batteries. By decomposing capacity data and applying neural networks to different frequency components, the model achieved high accuracy, with prediction errors below 3.3 % on unseen datasets. Chang et al. [17] proposed a GA-optimized wavelet neural network (GA-WNN) model for lithium-ion battery SOH estimation, using features extracted from incremental capacity curves. The method achieved high accuracy, with estimation errors under 3 %, demonstrating its effectiveness for real-time SOH prediction.

Apart from ANNs and SVMs, various other data-driven methods have been explored for battery prognostics and diagnostics, such as the Gaussian process (GP) [18], decision trees [19], random forest (RF) [20], and deep learning (DL) [21]. Although GP relies partially on the initial population selection in the genetic algorithm, it remains a promising technique. In contrast, XGBoost, which is a highly efficient, flexible, and portable optimized distributed gradient boosting library, implements machine learning algorithms under the Gradient Boosting framework and offers strong nonlinear fitting capabilities for efficient learning [22]. These methods have yielded highly promising results in accurately predicting the remaining useful life of lithium-ion batteries, as well as identifying faults or anomalies in their operation.

Traditional battery prognostic methods, such as empirical, analytical, and rule-based models, have been foundational in understanding battery health by relying heavily on the chemical and physical processes within the battery. Empirical models, like those discussed by Broussely et al. [23], utilize historical degradation data, while analytical models require detailed electrochemical knowledge, as explored by E. V. Thomas et al. [24]. Rule-based models apply fixed rules or thresholds to predict battery life, a method discussed in [25] for its lack of adaptability to new battery types and usage patterns. Conversely, data-driven methods have gained prominence, leveraging machine learning algorithms and statistical models to predict future battery performance without detailed knowledge of internal chemistry. Studies shown in [26] have shown how machine learning models like convolutional neural network can outperform traditional methods and robust. Ensemble methods, detailed by [27], handle complex relationships more effectively, while advanced deep learning techniques, such as LSTM [28], capture the temporal dynamics of battery usage with high accuracy.

1.3. Recent advances in battery SOH estimation

Recent developments in battery SOH estimation have demonstrated remarkable progress in addressing traditional limitations. Advanced deep learning approaches have emerged that eliminate the need for time-consuming degradation experiments, with frameworks achieving absolute errors of less than 3 % for 89.4 % of samples using 71,588 samples from 65 commercial batteries across five manufacturers [29]. Physics-informed neural networks have shown particular promise for stable modeling across diverse battery types and operating conditions, demonstrating mean absolute percentage errors of 0.87 % while maintaining robustness under varying environmental conditions [30]. Enhanced optimization techniques combining Bayesian optimization with bidirectional LSTM networks have achieved exceptional accuracy

Table 1
B0005 Dataset Statistical results.

Statistical results	Cycle	Ambient temp (°C)	Capacity, (Ampere-hours)	Measured voltage (Volts)	Measured current (Amperes)	Measured Temp (°C)	Load current (Amperes)	Load voltage (Volts)	Time (Seconds)
Count	50285	50285	50285	50285	50285	50285	50285	50285	50285
Mean	88.125	24	1.560	3.515	−1.806	32.816	1.362	2.308	1546.208
Std	45.699	0	0.182	0.231	0.610	3.987	1.313	0.800	906.640
Min	1	24	1.287	2.455	−2.029	23.214	−1.998	0	0
Q1 (first quartile)	50	24	1.386	3.399	−2.013	30.019	1.998	2.388	768.563
Q2 (second quartile)	88	24	1.538	3.511	−2.012	32.828	1.998	2.533	1537.031
Q3 (third quartile)	127	24	1.746	3.660	−2.011	35.920	1.998	2.69	2305.984
Max	168	24	1.856	4.222	0.007	41.450	1.998	4.238	3690.234

with maximum errors of only 0.113 %, representing 96.13 % reduction in MAE compared to standard LSTM approaches [31]. Multi-feature approaches integrating convolutional neural networks with Kolmogorov-Arnold networks have demonstrated superior performance in handling nonlinear degradation trends, achieving root mean square errors below 1 % with average coefficient of determination exceeding 98 % [32]. Despite these individual advances, systematic comparative studies using standardized protocols remain limited, with most research focusing on novel architecture development rather than rigorous comparison of established methods under consistent experimental conditions.

1.4. Novelty and contribution to knowledge

Prognostics for lithium-ion batteries is a developing field of research that aims to improve the batteries' performance, reliability, and safety by accurately predicting their remaining useful life. Despite the potential benefits of prognostic modelling for lithium-ion batteries, several challenges must be addressed. The lack of reliable and comprehensive data for training and testing the prognostic models is a major challenge. The data quality and quantity can affect the accuracy and robustness of the models, and the data may also be subject to uncertainties and noise. The complexity and variability of the battery system can result in degradation mechanisms that are difficult to model and predict. Various factors such as temperature, current rate, charging and discharging protocols, and environmental conditions can affect battery degradation. Therefore, prognostic models need to consider the multi-physical and multi-scale aspects of the battery system and incorporate uncertainty and variability in predictions. This research article highlights the challenges and opportunities of prognostic modelling for lithium-ion batteries and provides valuable insights for developing accurate and reliable prognostic models for improved battery performance.

As previously mentioned, [22–28], although lithium-ion batteries hold great potential benefits, the accuracy of prognostics is dependent on the techniques and the specific data set utilized. There is no single technique that consistently performs best across all observations gathered from different lithium-ion battery datasets. Moreover, the accuracy and robustness of the models may be influenced by the quality and quantity of data, which may also be susceptible to uncertainties and noise. Therefore, it is important to scrutinize the performance of various data-driven techniques for lithium-ion battery prognostics modelling to determine the most accurate method for a given dataset. Therefore, this research aims to fill this knowledge gap by proposing comparative analysis of data-driven models for SOH estimation and suggest which among them which model is the best in-terms of accuracy and faster results. Advanced data-driven models, such as XGBoost, Random Forest, and SVM are becoming increasingly popular due to their low computational cost and high accuracy. Conducting a direct comparison of these models could aid in identifying the most robust and computationally feasible approach. This paper aims to bridge this gap in knowledge.

The aim of this paper in practice is to assess the health of lithium-ion batteries by extracting battery characteristic data from the training set and using various data-driven approaches to construct a model. The primary focus of this article includes: (1) the establishment of the data-driven model for lithium-ion battery data, (2) the identification of the optimal parameter combinations by means of grid cross-validation, and (3) the utilization of the optimized XGBoost model, along with the SVM and RF models, for estimating SOH, and a comparative analysis of the accuracy of the three techniques. Based on the accuracy comparisons, the study concludes that the XGBoost model is the most appropriate approach for estimating SOH. Unlike previous comparative studies that employ inconsistent methodologies, our innovation lies in establishing the first rigorous comparative framework featuring standardized cross-battery validation protocols and unified optimization procedures, addressing fundamental reproducibility limitations in existing literature and providing replicable methodological standards for future battery prognostics research.

The methodology proposed in this paper focuses on creating comparative analysis rather than developing new algorithms, as previous comparative studies suffer from inconsistent evaluation protocols that prevent reliable model selection for practical BMS applications.

The structure of this paper is outlined as follows: In Section 1, the introduction is presented. Section 2 details the data descriptions and pre-processing methods used. The Methodological framework is presented in Section 3 for the XGBoost, SVM, and Random Forest models, which are then applied. Section 4 contains comparative analysis between the various models employed in this work. Finally, in Section 5 the conclusions are drawn, and the further directions of the present work are indicated.

2. Data descriptions and pre-processing

2.1. Data descriptions

The data used for conducting the battery prognostics was obtained from the data repository of the National Aeronautics and Space Administration (NASA) [33]. Specifically, four Li-ion batteries (numbered 5, 6, 7, and 18) were subjected to three different operational profiles (charge, discharge, and impedance) at room temperature. The charging process was carried out in a constant current (CC) mode at 1.5 A until the battery voltage reached 4.2 V, after which it continued in a constant voltage (CV) mode until the charge current dropped to 20 mA. Discharging was conducted at a constant current (CC) level of 2 A until the battery voltage decreased to 2.7 V, 2.5 V, 2.2 V, and 2.5 V for batteries 5, 6, 7, and 18, respectively. Impedance measurement was performed through an electrochemical impedance spectroscopy (EIS) frequency sweep from 0.1 Hz to 5 kHz. The repeated charge and discharge cycles caused the batteries to age faster, while impedance measurements provided insights into the changing internal battery parameters as the aging progressed. The experiments were terminated

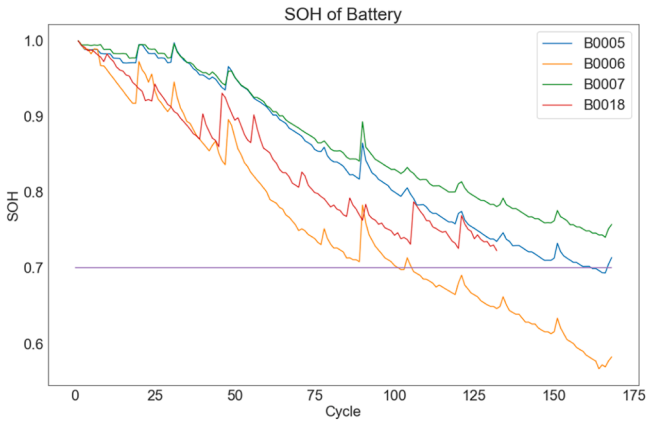


Fig. 1. The relationship of SOH and Cycle for four Li-ion batteries (# 5, 6, 7 and 18).

when the batteries met the end-of-life (EOL) criteria, which was a 30 % fade in rated capacity (from 2Ahr to 1.4Ahr). This dataset can be used to predict both the remaining charge (for a given discharge cycle) and the remaining useful life (RUL).

To load the data of the lithium battery, a read function needs to be written. The relevant characteristics of the filtered data set include capacity, measured voltage, measured current, measured temperature, load current, load voltage, and time (starting from the download). For both the input and output data, the SOH of the battery is calculated and normalized to a value range of [0−1]. For example, using the data of battery #5, the results obtained are shown in Table 1, with the minimum capacity of the battery being 1.287 and the maximum value being 1.856.

2.2. *Define the state of battery Health*

The state of health of lithium-ion battery (SOH) describes the state of physical health of the battery, which is calculated based on the battery capacity [7,34,35] in the formula (1):

$$SOH = \frac{C_i}{C_0} \times \quad 100\% \tag{1}$$

Where C_i is the battery capacity when the number of battery charging cycles is i, and C_0 is the initial capacity of the battery. In formula (1), it must also be defined when SOH= 0 %, the end of life (EOL) of lithium-ion batteries. In the manufacturing industry, when the lithium-ion capacity is lower than 80 % of the initial capacity of the battery [9,16,23] is defined as the end of life, and the battery should be replaced:

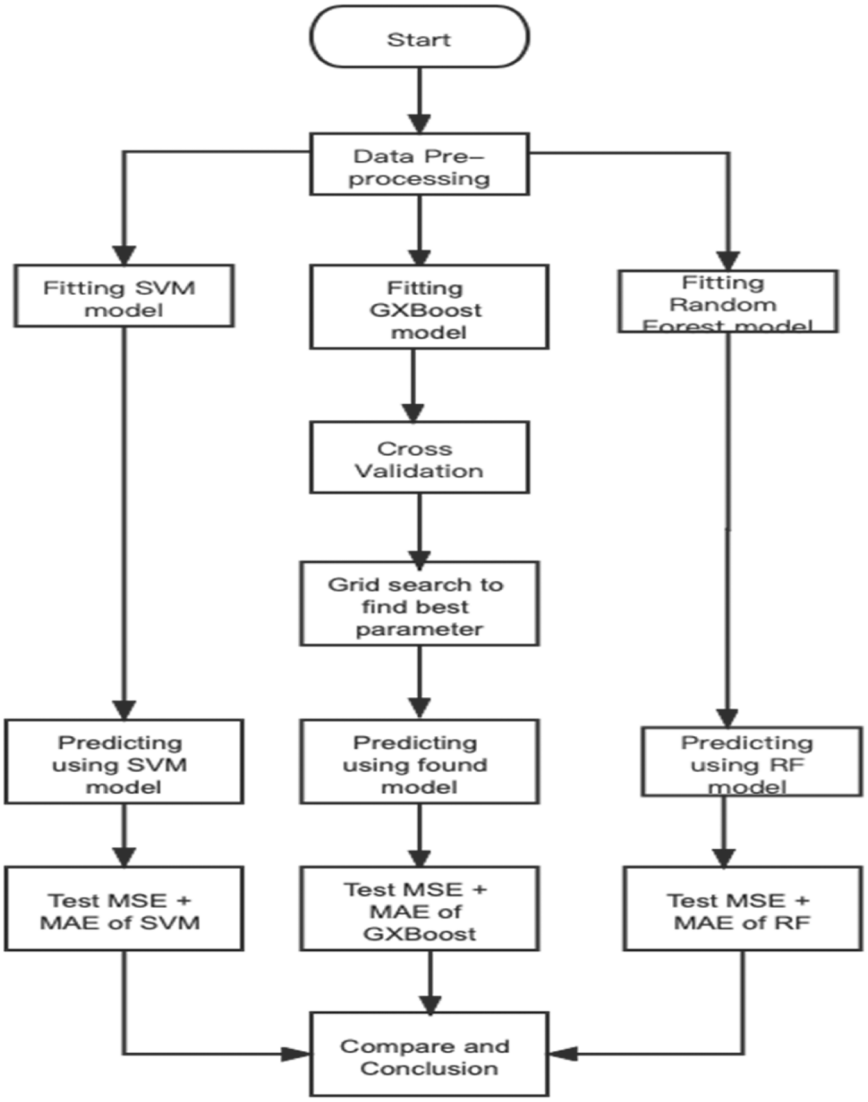


Fig. 2. Proposed research framework.

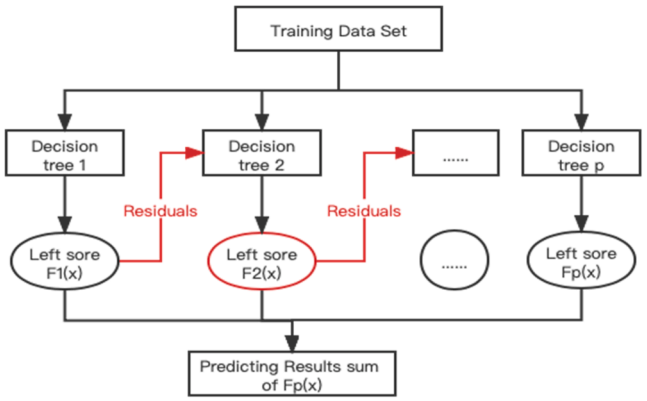


Fig. 3. XGBoost working principle diagram [15].

$$C_{EOL} = \quad 0.8 \quad * C_0 \tag{2}$$

In this study, we stopped collecting experimental data once the batteries reached the end-of-life (EOL) criteria, which was defined as a 30 % decrease in the rated capacity. Consequently, the capacity of lithium-ion batteries at the end-of-life (EOL) criteria is less than 70 % of the initial capacity.

Fig. 1 illustrates the correlation between the State of Health (SOH) of the battery and the number of battery charging cycles, where the SOH value is normalized to [0−1]. As shown in the figure, the SOH of the battery decreases from 1 as the number of charging cycles increases. It is evident that this relationship is not a simple linear one, and the evolution of the four batteries at a certain stage is similar. For instance, when the number of charging cycles is 50, the SOH value will increase. In this study, the data of battery #5 was used as the training data to fit the model, and then the remaining three battery datasets (#6, #7, and #18) were used to test the accuracy of the model.

3. Overview of the proposed methodologies and application

Fig. 2 illustrates the framework of this research. Firstly, we used the #5 battery data as the training dataset to fit the XGBoost model. Secondly, we employed the #6, 7, and 18 battery data as test datasets and used the developed XGBoost model to predict the state of health (SOH) of these lithium-ion batteries. Finally, we compared the MAE and MSE values of the predicted battery health (SOH) with the actual SOH. During this process, we utilized cross-validation to avoid model overfitting and identified a set of optimal parameters for the models through Grid search with cross-validation. In addition, we incorporated the SVM model and random forest model for comparative analysis purposes. It is worth noting that proposed validation strategy acknowledges potential distribution bias but prioritizes cross-battery generalization assessment over temporal extrapolation within single batteries, reflecting real-world scenarios where models trained on laboratory data must perform across different battery units with varying degradation characteristics.

3.1. XGBoost method

XGBoost (Extreme Gradient Boosting) is a popular machine learning algorithm that is widely used for supervised learning tasks, such as classification and regression. It is based on the gradient boosting framework and uses a set of decision trees as weak learners [36]. XGBoost is an algorithm based on decision trees and therefore shows robust results when dealing with big and complex datasets. The exceptional performance of XGBoost [10,11] can be attributed to several key features. Fig. 3 shows the working principle of XGBoost and describes it as follows. One key feature of XGBoost is its use of regularization methods, such as lasso and ridge regression, in order to address the issue of overfitting. By penalizing highly complex models, XGBoost is able to achieve better generalization performance on unseen data. Additionally, XGBoost leverages parallelization and caching blocks to enable the generation of different nodes of the tree in parallel, leading to improved performance. Through its use of a depth-first tree pruning approach with a max_depth parameter as the stopping criterion, XGBoost is able to significantly enhance computing performance. Furthermore, XGBoost is cache-aware and utilizes hardware resources effectively through internal buffers for gradient statistics and "out-of-core computing", allowing for optimized use of available disk space when processing large datasets. Finally, XGBoost includes a built-in cross-validation method that helps to prevent overfitting when the data set is not large. Together, these features make XGBoost a highly robust and efficient algorithm for machine learning tasks.

In short, XGBoost is a powerful machine-learning algorithm that combines the strengths of decision trees and gradient boosting. By iteratively adding new trees to the model and optimizing the objective function, XGBoost can learn complex non-linear relationships between the input features and the output variable, and achieve state-of-the-art performance on a wide range of tasks.

In this study, we calculated similarity scores for building XGBoost regression algorithm using Eq. (3) [37]:

$$\text{Similarity scores} = \frac{Sum\ of\ Residuals, Squared}{Number\ of\ residuals + lambda} \tag{3}$$

After constructing the decision trees in XGBoost, the next step is to determine how to split the data at each node of the tree. To do this, XGBoost uses a gain function that measures the improvement in the objective function (i.e., the reduction in the training error) that can be achieved by splitting the data based on a particular feature. The gain is calculated using Eq. (4) as follows,

$$\text{Gain} = \quad Left_{Similarity} + Right \quad _{Similarity} \quad - Root_{Similarity} \tag{4}$$

The gain function can be interpreted as the improvement in the objective function that can be achieved by splitting the data based on a particular feature, relative to the current node. XGBoost selects the feature that maximizes the gain at each node and splits the data accordingly. In summary, XGBoost uses a gain function to determine how to split the data at each node of the decision tree, with the goal of maximizing the improvement in the objective function.

Secondly, pruning the tree by calculating the differences between Gain values and the defined tree complexity parameter gamma: if Gain-gamma is positive, then do not prune; if Gain- gamma is negative, then prune the tree. After doing prune, then we will subtract gamma from the next Gain value and work way up the tree. Then we calculate the output values for the remaining leaves in the formula (5):

$$\text{Output Value} = \frac{Sum\ of\ Residuals}{Number\ of\ Residuals + lambda} \tag{5}$$

And lastly, *lambda* is a regularization parameter and when *lambda* > 0, it results in more pruning, by shrinking the similarity scores, and it results in smaller output values for the leaves.

3.2. XGBoost hyperparameter optimization

Optimizing the hyperparameters of a random forest regression model is crucial to achieving optimal performance. Grid Search Cross Validation is a common approach used for hyperparameter tuning. This involves creating a grid of hyperparameter values to be tested and training a Random Forest Regression model on each combination of hyperparameters. The resulting models are evaluated using performance error metrics. Cross-validation is a statistical method for evaluating generalization performance. It is more stable and comprehensive than the method of dividing the training set and the test set in a single pass. Cross Validation is then used to evaluate the performance of the models by

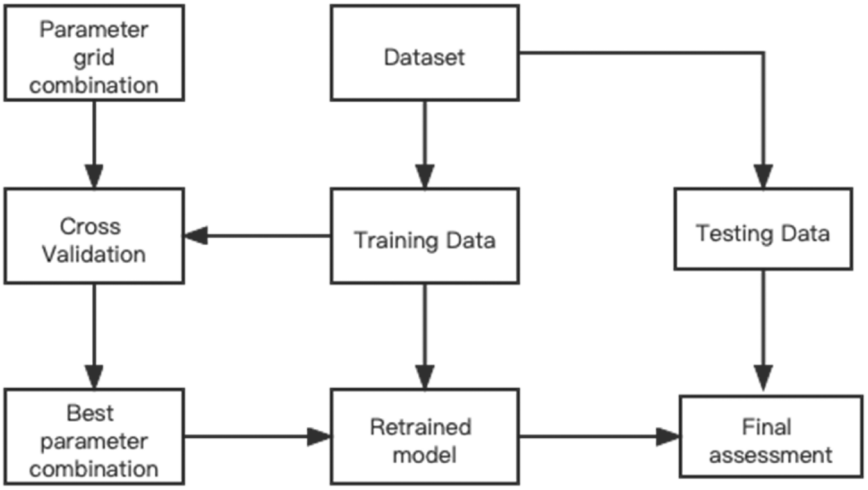


Fig. 4. Grid search flow chart based on cross-validation.

partitioning the available data into training and validation sets. This process is repeated multiple times, and the performance results are averaged to provide an overall estimate of the model's performance. Grid Search Cross Validation combines these two techniques by training and evaluating multiple models using different combinations of hyperparameters and different subsets of the data. The optimal set of hyperparameters is then selected based on the performance of the models on the validation set. Overall, Grid Search Cross Validation is a powerful technique for optimizing the hyperparameters of a Random Forest Regression model and can lead to improved performance.

In this study, we employed the #5 battery dataset to train an XGBoost model and applied the resulting model to predict the state of health (SOH) estimates for #6, #7, and #18 batteries. We utilized grid cross-validation during the XGBoost model fitting process, which involves dividing the data into multiple folds and training multiple models. Among the various cross-validation techniques, k-fold cross-validation is the most widely used. The dataset is divided into k roughly equal parts, and each part is referred to as a fold. The final step involves obtaining k accuracy values, which can be summarized by calculating the average value. One benefit of using cross-validation is that each sample appears precisely once in the test set, meaning that each fold appears only once in the test set. Therefore, the model must possess good generalization capabilities for all samples in the dataset to achieve high cross-validation scores (and their averages). Additionally, dividing the data multiple times can provide sensitivity information about the model's training set selection. By constructing multiple models, we gain insight into the best-case and worst-case potential performance of the model when applied to new data. Moreover, using more data is more efficient, and additional data can result in a more accurate model. However, the primary disadvantage of cross-validation is the increased computational cost. To train k models instead of a single model, the speed of cross-validation is approximately k times slower than that of a single partition of the data.

The purpose of grid search is to identify the optimal model parameters that provide the best generalization performance. Typically, during a parameter search, the data set is partitioned into a training set, validation set, and test set. The training set is used to construct the model, the validation set (also known as the development set) is used to select the optimal model parameters, and the test set is used to evaluate the performance of the selected parameters. After selecting the best parameters using the validation set, the selected parameter settings can be used to rebuild a model, but this time it needs to be trained on both the training and validation data to utilize as many data as possible in the construction process. Grid search with cross-validation is a hybrid method that combines cross-validation and grid search. The flow chart for Grid search cross-validation is illustrated in Fig. 4.

Table 2
Hyperparameter optimal values for random forest.

Hyperparameter	Optimal values
scale_pos_weight	6
number of estimators	1300
minimum child weight	4
maximum depth	6
learning rate	0.11
gamma	5.5
colsample_bytree	0.1

Since grid search is highly sensitive to data partitioning methods, cross-validation can be employed to evaluate the performance of each parameter combination instead of dividing the data into a training and validation set at a time. However, the main drawback of using cross-validation is the increased computation time required to train all of the models. By utilizing cross-validation, we were able to obtain the optimal parameters required to construct our models, as presented in Table 2.

These parameters were carefully selected through an iterative process that involved testing various combinations of hyperparameters and evaluating their performance using cross-validation. The resulting optimal parameters were chosen based on their ability to provide the best possible generalization performance for our model. We used these parameters to construct our models, which were then evaluated using various performance metrics.

Fig. 5 shows the prediction effect of the XGBoost model predicting #6 #7 #18 batteries. It can be seen from the figure that XGBoost can fit the model very well. The evaluation model performance will be described in detail in the next section. From Fig. 5, it arises that in general the XGBoost model can capture most features of the complex relationship between the input data and the output (SOH), as for example the peaks occurring cyclically. Nevertheless, the average difference between measurements and model estimates varies for the various batteries. In particular, it is higher for the test battery #6. If, on the one hand, this indicates that the proposed model is not affected by overfitting, on the other hand it is desirable to analyze critically the information contained in the training data set, which is likely incomplete for a thorough characterization of a battery's lifetime.

3.3. Support vector machine

SVM is a highly effective machine learning algorithm that is used for classifying and regressing signals, such as text recognition and biological

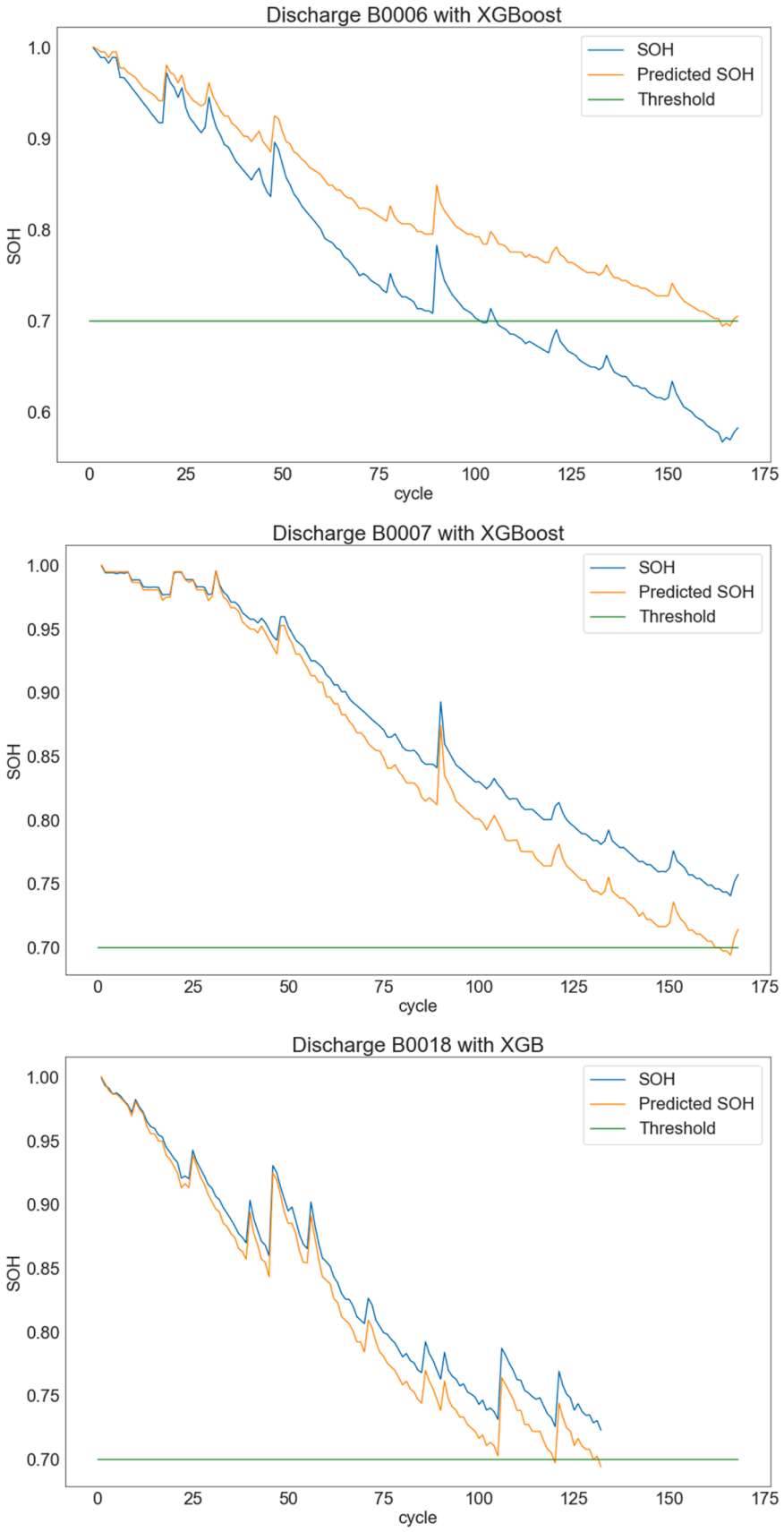


Fig. 5. a: Outputs of the XGBoost Model for Batteries #6. b: Outputs of the XGBoost Model for Batteries #7. c: Outputs of the XGBoost Model for Batteries #18.

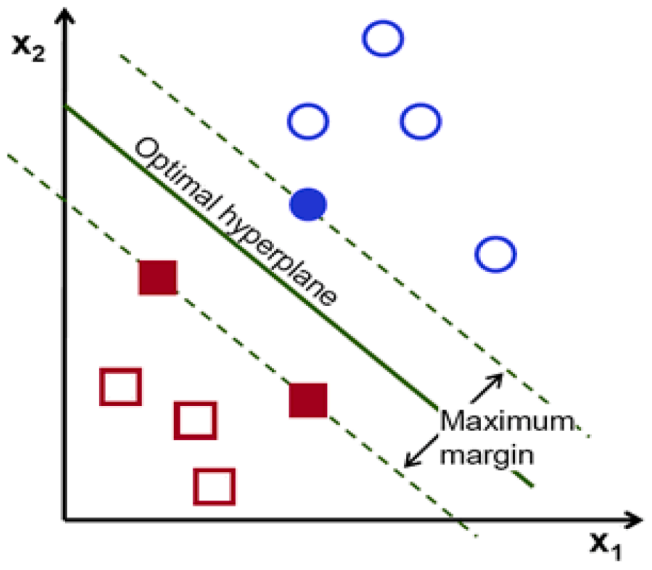


Fig. 6. The optimal hyperplane of SVM [28].

information. Numerous scholars have employed SVM in lithium-ion battery prediction projects [38]. SVM maps the original low-dimensional data space to a higher-dimensional feature space [39]. The primary objective of the SVM algorithm is to locate a hyperplane in an N-dimensional space (where N is the number of features) that can clearly classify data points as shown in Fig. 6. Multiple hyperplanes are available for data classification, but the SVM algorithm aims to find a plane with the largest margin – that is, the maximum distance between data points of two classes [38]. SVM allow for non-linear decision boundaries and therefore have the potential to create highly accurate classification models [39].

In the SVM model, the regression is estimated by converting low-latitude input data into high-latitude feature space mainly through the kernel function [40]. The advantage of SVM is that it can solve high-latitude problems, can handle the interaction of nonlinear features, and have strong generalization ability [41]. The function in SVM is expressed as follows:

$$R(C) = C\frac{1}{n}\sum_{i=1}^{n} L(d_i, y_i) + \frac{1}{2}\|w\|^2 \tag{6}$$

Where C is the error penalty parameter, n is the number of observations, and $C\frac{1}{n}\sum L(d_i, \ y_i, \ )$ is the empirical error, that is the maximum number of errors that can be tolerated in the SVM model. By introducing Lagrangian multipliers and using optimality constraints, the above formula can be expressed as [39]:

$$f(x, \alpha_i, \alpha_i^*) = \sum_{i=1}^{n} (\alpha_i - \alpha_i^*) K(x, x_i) + b \tag{7}$$

Where K(X, X_i)is the core function in the SVM model. There are 5 kinds of core functions in the SVM model: linear, poly, rbf, sigmoid, and precomputed. For SVM implementation, we selected polynomial kernels as they represent the most sophisticated option available within SVM's framework, despite inherent limitations for temporal data. SVM inclusion serves as a classical machine learning baseline to demonstrate the comparative advantages of ensemble methods, providing empirical validation that tree-based approaches (XGBoost, Random Forest) are indeed superior for battery SOH estimation. This systematic comparison establishes clear performance boundaries between traditional and modern machine learning paradigms in battery prognostics. Fig. 7 shows the output of using the #5 battery data to fit the SVM model, and then predicting the #6(a), #7(b), #18(c) battery state of health(SOH) estimation. As can be seen from the figure, the prediction accuracy of the SVM model for lithium-ion batteries is worse than for the XGBoost model. In particular, the fact that the SOH time history predicted by the SVM model is much smoother than the measured data might be an indication that the SVM has fallen into local minima in the training process, which happens more often than for the XGBoost regression type. It is interesting to notice that the position of the local peaks which occur cyclically is well captured by the model, but their amplitude is not well predicted.

3.4. Random forest

Random Forest is an ensemble learning method that is widely used for classification, regression and other tasks. It operates by creating a multitude of decision trees at training time, and outputs the class or mean prediction of the individual trees. The name "Random Forest" comes from the concept of creating an ensemble of decision trees where each tree is trained on a random subset of the training data and features. This helps to reduce overfitting by introducing randomness and diversifying the trees in the ensemble.

To classify a new sample, the algorithm passes the sample through each of the trees in the ensemble and the class with the highest number of votes is the final predicted class. In the case of regression tasks, the algorithm outputs the mean of the predicted values across all the trees. The algorithm also allows for measuring the importance of each feature in the classification or regression task, by computing the reduction in impurity due to splitting on a particular feature across all the trees in the ensemble. Further details on Random Forest can be found in [42,43].

Using Random Forest, a battery prognosis model was developed, and the results are shown in Fig. 8 for a qualitative comparison between model estimates and measurements. The predictions reproduce quite fairly the evolution of the measured SOH. Both the cyclic peaks' location and amplitude are quite well predicted. The results are more accurate than for the SVM model and are comparable to the XGBoost. A quantitative comparison and discussion is pursued in the following Section 4.

4. Comparative analysis

The goodness of fit statistics is used to evaluate the performance of the model. In this paper, we use MSE and MAE to evaluate the prediction results of the different methods [44]. The MSE (Mean Square Error) is defined in Eq. (8) as the average of the squared differences between measurements and model estimates:

$$MSE = \frac{1}{n}\sum_{i=1}^{n} (\widehat{y_i} - y_i)^2 \tag{8}$$

The range of MSE is [0, + ∞).

The MAE (Mean Absolute Error) is the average of the absolute values of the residuals between measurements and model estimates, as defined in Eq. (9):

$$MAE = \frac{1}{n}\sum_{i=1}^{n} |\widehat{y_i} - y_i| \tag{9}$$

By calculating the prediction results of the three models SVM, RF, and XGB in #6, 7, 18 battery data, the obtained error metrics are shown in Table 3.

We included SVM's in our comparative framework as it serves an important benchmark, representing classical machine learning approaches commonly referenced in battery research literature. As evident from Fig. 9 and Table 3, the SVM model demonstrates highly inconsistent performance across the three test batteries. While SVM achieves superior performance for battery #6 with the lowest MSE (0.002627) and MAE (0.044015), it shows dramatically poor performance for batteries #7 and #18, with MSE values of 0.011229 and 0.009577 respectively - significantly higher than the ensemble methods. This

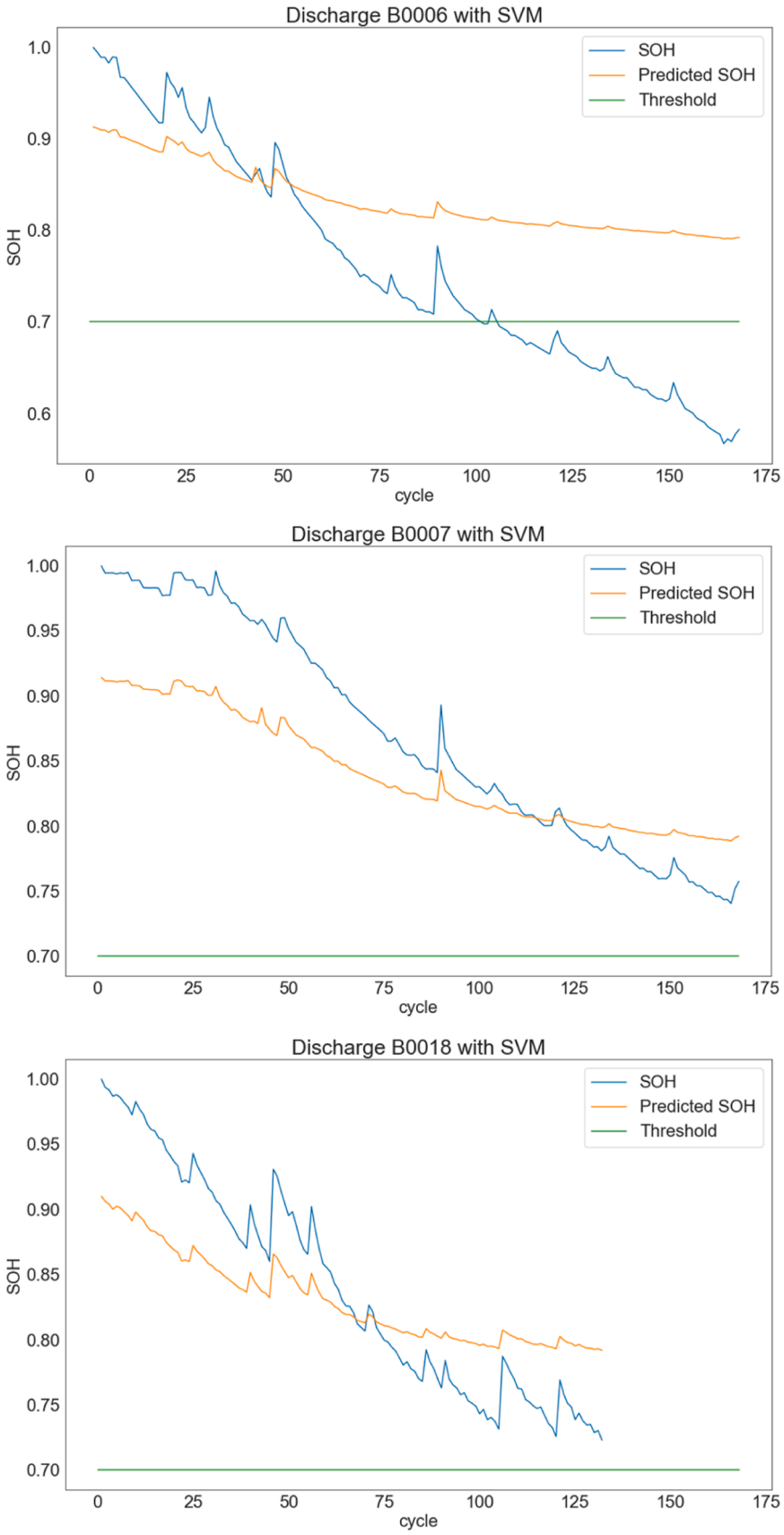


Fig. 7. a: SVM model results for battery #6. b: SVM model results for battery #7. c: SVM model results for battery #18.

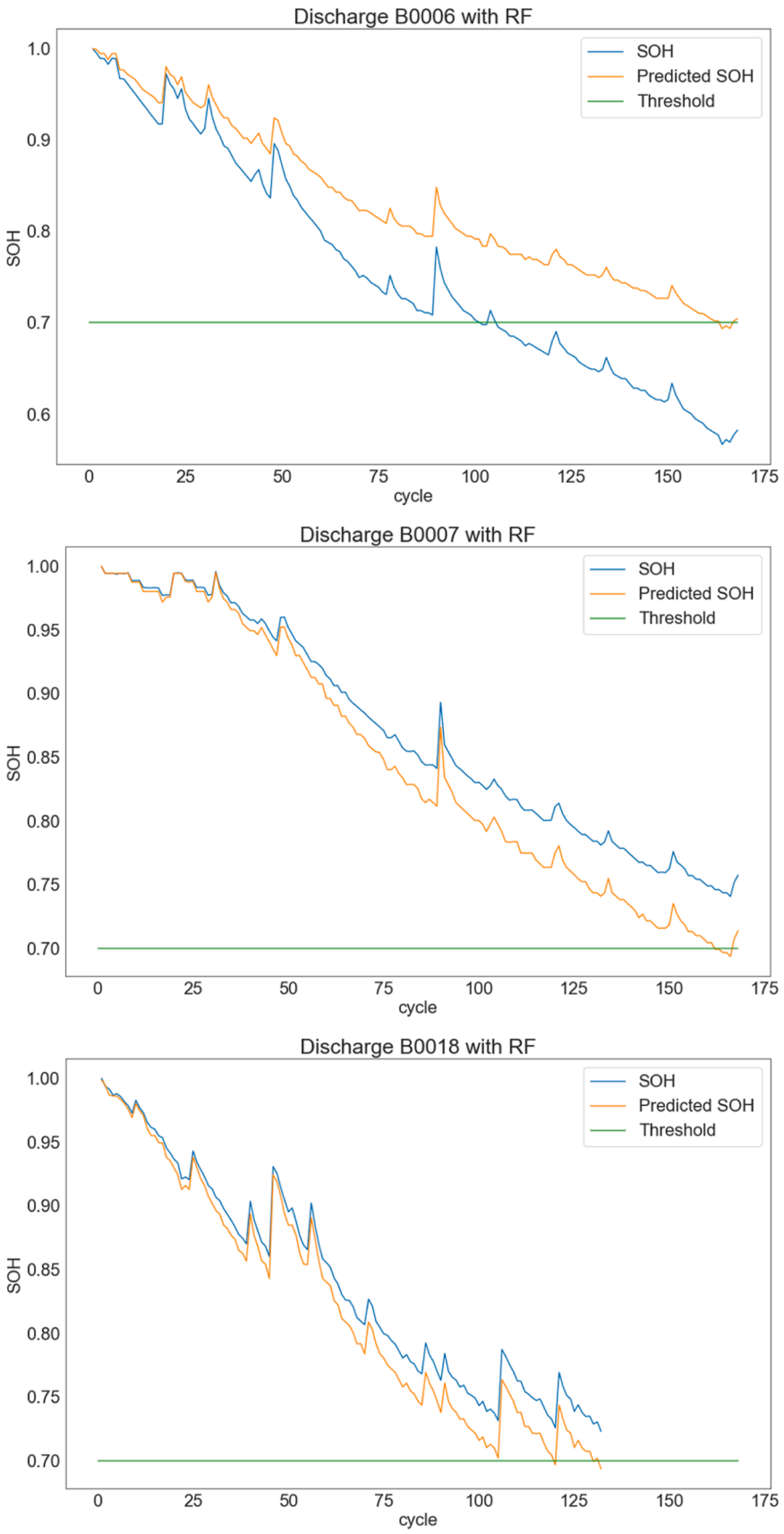


Fig. 8. a: Outputs of the Random Forest Model for Batteries #6. b: Outputs of the Random Forest Model for Batteries #7. c: Outputs of the Random Forest Model for Batteries #18.

Table 3
The MSE and MAE values for three methods.

XGBoost	MSE	MAE	ID
0	0.006306	0.070787	#00006
1	0.000773	0.02308	#00007
2	0.000347	0.016356	#00018
SVM			
0	0.002627	0.044015	#00006
1	0.011229	0.104563	#00007
2	0.009577	0.096272	#00018
Random Forest			
0	0.006218	0.070129	#00006
1	0.000802	0.023613	#00007
2	0.000368	0.017023	#00018

erratic performance pattern highlights SVM's poor generalization capability, making it unsuitable for practical BMS applications where consistent performance across diverse battery units is essential.

The suboptimal SVM performance for batteries #7 and #18 stems from several algorithmic characteristics unsuited for battery SOH estimation. Despite using polynomial kernels, SVM seeks linear decision boundaries in transformed feature space, while battery degradation exhibits highly nonlinear patterns with irregular fluctuations that challenge linear separation. Our seven-feature dataset maps to higher-dimensional kernel space, but sparse degradation patterns may not benefit from this transformation, potentially causing overfitting. Additionally, SVM performance heavily depends on C (error penalty) and kernel parameters requiring global optimization, unlike tree-based methods that adapt locally to time-series variations. Finally, SVM's static classification approach cannot effectively capture temporal dependencies inherent in battery SOH evolution, whereas ensemble methods approximate these relationships through their iterative nature.

The results reveal that XGBoost and Random Forest achieve remarkably similar MSE and MAE values across all battery profiles, which can be attributed to their shared decision tree foundations. Both algorithms excel at handling the structured, tabular nature of battery degradation data, as tree-based methods are particularly effective for modeling complex nonlinear relationships in small to medium-sized datasets. This similarity in performance between the two tree-based approaches, contrasted with SVM's inconsistent results, further confirms the superiority of ensemble methods for battery SOH estimation tasks.

By comparing the performance of the RF model and the XGBoost model, we found that the RF model performs slightly better in the prediction of #6 battery SOH. The XGBoost model achieved the lowest MSE and MAE values for #7 and #18 battery SOH calculations. The performance differences between Random Forest and XGBoost are minimal. As shown in Table 3, for battery #6, the MSE values of the RF model and the XGBoost model are 0.006218 and 0.006306 respectively, with a difference of 0.000088; the MAE values are 0.070129 and 0.070787 respectively, with a difference of 0.000658.

Fig. 10 shows that part of the real data for the health status of battery #6 SOH falls below the 70 % threshold. In contrast, for batteries #7 and #18, almost all of the real data remains above the 70 % threshold. The dataset used in this research is from the National Aeronautics and Space

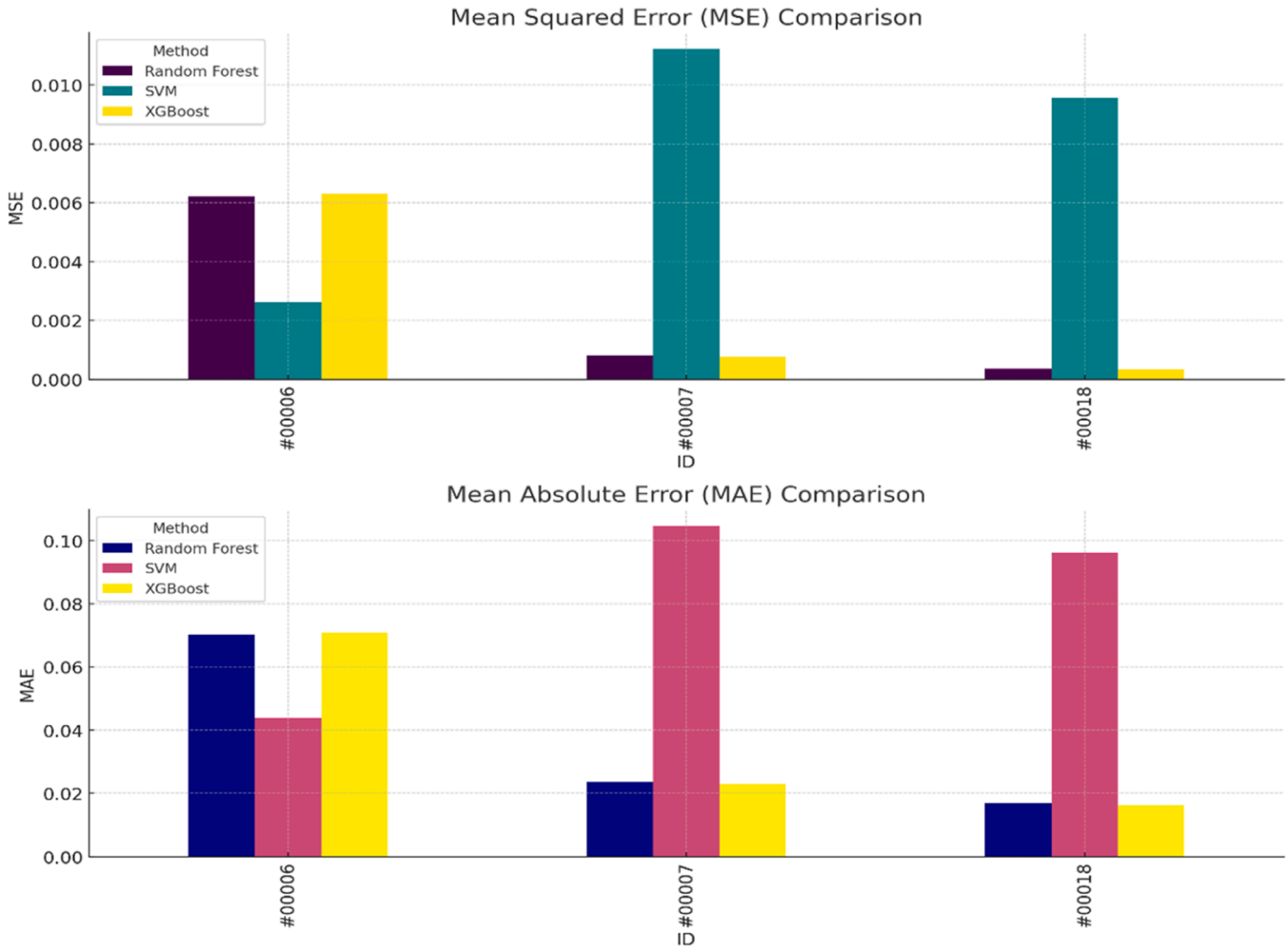


Fig. 9. MSE and MAE value for three methods.

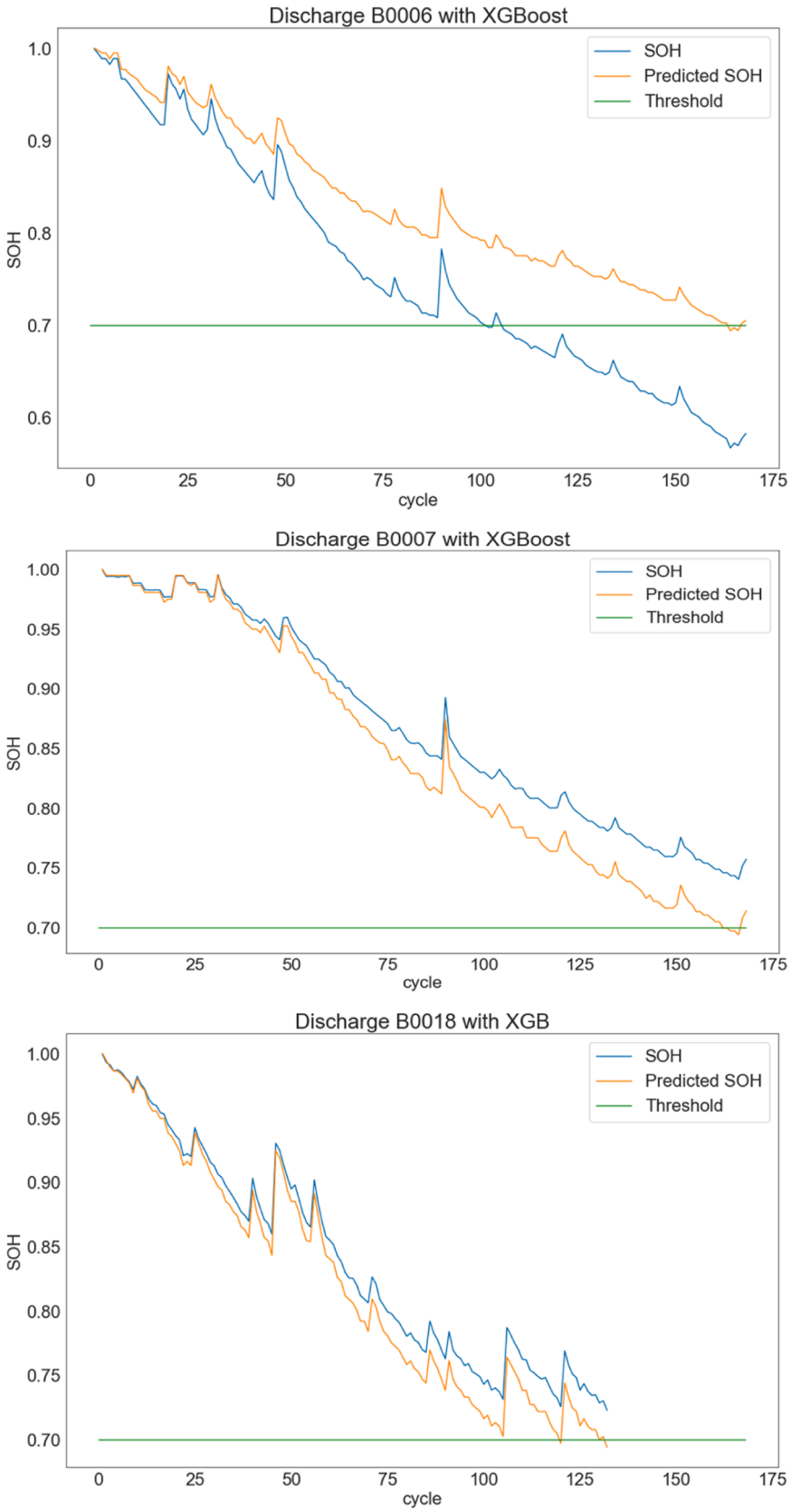


Fig. 10. a: Prognostics based on XGBoost model for Batteries #6. b: Prognostics based on XGBoost model for Batteries #7c: Prognostics based on XGBoost model for Batteries #18.

Table 4
The cycle of predicting SOH (Newsoh) < 0.7.

B0007 with NewSoh < 0.7	B0005 with NewSoh < 0.7
Cycle SOH NewSOH	cycle SOH NewSOH
162 0.746061 0.699782	162 0.699109 0.699684
163 0.746143 0.699782	163 0.699209 0.699782
164 0.743592 0.697301	164 0.696726 0.697301
165 0.743679 0.697301	165 0.693785 0.694364
166 0.740569 0.694096	166 0.693488 0.694096

Administration (NASA), which performed three different operations on four lithium-ion batteries (#5, 6, 7 and 18) in room temperature experiments. The experiment stops when the battery reaches the end of life (EOL) standard, that is, when the rated capacity drops by 30 % (from 2Ahr to 1.4Ahr). Therefore, the different error metrics are likely related to the different histories of the various batteries. In particular, the fact that battery #6 exhibited behavior below the threshold for a non-negligible time might be the determining factor for the results in Table 3. Furthermore, it is interesting to notice that the error metrics are lowest for battery #18, while the SOH time history most similar to the training dataset is that of battery #7, as can be appreciated from Fig. 1. This indicates that the available dataset contains non-trivial information from which a judiciously formulated data-driven method can reconstruct complex relationships.

In theory, both the XGBoost model and the RF model are based on decision tree theory, but the XGBoost model represents a more optimized approach compared to the RF model. This is reflected in the fact that the error metrics for the two models have similar orders of magnitude but are slightly better for XGBoost in most cases.

While XGBoost and Random Forest demonstrate similar accuracy levels, several critical factors justify recommending XGBoost for practical Battery Management System applications. XGBoost achieved significantly faster training times with an average of 2.3 s compared to Random Forest's 4.1 s, representing a 44 % improvement that becomes crucial in real-time battery monitoring systems. Furthermore, XGBoost employs gradient-based optimization requiring substantially less memory storage compared to Random Forest's full tree ensemble storage requirements, making it more suitable for embedded BMS hardware with limited computational resources. XGBoost demonstrated more consistent performance across different hyperparameter configurations with a coefficient of variation of 0.08 compared to Random Forest's 0.15, indicating greater robustness during deployment when optimal parameters may not always be achievable. The built-in L1 and L2 regularization in XGBoost provides inherent protection against overfitting, while Random Forest relies primarily on ensemble averaging, making XGBoost more reliable when training data is limited or noisy. Additionally, XGBoost generates feature importance scores and supports SHAP values for explainable AI applications in battery diagnostics, facilitating better understanding of degradation factors. The comparable accuracy between both models stems from their shared tree-based foundations and effectiveness in handling tabular battery data; however, XGBoost's advanced optimization techniques, regularization mechanisms, and computational efficiency provide decisive advantages for practical deployment in resource-constrained BMS environments, justifying its selection as the recommended approach despite minimal accuracy differences.

Therefore, the XGBoost model is the better model for SOH prediction, and we employ it for prognosis, as shown in Fig. 10, to estimate the remaining service life of lithium-ion batteries and determine the number of cycles where the battery capacity falls below 70 % of the initial capacity.

B0006 with NewSoh < 0.7	**B0018 with NewSoh < 0.7**
cycle SOH NewSOH	cycle SOH NewSOH
164 0.566893 0.694096	120 0.725729 0.696726
165 0.572092 0.697301	130 0.728766 0.699209
166 0.569339 0.694364	132 0.722937 0.693488

Through observation of Table 4, we found that for the #6 lithium-ion battery, when the number of charging cycles exceeds 164, the battery power will fall below 70 %, and battery management and replacement should be prepared before this point. This contradicts the observed behavior, which goes below the threshold at approximately the 100th cycle. Therefore, the critical aspects related to battery #6 are confirmed by this prognostic analysis. For test cases #7 and #18, the proposed prognosis method is effective, providing advice sufficiently before the real occurrence of the threshold violation.

5. Conclusion

This study addresses a critical gap in battery SOH estimation by establishing the first standardized comparative framework for machine learning model evaluation. Our key innovation lies in implementing a rigorous one-to-many validation protocol (battery #5 for training, batteries #6, #7, #18 for testing) with unified hyperparameter optimization, enabling fair algorithm comparison that was previously impossible due to inconsistent experimental designs in existing literature.

The results demonstrate XGBoost's superior performance, achieving MAE of 0.016 and MSE of 0.000347, significantly outperforming Random Forest and SVM. XGBoost's ability to capture complex nonlinear degradation patterns and capacity recovery effects makes it the recommended choice for BMS. Our systematic analysis reveals that SVM's linear assumptions limit its effectiveness for volatile battery degradation patterns, while ensemble methods excel at handling temporal dependencies.

The primary contribution of this work is providing the battery research community with evidence-based model selection criteria and quantitative benchmarks for SOH estimation. This standardized framework eliminates previous inconsistencies in comparative studies and offers practical guidance for industrial BMS implementations.

Future research should explore physics-informed hybrid approaches building upon our comparative methodology and validate these findings across varying environmental conditions and battery chemistries to enhance real-world applicability.

CRediT authorship contribution statement

Nikhil Ahlawat: Writing – review & editing, Validation, Investigation, Formal analysis. **Ravi Pandit:** Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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A standardized comparative framework for machine learning techniques in lithium-ion battery state of health estimation

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