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Precision Forecasting: Optimizing Lithium-ion Battery Remaining Usable Life Estimation with Cutting-Edge Machine Learning

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Abstract: - This study seeks to estimate the remaining life span of lithium-ion batteries, which is an essential component of early failure prevention. The paper demonstrates how advanced machine learning tools like CatBoost and LightGBM are superior when it comes to handling complex data patterns. In assessing the accuracy of prediction, several key performance metrics such as Mean Squared Error (MSE), Mean Absolute Error (MAE) and Root Mean Squared Error (RMSE) were used. Experimental validation using NASA's 18650 lithium-ion battery datasets reveals a 25% improvement in prediction accuracy, with CatBoost consistently outperforming LightGBM. This implies that these approaches have the potential to improve RUL predictions and thus battery management policies.

Keywords: Lithium-ion batteries, RUL, Machine learning, Neural networks, Data-driven, Prediction, CatBoost, LightGBM, MSE, MAE, RMSE.

I. Introduction

Electric propulsion systems cannot do without Energy Storage Systems (ESS) that are also essential in running drones and aircraft. The growing environmental concerns and unpredictable oil prices have led to a soaring demand for electric propulsion technology in the aviation sector. This boom highlights why ESS should be used to improve efficiency as well as minimize environmental footprints.

Therefore, many attempts have been made to predict the Remaining Useful Life (RUL) of lithium-ion batteries, which are the indispensable components of ESS necessary for ensuring their reliability and longevity. For example, [1] suggest applying machine learning for predicting lifetime of NMC-LCO batteries using data from Hawaii Natural Energy Institute. Similarly, [2] present LightGBM-based system to forecast battery life under specified operating conditions involving electrochemical impedance spectroscopy (EIS), impedance-capacity discharge voltage (IC-DV) curves for accurate estimations on RUL.

To build on this, a CatBoost model introduced by [3] helps improve prediction accuracy and diagnosis of Li-ion battery. [4] also combined stream learning with LightGBM to estimate SOH and RUL, resulting in better performance over the existing models. These studies underscore the need for accurate battery life prediction especially when it comes to electric propulsion systems.

These are not the only applications of machine learning in battery prognosis. For in-stance, [8] examine deep learning and machine learning paradigms applied solar radiation forecasting while [10] use machine learning algorithms to assess ecological suitability demonstrating how versatile these methods can be.

Nevertheless, despite several approaches available, accurately predicting the lifespan of Lithium-Ion batteries remains a significant hurdle. This research employs CatBoost as well as LightGBM algorithms for battery life prediction based on their strong feature se-lection capabilities and suitability in handling time series data. The study compares and evaluates the forecast performance of LightGBM and CatBoost using NASA dataset about 18650 Lithium-ion Batteries.

In the preliminary results, it was observed that CatBoost is better than LightGBM as it consistently gives much lower RMSE values and more precise predictions on RUL [17]. These approaches have improved long-term forecasting capabilities and outperformed existing ones.

The next paragraphs present a concise overview of the CatBoost and LightGBM algorithms, after which they take an in-depth look at the RUL estimation methods with NASA's data on 18650 lithium-ion batteries. The accuracy and efficiency of predicting remaining useful life for lithium-ion batteries using CatBoost and LightGBM are demonstrated through experimental results and performance comparisons.

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II. METHODOLOGY

Gradient boosting algorithms, such as CatBoost and LightGBM, offer several advantages over neural network or LSTM algorithms, particularly in the context of predicting the Remaining Useful Life (RUL) of lithium-ion batteries. Here are the key reasons, [25]

When dealing with structured, tabular data, gradient boosting algorithms excel by efficiently capturing complex feature interactions with minimal feature engineering. In contrast, neural networks, and LSTMs, while powerful for unstructured data like images, text, or time-series, often necessitate significant preprocessing and feature extraction when applied to structured data.

Gradient boosting models, such as CatBoost and LightGBM, are advantageous due to their interpretability. They provide clear insights into feature contributions through feature importance scores and partial dependence plots, making them easier to understand and explain. Neural networks and LSTMs, on the other hand, are often considered "black boxes" because of their complex architectures, making it challenging to interpret individual feature influences on the output.

Regarding handling missing values and outliers, gradient boosting algorithms are robust and can manage these issues effectively without extensive preprocessing. For instance, CatBoost can directly handle missing values, and robust loss functions help mitigate the impact of outliers. Conversely, neural networks and LSTMs typically require additional preprocessing steps like imputation or normalization, adding complexity to the modeling process.

In terms of training time and resource efficiency, gradient boosting models generally require less computational power and time compared to neural networks and LSTMs. Optimized implementations like LightGBM enhance efficiency, making them practical for situations with limited computational resources or the need for quick results. Neural networks and LSTMs often demand extensive computational resources and longer training times, especially for deep architectures, along with careful hyperparameter tuning, which can be time-consuming.

Gradient boosting models incorporate built-in regularization techniques to prevent overfitting, such as early stopping, tree pruning, and shrinkage (learning rate). These methods enhance generalization and help avoid overfitting. Although neural networks and LSTMs also have regularization methods like dropout and weight decay, they are still prone to overfitting, especially with small to medium-sized datasets, requiring meticulous tuning to manage effectively.

Scalability and parallelization are strengths of gradient boosting algorithms like LightGBM, which are designed to handle large datasets efficiently through parallel and distributed training. This capability makes them suitable for big data applications. While neural networks and LSTMs can also scale, training large models often requires specialized hardware, such as GPUs, and frameworks like TensorFlow or PyTorch to manage parallelization, increasing complexity and cost.

Hyperparameter tuning in gradient boosting models is more straightforward and less sensitive compared to neural networks. The process is faster and more reliable, simplifying model optimization and accelerating deployment. In contrast, neural networks and LSTMs have numerous hyperparameters, including learning rates, batch sizes, and the number of layers and units per layer. Tuning these parameters is complex and time-intensive, demanding significant expertise and computational resources to achieve optimal performance.

In summary, gradient boosting algorithms such as CatBoost and LightGBM offer advantages in terms of handling structured data, interpretability, robustness to missing values and outliers, training efficiency, regularization, scalability, and ease of hyperparameter tuning. These strengths make them particularly well-suited for tasks like RUL prediction of lithium-ion batteries, where structured data is prevalent and model interpretability is crucial. While neural networks and LSTMs have their place in machine learning, especially for unstructured data and sequential tasks, gradient boosting remains a powerful and often more practical choice for many predictive modeling tasks.

III. PROPOSED ALGORITHM TECHNIQUES

The study uses machine learning algorithms, LightGBM and CatBoost, to improve lithium-ion battery lifespan prediction, crucial for electric vehicle performance and sustainability. The process involves data importation, preprocessing, training, evaluation, prediction, interpretation, and conclusion, providing valuable insights into lithium-ion battery forecasted lifespan for electric vehicle applications.

LightGBM

LightGBM (Light Gradient Boosting Machine) is a high-performance, open-source gradient boosting framework developed by Microsoft. It is designed for efficiency and scalability, particularly suitable for large datasets and high-dimensional data. LightGBM incorporates several novel techniques to enhance its performance compared to other gradient boosting libraries like XGBoost

Traditional Gradient Boosting: In traditional gradient boosting, the decision trees are built using exact greedy algorithms, which can be computationally expensive and memory-intensive for large datasets.

LightGBM's Approach: LightGBM uses a histogram-based decision tree learning algorithm. It discretizes continuous feature values into a finite number of bins (histograms), significantly reducing memory usage and speeding up the training process. This approach allows LightGBM to handle large datasets efficiently.[27]

LightGBM is a highly effective model for lithium-ion battery lifetime prediction, utilizing advanced techniques to optimize model performance and control complexity [9,11,13]

Mathematical Formulation of LightGBM

Gradient boosting is an ensemble technique that builds models sequentially, with each new model correcting errors made by previous ones. The objective is to minimize a loss function L(y, F(x)), where y is the true value and F(x) is the predicted value. For a given iteration t, the objective is to fit a new model ht(x) to the negative gradient of the loss function:

$$h_t(x) = -\left.\frac{\partial L(y,F(x))}{\partial F(x)}\right|_{F(x)=F_{t-1}(x)} \qquad (1a)$$

The model is updated as:

$$F(x) = F_{t-1}(x) + \eta \cdot h_t(x) \qquad (1b)$$

where η is the learning rate.

For each feature, LightGBM builds histograms and uses them to find the best split points. The split gain for a potential split s at node j is given by:

$$Gains(s) = \frac{1}{2}\left(\frac{G_L^2}{H_l+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{(G_L+G_R)^2}{H_L+H_R+\lambda}\right) - \gamma \qquad (1c)$$

CatBoost

CatBoost (Categorical Boosting) is a high-performance, open-source gradient boosting on decision trees library, developed by Yandex. It is designed to handle categorical features more effectively than other gradient boosting libraries. CatBoost incorporates several innovative techniques that enhance its performance and usability, particularly in scenarios with a high number of categorical variables.

Ordinary Gradient Boosting: Traditional gradient boosting algorithms, such as XGBoost or LightGBM, require categorical features to be converted to numerical values, often using one-hot encoding or label encoding. This can lead to loss of information or significant increase in dataset dimensionality.

CatBoost's Approach: CatBoost uses a technique called "Ordered Target Statistics". It calculates mean target values for categorical features, ensuring that the calculation is performed in an ordered fashion to avoid data leakage. This is achieved using a process called "ordered boosting", where each instance is processed based on its position within the dataset. [26]

With customized grid search algorithms and robust parameter setups, CatBoost optimizes hyperparameters to improve model performance. Additionally, CatBoost uses sophisticated techniques to manage model complexity and choose characteristics to provide reliable and accurate battery lifetime estimates [12,14,15,16]

In CatBoost, the handling of categorical features involves calculating the target statistics in an ordered manner to avoid leakage. For a categorical feature c with possible values {c1, c2, . . . , ck}, CatBoost computes the following for each value ci :

$$TargetStatistic(c_i) = \frac{\sum_{i\in PastData} y_j \cdot \mathbb{I}[c_j=c_i]}{\sum_{i\in PastData} \mathbb{I}[c_j=c_i]} \qquad (2)$$

where 𝕀 is the indicator function and “Past Data” represents the subset of data points preceding the current data point to ensure ordered boosting

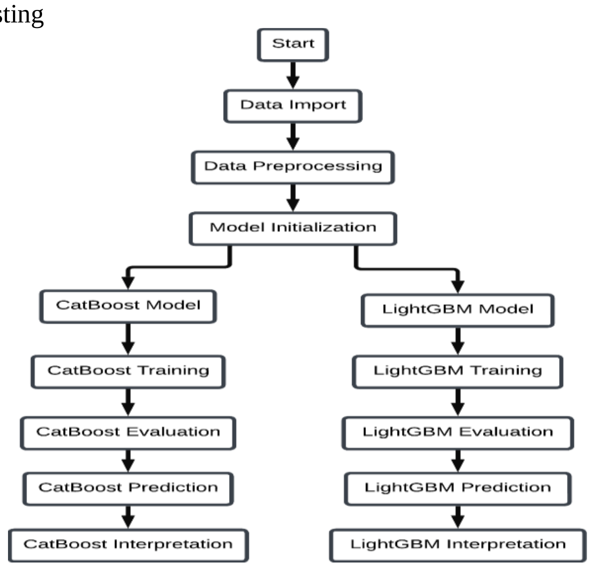

Figure 1. Flowchart of the proposed algorithm techniques

IV. RESULTS AND DISCUSSION

Before Remaining Useful Life (RUL) is the maximum battery capacity before capacity loss, while Out of Life (EOL) occurs when a capacitor reaches 70%-80% of its nominal capacity) [5,6,7].

RUL =T_EOL-T_cc (3)

Where:

RUL is the Remaining Useful Life,

T_EOL shows the cycle number at which the End of Life (EOL) criterion is reached by the capacity.

T_cc indicates the battery's capacity's current cycle number.

The experimental dataset from NASA's Prognostics Center of Excellence was used to assess 18650 lithium-ion batteries during charge, discharge, and impedance operations at a constant temperature. [23,24]

The experiment was terminated when the measured values were less than 70% to 80% of the battery's rated capacity.

Table 1. Nasa 18650 Lithium-ion battery description

Battery	Constant charge current	Discharge current	Minimal charge current	Rated capacity	Charge/ discharge cutoff voltage
BATTERY5	1.5A	2A	20mA	2Ah	4.2/2.7V
BATTERY6	1.5A	2A	20mA	2Ah	4.2/2.7V
BATTERY7	1.5A	2A	20mA	2Ah	4.2/2.7V
BATTERY18	1.5A	2A	20mA	2Ah	4.2/2.7V

The algorithm's performance in RUL prediction is evaluated using various metrics such as MSE, MAE, MSLE, RMSE, MPE, EV, MSPE, RE, and R^2. [19] They are:

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \tag{4}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \tag{5}$$

$$MSLE = \frac{1}{n}\sum_{i=1}^{n}(\log(y_i + 1) - \log(\hat{y}_i + 1))^2 \tag{6}$$

$$RMSE = \sqrt{MSE} \tag{7}$$

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i}\right| x\ 100\% \tag{8}$$

$$EV = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2} \tag{9}$$

$$MSPE = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{y_i}\right)^2 x\ 100\% \tag{10}$$

$$RE = \frac{\sum_{i=1}^{n}|y_i - \hat{y}_i|}{\sum_{i=1}^{n} y_i} x\ 100\% \tag{11}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2} x\ 100\% \tag{12}$$

Where:

n is an observations number,

y_i *is an i-th observation's true value,*

$\hat{y}_i$ *is an i-th observation's predicted value,*

$\bar{y}_i$ *is the mean value of true* y_i.

The algorithm consists of three phases: data preparation, training, and validation. It uses hyperparameters like n_estimators, random_state, batch_size, learning_rate, epochs, window_size, iterations, and verbose. The average execution time is around 300 seconds for each data set. After training cycles, the algorithms consistently work. The RUL prediction results show the End of Life (EOL) threshold, validation data, actual values, and predictions. This part compares the accuracy of the LightGBM and CatBoost algorithms in estimating the Remaining Useful Life (RUL) of different Li-ion batteries [20] Four batteries (B0005, B0006, B0007, and B0018) are utilized for RUL prediction. The datasets are separated between validation and training sets, with each set of data beginning at a different point for every battery.

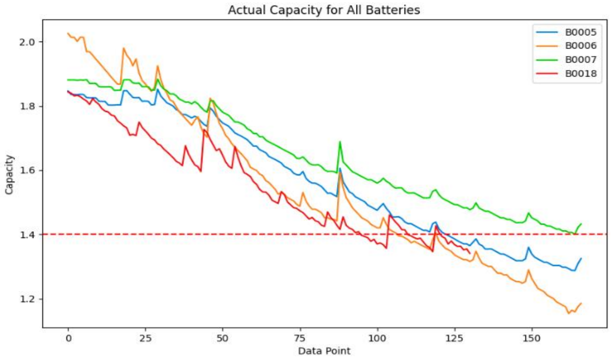

Figure 2. Battery degradation curve for NASA dataset

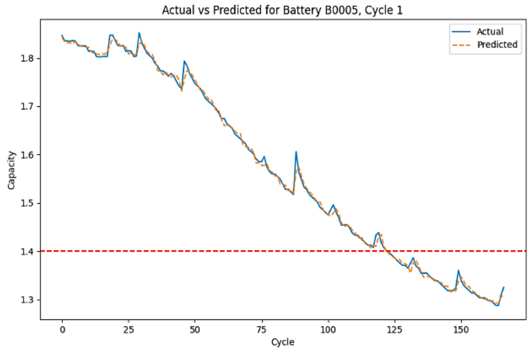

Figure 3. CatBoost based RUL prediction for B0005 dataset

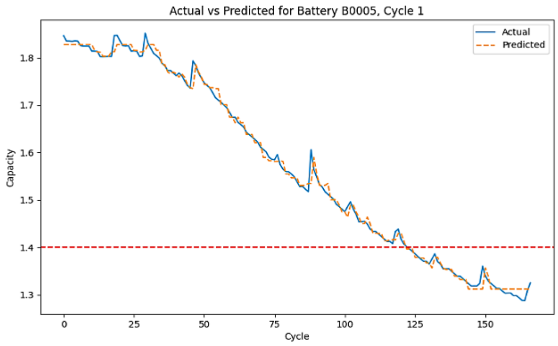

Figure 4. LightGBM based RUL prediction for B0005 dataset

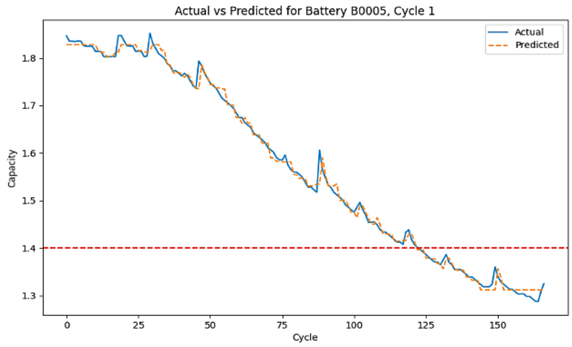

Figure 5. LightGBM based RUL prediction for B0005 dataset

The B0005 Li-ion battery's Remaining Useful Life (RUL) is estimated using CatBoost and LightGBM algorithms. Both methods show good performance during validation, but CatBoost consistently outperforms LightGBM in terms of Mean Absolute Error and Root Mean Square Error, indicating better prediction accuracy.

The CatBoost and LightGBM algorithms are used for the second Li-ion battery, B0006, and their performance is compared to LightGBM. CatBoost outperforms LightGBM in terms of capacity deterioration, prediction, and R-squared values.

The CatBoost and LightGBM algorithms are evaluated for the third Li-ion battery, B0007. CatBoost higher R^2 value and lower MAE and RMSE values demonstrate better prediction accuracy, as shown in Figure. 7.

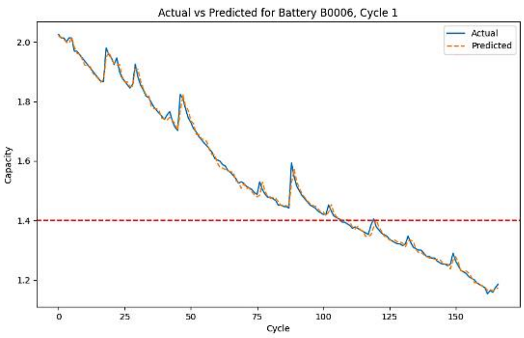

Figure 6. CatBoost based RUL prediction for B0006 dataset

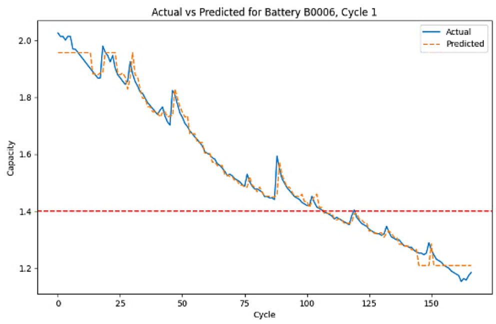

Figure 7. LightGBM based RUL prediction for B0006 dataset

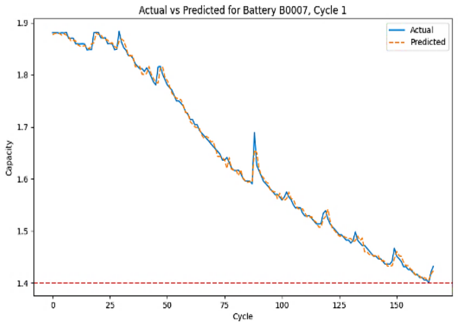

Figure 8. CatBoost based RUL prediction for B0007 dataset

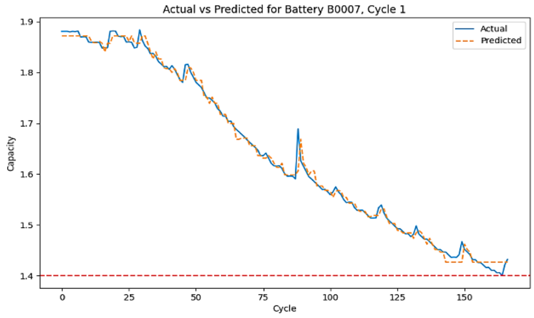

Figure 9. LightGBM based RUL prediction for B0007 dataset

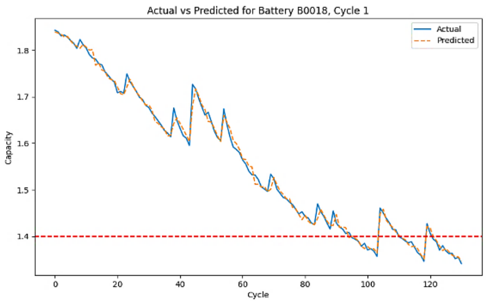

Figure 10. CatBoost based RUL prediction for B0018 dataset

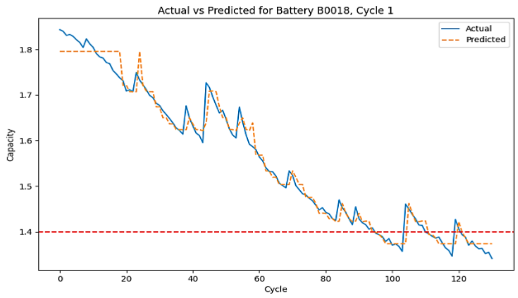

Figure 11. LightGBM based RUL prediction for B0018 dataset

The fourth Li-ion battery, B0018, faces challenges, but CatBoost outperforms LightGBM in performance, wit between prediction curves and actual capacity decline curve compared to LightGBM.
Tables 2 and 3 show that CatBoost outperforms LightGBM in performance indicators like MSE, MAE, MSL MAPE, EV, MSPE, RE, and R-squared for all batteries. CatBoost significantly improves battery performance accuracy compared to LightGBM, as it consistently outperforms LightGBM in terms of R-squared values.
The CatBoost and LightGBM algorithms effectively capture the dynamic characteristics of Li-ion batteries [18,21,22]. Comparing our prediction findings with previous NASA datasets, our results show superior performance compared to previous articles. However, our suggested approach, which uses CatBoost and LightGBM, outperforms the others, highlighting the superiority of our approach in predicting RUL for each battery.

Table 2. CatBoost Error Metrics of RUL Prediction

	B0005	B0006	B0007	B0018
MSE	0.00007007	0.00017349	0.00005876	0.00010974
MAE	0.00603363	0.00924179	0.00560260	0.00728351
MSLE	0.00001055	0.00002616	0.00000840	0.00001654
RMSE	0.00837093	0.01317164	0.00766570	0.01047560
MAPE	0.38627801	0.60004415	0.34368406	0.46809943
EV	0.99804125	0.99720574	0.99769920	0.99529280
MSPE	0.00283229	0.00704674	0.00217984	0.00441191
RE	0.00160704	-0.00416472	0.00080289	0.00117640
R^2 (%)	99.80	99.72	99.76	99.52

Table 3. LightGBM Error Metrics of RUL Prediction

	B0005	B0006	B0007	B0018
MSE	0.000162884	0.000761481	0.000141610	0.000510516
MAE	0.008461430	0.018237383	0.007915726	0.015295248
MSLE	0.000024731	0.000112987	0.000020584	0.000074834
RMSE	0.012762600	0.027594943	0.011899987	0.022594610
MAPE	0.546213303	1.171411934	0.486403094	0.960284776
EV	0.995446507	0.987735010	0.994455072	0.978098226
MSPE	0.006655668	0.030673735	0.005352821	0.019613045
RE	-0.007651998	-0.033401813	-0.006006861	-0.021927052
R^2 (%)	99.54	98.77	99.45	97.81

Table 4. Comparison of Error metrics in Prediction

Batteries	Methods	RMSE	R	MAE
BATTERY5	CNN-LSTM-DNN [28]	0.01457	98.313	0.00826
	LightGBM	0.01276	99.545	0.00846
	CatBoost	0.00837	99.804	0.00603
BATTERY6	CNN-LSTM-DNN [28]	0.01992	96.096	0.00872
	LightGBM	0.02759	98.774	0.01824
	CatBoost	0.01317	99.721	0.00924
BATTERY7	CNN-LSTM-DNN [28]	0.01722	96.900	0.01199
	LightGBM	0.01190	99.446	0.00792
	CatBoost	0.00767	99.770	0.00560
BATTERY18	CNN-LSTM-DNN [28]	0.02033	74.686	0.00966
	LightGBM	0.02259	97.810	0.01530
	CatBoost	0.01048	99.529	0.00728

Table 5 shows the RMSE increase in RUL prediction with CatBoost and LightGBM approaches, focusing on top article outcomes. Table VI shows the optimal RUL prediction result, increasing the RMSE improvement percentage for both NASA batteries from 33% to 55%.

Table 5. Enhanced RMSE prediction

Battery	Algorithm	RMSE	RMSE Improvement	
			CatBoost	LightGBM
BATTERY5	CNN-LSTM-DNN	0.01457	42.56%	12.43%
	LightGBM	0.01276		
	CatBoost	0.00837		
BATTERY6	CNN-LSTM-DNN	0.01992	33.89%	-38.51%
	LightGBM	0.02759		
	CatBoost	0.01317		
BATTERY7	CNN-LSTM-DNN	0.01722	55.46%	30.90%
	LightGBM	0.01190		
	CatBoost	0.00767		
BATTERY18	CNN-LSTM-DNN	0.02033	48.46%	-11.12%
	LightGBM	0.02259		
	CatBoost	0.01048		

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V. CONCLUSION

The study compares CatBoost and LightGBM performance with CNN-LSTM-DNN on datasets BATTERY 5, 6, 7, and 18. CatBoost significantly improves RMSE by 42.56%, 33.89%, 55.46%, and 48.46%, while LightGBM shows improvements of 12.43%, -38.51%, 30.90%, and -11.12%. The study concludes that the CatBoost and LightGBM technique used in this study is reliable, offering an average increase in prediction accuracy of 25% and maintaining long-term predictive capabilities within an execution time average of 300

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