Accurate Battery Lifetime Estimation for Electric Vehicle Using Machine Learning Models

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Abstract. Specific determination of battery capacity is fundamental to enhance the safety, dependability and durability of electric vehicles (EVs). This paper presents a machine learning based data-driven approach to predicting the capacity, as determined by the State of Health (SOH) of lithium-ion batteries. With the help of XJTU battery degradation data, the authors evaluate six machine learning algorithms and harvest pertinent features: CatBoost, Random Forest, K-Nearest Neighbors (KNN), LightGBM, XGBoost, and Decision Tree. Four regression measures are applied to measure performance, including MSE, RMSE, MAE, and R^2. Of these, CatBoost proves to have better predictive performance with minimal error and highest, R 2. The strength of our method is justified by a comparative study with previous researches and the applicability of ensemble-based models in estimating battery capacity in the real world. In addition to demonstrating the effectiveness of these models, this study highlights how data-driven approaches can reduce the need for extensive physical testing, ultimately improving the efficiency of battery health assessment.

Keywords: Battery · Machine Learning · Charging · EV · Capacity · Catboost.

1 Introduction

The concept of machine learning has become the cornerstone technology given its flexibility and scalability. It is an important tool of the era of big data and has been largely used in various sectors, such as education [8], banking, and energy systems[2]. Lithium-ion batteries are critical to electrical cars, cellphones,

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and mobile energy storage and smart grids due to their low self-discharge, high power and energy density, and low weight, which results in high power to mass and power [5], [4]. A battery management system is critical in ensuring safety and reliability of lithium-ion batteries are maintained at acceptable standards as well as reliability of the battery system used in electronic devices like cell phones and other electronic devices such as devices that run on electrical power [9]. This causes a slow wearing out of the physical and chemical characteristics of a battery to cause reduction in capacity and output power with prolonged use of a battery [20], [15].

The battery management system (BMS) must be able to reliably and accurately see the State of Health (SOH) of the battery to ensure an aging process is monitored and the correct actions are undertaken to compensate. In this regard, data-driven strategies are gaining more significance in facilitating accurate health prognostics in future battery systems [20]. Lithium-ion batteries are used in the automotive sector in support of electric vehicles (EVs). Not only does the extended energy density make better use of the driving range, but the weight of the vehicle is also less than that of older lead-acid battery systems. These benefits have greatly enhanced electric cars, which are far more attractive and environmentally secure, not to mention competitive to traditional fuel-driven cars. Although internal combustion engines are still the common ones, they are also linked with high noise and emissions as evidenced in the research on biodiesel blends in regular engines [7]. In contrast, electric vehicles powered by lithium-ion batteries offer a cleaner, quieter, and more sustainable alternative with zero tailpipe emission. The growing intersection between automation, predictive analytics, and everyday systems from smart homes [1] to EVs further highlights the expanding role of machine learning in shaping energy efficient futures. Renewable energy storage has significant applications. Energy from solar panels and wind turbines can be stored in lithium-ion batteries [4]. The SGLS system can efficiently be supported by deploying this stored energy during times of high demand or low production [9], [17]. Since they can provide a strong and rechargeable option for equipment used at home and in the workplace, lithium-ion batteries are also found in the outdoor power industry. Because of their longevity and dependability, it is also utilized in the medical field to guarantee the steady operation of these life-saving tools. Overall, lithium-ion batteries' adaptability and high efficiency make them essential for a variety of uses, spurring innovation and advancing sustainability across numerous industries. Battery SOH, which is used as a gauge to assess battery deterioration and predict future battery performance, is defined as the ratio of the present available capacity to the initial capacity [25], [22], [16]. There are two types of capacity estimating techniques: model-based techniques and data-driven techniques [11]. There are three categories of model-based approaches, where electro chemical models offer high accuracy by simulating internal chemical reactions but are computationally intensive and less suitable for real-time use [6]. Alternatively, equivalent circuit models simplify battery behavior into electrical analogs which allow faster, online estimations with reasonable accuracy. Unlike previous work that focuses on smooth laboratory cycling, our study evaluates models on the Random-Walk discharging profile of XJTU Batch-5, which closely resembles real EV operating conditions. This makes the evaluation more meaningful for practical deployment. Furthermore, we present a unified comparison of six supervised ML models on the same engineered feature set, an analysis not previously reported in literature. A limitation of this work is the reliance on a single dataset (XJTU Batch-5).

Lastly, empirical, and semi-empirical models track observable trends like capacity decline or resistance growth over time using fitting algorithms such as particle filters or particle swarm optimization [24]. Given that these methods are quite straightforward and effective, they lack resilience, are vulnerable to noise, and when copious amounts of data are needed. Also the models that are designed to operate on a single type of battery might not be generalized to other types of chemistries. Data-driven approaches to predicting battery capacity have emerged rapidly and in large numbers in recent years by modeling SOH as a black box where external factors such as voltage, current and temperature are the inputs, and the SOH is estimated by processing the data (e.g. algorithmically) [24].

2 Meethodology

The approach used in the present study is a systematic workflow based on the prediction of the SOH of lithium-ion batteries based on the machine learning models. As presented in Fig. 1, the methodology involves first the collection of data based on a publicly available dataset of battery degradation, preprocessing, and feature engineering. Three machine learning models, K-Nearest Neighbors (KNN), XGBoost and Decision Tree, were trained and tested with respect to their capacity prediction effectiveness. The performance of each model was compared using metrics such as Mean Squared Error (MSE) and the R-squared score (R^2). Such a framework of methodology leads to the same predictive power of various algorithms within the same dataset and conditions, which can be re produced.

2.1 Data Collection and Preprocessing

Eight lithium-nickel-cobalt-manganese-oxide (NCM) batteries from Batch 5 of the XJTU battery dataset [22] were used in this investigation. With cut-off voltages of 4.2 V (charge) and 2.5 V (discharge), these batteries, each with a nominal capacity of 2000 mAh and a nominal voltage of 3.6v, were cycled until failure at room temperature. The experimental protocol for Batch 5 involved Random walking discharging under conditions of full charge but not necessarily full discharge. This approach is particularly suitable for the study, as it closely simulates the typical daily usage patterns of an EV battery. Before comparing model performances, it is necessary to visualize the actual degradation trend of the battery over successive charge-discharge cycles. Fig. 2 illustrates the battery

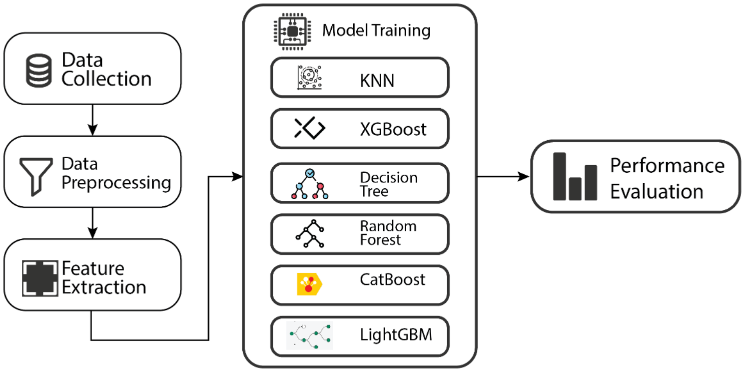


Fig. 1: Workflow of the proposed battery capacity prediction methodology

degradation curve obtained from the XJTU dataset, where capacity is plotted against the number of cycles. The plot highlights a gradual decline in capacity with increasing cycles, reflecting typical lithium-ion aging behavior. This trend serves as the ground truth against which the predictions of machine learning models are evaluated. The features were first extracted into an excel worksheet, after that missing values were removed, and data was split using stratification by battery ID to maintain representative distributions. To conserve data, the dataset was stratified by battery ID and divided into training (80%) and testing (20%) groups. Features were standardized using Standard Scaler before model training.

2.2 KNN Algorithm

A popular nonparametric, slow learning model for classification and regression applications is the K Nearest Neighbors (KNN) algorithm. It is based on the intuitive idea that similar data points are more likely to be found near one another in the feature space [19]. KNN is utilized in capacity prediction due to its ease of use and efficiency when the dataset displays localized structures or patterns. It does not require an explicit training phase, making it computationally lightweight during training. However, it becomes more intensive during the prediction stage, as it must compute distances to all training points. One key limitation of KNN is its sensitivity to irrelevant features and noise, which can affect its accuracy if not properly preprocessed [19]. In our implementation, KNN used 5 neighbors ($n_{neighbors}$=5) with Euclidean distance metric, balancing local pattern capture and noise robustness.

2.3 XGBoost

The advanced machine learning algorithm is gradient boosting decision trees and is named XGBoost [18]. Compared to classical methods of boosting, XGBoost

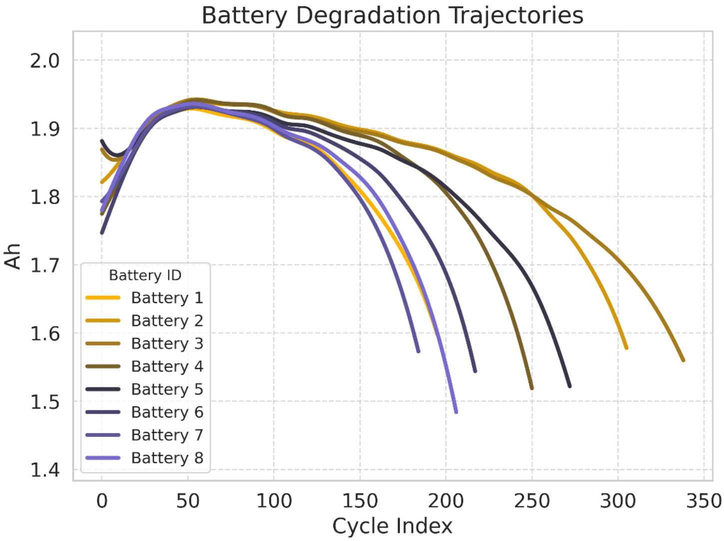


Fig. 2: Battery Degradation Trend

also has a variety of improvements, such as L1 and L2 regularization, parallel processing and tree pruning. These modifications are very effective in improving the accuracy and speed of the model. The use of XGBoost in SOH prediction is probably explained by its resistance to overfitting and the ability to operate with high-dimensional and noisy data. It is an acceptable alternative when the selection of features is important in datasets since it also gives the rank of feature relevance and automatically handles missing values. XGBoost is also suitable when dealing with large datasets with sufficient samples and features as it has been demonstrated that it is effective in a wide range of applications, one of them being financial fraud detection [18]. The authors have used 200 gradient-boosted trees ($n_{estimators} = 200$) with a shallow depth of 4 and a conservative learning rate of 0.05 to avoid overfitting whilst learning nonlinear trends.

2.4 Decision Tree

A supervised learning model called the Decision Tree algorithm makes judgments using a structure like a tree. Using factors like information gain, Gini index, or entropy to help choose the optimal split at each node, it divides the dataset into branches based on feature values [3]. The resulting structure allows the model to search from the root node to a leaf node to arrive at a decision. In battery capacity prediction, decision trees are particularly useful due to their ability to model nonlinear relationships and handle both numerical and categorical data [3], [14]. To mitigate overfitting, our Decision Tree was constrained to maximum depth 5 ($\max_{depth}$=5) and used Gini impurity for splits. Even with limited pre-processing, they can compute efficiently and perform well. Their propensity to overfit the training set, particularly if the tree gets too deep or is not sufficiently trimmed, is a significant disadvantage [3].

2.5 RandomForest

Random Forest is an ensemble learning method that builds many decision trees and then aggregates their results to improve prediction and reduce overfitting. In the application of the battery SOH prediction problem, it employs bootstrapped sampling and randomness in features to maintain diversity among individual trees such as to capture nonlinear complex interactions within data. The Random Forest was constructed by 300 trees ($\mathrm{n}_{estimators}$=300), maximum depth 8, and a minimum of 5 samples per split ($\min_{samplessplit}$=5) to be able to generalize. Every tree in the forest makes a prediction, which is then averaged to provide the final result. This ensemble strategy makes Random Forest particularly robust to noise and outliers, which are common in real-world battery datasets [21]. Moreover, it naturally handles high-dimensional feature spaces and provides insights through feature importance scores, aiding in interpretability and feature selection. While it is computationally more intensive than single-tree models, its improved generalizability and strong performance make it a competitive candidate for SOH estimation tasks.

2.6 CatBoost

CatBoost is a gradient boosting library by Yandex that internally manages categorical variables and does not a require significant amount of pre-processing. Though the features used in this work are numerical, fast accurate implementation and advanced boosting techniques like Ordered Boosting & minimal variance sampling bring CatBoost as one of the top candidates for SOH prediction. The algorithm provides the capability of reducing overfitting while keeping a high level of accuracy, particularly useful on problems with small but high-quality feature sets akin to those engineered here. Toward driving deeper pattern discovery into battery degradation behavior, support both natively for missing values as well as automatic feature combination are provided. Our CatBoost model used 300 iterations (iterations=300), depth-6 trees (depth=6), and learning rate 0.05 to efficiently model degradation patterns. As demonstrated in the results, CatBoost closely follows the capacity degradation trend, providing a smooth and consistent prediction trajectory that validates its applicability in battery health prognosis.

2.7 LightGBM

Gradient boosting architecture that focuses on Efficient and Faster, i.e., Light Gradient Boosting Machine (LightGBM). It brings techniques such as Gradient based One-Side Sampling (GOSS) and Exclusive Feature Bundling (EFB) to significantly reduce training time without losing accuracy [23]. LightGBM is normally tuned with 300 estimators available, Depth-5 trees, 20 leaves in a tree, and learning rate of 0.05 to make it run fast yet accurate. LightGBM shines out when talking about the SOH prediction task because this model supports large-scale data with low memory consumption and high speed-a perfect fit for real-time applications like an electric vehicle battery management system. It detects complex interactions quite well and has built-in ways of regularization therefore lowering the risk of overfitting.

3 Results and Analysis

To comprehensively evaluate the performance of the proposed models, four well-known regression metrics were used to measure how well they performed. These include the coefficient of determination, R^2, Mean Squared Error (MSE), Root Mean Squared Error (RMSE), and Mean Absolute Error (MAE). The mean squared error represents the average squared difference between the actual value and the predicted value placing more weight on larger errors. It can be mathematically represented as[10],

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

where N denotes the number of samples, y_i represents the actual or observed values, and $\hat{y}$ indicates the corresponding predicted values generated by the model. The squared error expresses how much each prediction deviates from the corresponding true value of outcome for every sample. Large errors are more heavily penalized due to squaring. RMSE expresses MSE in terms of original units of measurement and hence is easier to interpret intuitively. MAE expresses average absolute deviation and is less sensitive to outliers[13],

$$\mathrm{MAE} = \frac{1}{N}\sum_{i=1}^{N}|y_i - \widehat{y_i}| \tag{2}$$

Finally, the R^2 metric shows the percentage of the dependent variable's variance that the model can account for. It is described as [12],

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \widehat{y_i})^2}{\sum_{i=1}^{N}(y_i - \overline{y})^2} \tag{3}$$

where N denotes the sample size, y_i represents the observed capacity, $\hat{y}$ the predicted capacity. and $\overline{y}$ the mean capacity. The predictive capability of six machine learning models; CatBoost, LightGBM, XGBoost, Random Forest, K-Nearest Neighbors (KNN), and Decision Tree was systematically assessed using extracted features derived from the XJTU dataset. Table I summarizes the key results, revealing significant disparities in performance across the models. Among these, ensemble boosting algorithms demonstrated superior performance. CatBoost achieved optimal metrics with an MSE. of 0.000068 and an R^2 of 0.992952.

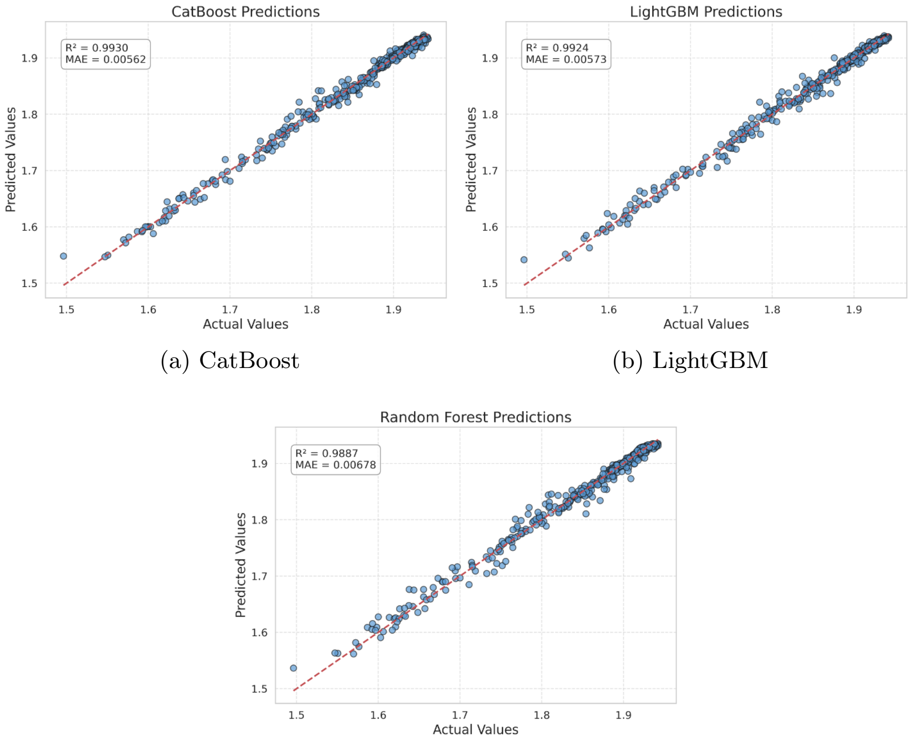
LightGBM closely followed, attaining an MSE of 0.000073 and an R^2 of 0.992402. XGBoost also maintained competitive accuracy with an MSE of 0.000084 and a R^2 of 0.991306. In contrast, the Random Forest model yielded moderate results, with an MSE of 0.000109 and an R^2 of 0.988722. Traditional models, specifically KNN and Decision Tree, exhibited inferior performance with notably higher errors, for KNN: MSE $=$ 0.000249, $R^2 = 0.974284$; and for Decision Tree model: MSE $=$ 0.000407, $R^2 = 0.957873$.

CatBoost feature importance reveals that the most dominant features toward predicting SOH are discharge duration, voltage-based indicators, and the cycle index. This is consistent with degradation physics. CatBoost has proven to be a valid degradation curve delivering predictions as smooth and accurate even during sharp transitions in capacity periods as seen in Fig. 3(a). This type of minimal deviation yet explicit power speaks to the generalization capabilities at their best here. LightGBM delivers near identical accuracy explicitly finding fast drops in capacity with just a small deviation as indicated in Fig. 3(b). The combination of efficiency and predictive accuracy (MSE $=$ 0.000073, R^2 $=$ 0.992402) supports its potential for real-time Battery Management System (BMS) applications. XGBoost shown in Fig. 3(c) shows successful tracking the overall degradation trend but displayed slight fluctuations during transitional cycles, indicating some sensitivity to localized variations. Nevertheless, its overall performance remained robust (MSE $=$ 0.000084, $R^2 = 0.991306$).

Table 1: Performance Comparision of Machine Learning Models

Model	**MSE**	**RMSE**	**MAE**	$\mathbf{R^2}$
CatBoost	0.000068	0.008253	0.005617	0.992952
LightGBM	0.000073	0.008569	0.005730	0.992402
XGBoost	0.000084	0.009166	0.006327	0.991306
Random Forest	0.000109	0.010439	0.006780	0.988722
KNN	0.000249	0.015764	0.010207	0.974284
Decision Tree	0.000407	0.020176	0.013901	0.957873

The conventional KNN model demonstrated in Fig. 5 deviated about the actual capacity mostly at the mid and late cycles. Higher MSE and a lower R^2 for this model are indicators of its inability toward mapping complicated, nonlinear degradation processes properly. Among all the models, variance in prediction from Decision Tree was highest which is visible as error variations at later cycles thus validating overfitting through it. Comparative insights are synthesized in Fig 4, consolidating model performance metrics to underscore the unmistakable superiority of ensemble boosting approaches. A bar plot in Fig. 5 with two axes clearly presents the considerable gap in accuracy between the boosting models (CatBoost, LightGBM, XG Boost) and simpler more traditional approaches (KNN, Decision Tree). CatBoost consistently outperformed all other models across both MSE and R^2 metrics, with Random Forest occu-



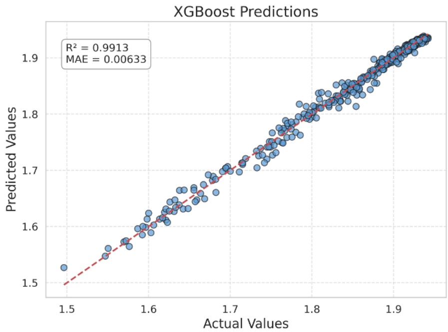
(a) CatBoost (b) LightGBM

(c) XGBoost

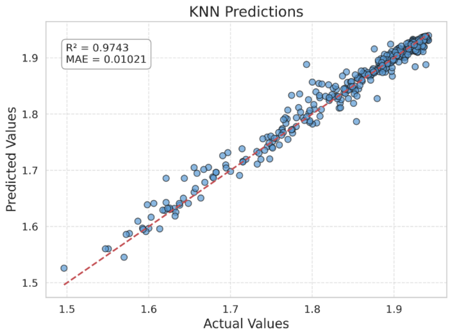
Fig. 3: Prediction vs. actual capacity for boosting models.

pying an intermediary position by outperforming the simpler models but falling short of the advanced boosting techniques. These findings affirm that modern gradient-boosting architectures incorporating techniques such as regularization, feature bundling, and ordered learning are highly effective in modeling complex, nonlinear battery degradation dynamics.

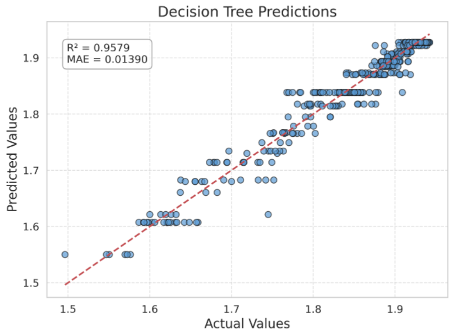
Several key observations can be drawn from the analysis. Firstly, the boosting models achieved R^2 scores exceeding 99%, demonstrating near-perfect variance explanation. Secondly, the engineered features contributed to high generalizability across the boosting models. Thirdly, LightGBM's favor able trade-off between computational efficiency and predictive accuracy positions it as a strong candidate for embedded BMS deployment. Lastly, the underperformance of KNN and Decision Tree models underscores their limitations in handling localized noise and nonlinear trends, consistent with their theoretical constraints. To contextualize these results, Table II benchmarks the proposed models against recent studies in the literature. Notably, the sub-0.0001 MSE values achieved by CatBoost and LightGBM in this study surpass those reported in prior works, such



(a) Random Forest



(b) KNN



(c) Decision Tree

Fig. 4: Prediction vs. actual capacity for traditional models.

as Xingjia Li et al. [10] (MSE = 0.0064) and Mishra et al. [12] (MSE = 0.0002), thereby demonstrating the efficacy of the proposed feature engineering pipeline. Furthermore, the R^2 values exceeding 0.99 for all boosting models further validate their superior predictive capability. Collectively, these results position the proposed framework as a state-of-the-art, data driven solution for electric EV battery prognostics.

4 Practical Considerations for Real-Time Deployment

CatBoost and LightGBM exhibit low-latency inference, making them suitable for execution on resource-constrained Battery Management System (BMS) microcontrollers. Their built-in handling of missing values and robustness to noisy measurements allow stable predictions under fluctuating load currents and partial charge/discharge events typical in EV operation. For real-time deployment, features such as voltage, current, and temperature can be continuously streamed,

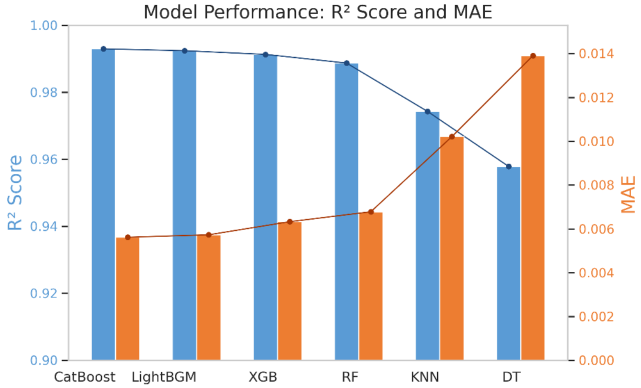


Fig. 5: Comparative performance of all models.

Table 2: Comparison of the Proposed Method with Previous Studies

Study	**Dataset**	**Method**	**MSE**	$\mathbf{R^2}$
This Study	XJTU	CatBoost	0.000068	0.9929
	XJTU	LightGBM	0.000073	0.9924
	XJTU	XGBoost	0.000084	0.9913
[10] Xingjia Li et al. (2024)	CALCE battery dataset	XGBoost	0.0064	0.9987
[13] Sachin et al. (2024)	Experimental	Linear Regression	0.1870	0.9908
[12] Mishra et al. (2023)	NASA Battery Dataset	Stepwise Linear Regression	0.0002	0.987

enabling online SOH estimation without full charge cycles. Future work will validate the models under dynamic driving profiles (UDDS, WLTP) and evaluate memory usage, model update mechanisms, and sensor-noise resilience to ensure practical integration into commercial EV BMS platforms.

5 Conclusion

This work used designed variables from the XJTU battery dataset to show how well machine learning algorithms predict the SOH of lithium-ion batteries. With the lowest MSE and greatest R^2 score among the three models assessed, the CatBoost method had the best predictive accuracy, closely tracking the actual battery capacity trend. XGBoost and Decision Tree models also performed well, offering reliable predictions with relatively low computational requirements. The results validate the role of data-driven models in battery health monitoring and reinforce the importance of careful feature engineering in achieving robust outcomes. A comparative evaluation with previous studies further confirmed the competitiveness of our approach, with the KNN model achieving better or comparable performance in terms of both MSE and R^2. Deep learning architectures may be investigated in future research, and hybrid ensemble models to improve generalization and prediction accuracy even more across various battery chemistries and operational conditions. Real-time deployment and integration into battery management systems also remain promising directions for continued research.

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