Fast hybrid FNN-GPR modeling for state of health estimation in Lithium-Ion cells using early charge data: addressing performance variability

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Abstract– Accurate State of Health (SOH) estimation is essential for optimizing lithium-ion battery performance, especially in second-life applications. This paper introduces a fast SOH estimation method using the first 10 seconds of charge voltage data, followed by polynomial regression to extract features for AI algorithms. A hybrid model combining Feed-Forward Neural Networks (FNN) and Gaussian Process Regression (GPR) is proposed. This model was more accurate in detecting the SOH using just 10 seconds of charge voltage data, compared to other references that use approximately 6000 seconds of data. Using the Oxford Battery Dataset, we show that FNN excels in early-cycle estimations, while GPR performs better over full cycles. After detecting and excluding poorly performing cells, the combined model achieves superior accuracy, highlighting its potential for second-life battery applications and cell balancing strategies.

Keywords - State of health, Polynomial regression, Artificial intelligence, Cell balancing.

1. Introduction

Second-life usage of lithium-ion batteries involves repurposing degraded batteries from electric vehicles or other sources for less demanding applications, such as stationary energy storage.

In these applications, fast SOH estimation is critical to assess the remaining capacity and ensure safe and efficient operation.

The SOH (%) is expressed as:

$$SOH = \frac{C_{\max}}{C_{\text{nominal}}} \quad (1)$$

where C_{max} and $C_{nominal}$ are the current maximal and nominal capacities of the battery, respectively.

Additionally, accurate SOH estimation supports effective cell balancing strategies, which are essential for prolonging the life and performance of second-life battery packs by managing the variability in cell degradation.

Fast SOH estimation methods are particularly valuable in both first and second-life battery applications, as they reduce the need for extensive testing and allow for real-time monitoring. Traditional SOH estimation approaches often rely on full charge-discharge cycles, which can be time-consuming and impractical in real-world scenarios. Fast SOH techniques focus on utilizing early-stage data, such as the first few seconds of charge or discharge, to estimate battery health more efficiently, enabling proactive maintenance and better system management.

Fast SOH estimation techniques enable proactive maintenance, enhance system management, and reduce time and energy costs compared to traditional methods.

In second-life applications, where batteries are reused after their initial lifecycle in electric vehicles or other devices, effective cell balancing becomes crucial. Cell balancing ensures that all cells within a battery pack degrade evenly and function at similar performance levels, preventing the accelerated degradation of weaker cells.

By incorporating fast SOH estimation, second-life battery systems can be better managed, improving both the longevity and safety of repurposed batteries. Accurate SOH estimation also supports advanced cell balancing strategies, helping to extend the useful life of second-life battery packs.

The primary classifications focus on using either physical models or mathematical models within AI techniques to estimate the SOH of a battery and select the most suitable AI approach.

For instance, equivalent circuits which are types of physical modelling, simulate battery behavior using predefined physical components, while data-driven models utilize machine learning to identify complex patterns from battery measurement data. Data-driven methods offer several advantages, such as flexibility in handling non-linearities, minimal reliance on detailed physical understanding, and improved accuracy as more data becomes available, making them ideal for real-time SOH estimation across varying conditions [1]. The selection of data-driven models, such as SVM [2], Back-propagation Feed-forward neural network (BPFNN), GPR, LSTM (using approximately 6000 seconds of data) [3], Random Forest [4], or linear regression (using 30 seconds of data) [5], depends on various factors, including the available measured parameters, feature engineering techniques, and the quality and quantity of data [6]. However, we have successfully developed an SOH estimation model using only 10 seconds of data, enabling the creation of a cell classification strategy for cells based on their performance on a specific cycle.

In Section 2, we will detail the machine learning models used for SOH estimation. Section 3 will cover the selected feature extractions and methodology, including a discussion of the methods and presentation of the results. Section 4 will focus on the application and validation of the model using the Oxford dataset. The study will conclude with a summary of the findings and their implications in Section 5.

2. Proposed ML approaches for SOH estimation

In this study, various machine learning techniques were employed to fast estimate the SOH percentage of batteries and to identify poorly performing cells after reconstructing the database. Multivariable polynomial regression has proven effective for estimating the SOH [7]. Additionally, GPR and FNN were widely utilized, demonstrating superior accuracy and reliability in estimating battery health. GPR offers the advantage of providing probabilistic predictions, making it suitable for scenarios with uncertainty in the data, while FNN excels in capturing complex non-linear relationships between inputs and outputs, making it highly effective for handling large datasets [3]. Together, these methods form a robust approach to SOH estimation, with GPR contributing uncertainty quantification and FNN delivering strong predictive power.

GPR is a machine learning method based on Bayesian and statistical learning theories, well-suited for handling the complex nonlinear problems associated with battery degradation. It provides an effective way to estimate the SOH of a battery by learning the relationship between input and output data. GPR can be viewed as a supervised learning approach where a collection of random variables follows a joint Gaussian distribution. As a non-parametric model, GPR performs regression by incorporating both noise and prior information, solved through Bayesian inference. Its ability to offer accurate predictions and quantify uncertainty makes GPR particularly valuable for SOH estimation, especially in scenarios with high data variability [8].

FNN is widely used in machine learning, especially for predicting the SOH in batteries. Unlike recurrent neural networks, FNNs process data in one direction—from the input layer through one or more hidden layers to the output layer—without looping back. Each layer consists of neurons that apply activation functions to learn patterns from the data. FNNs are particularly effective for modeling complex relationships in battery data due to their ability to approximate nonlinear functions. By training the network on historical battery measurements, FNNs can capture the underlying patterns that indicate battery health degradation. Their simplicity, robustness, and adaptability make them well-suited for SOH estimation, providing accurate predictions even in dynamic environments [7]. The FNN model employed in this paper is identical to the one utilized in our prior research [10].

This study leverages state-of-the-art machine learning techniques, including GPR and FNN, to advance the estimation of battery SOH. While GPR is renowned for its probabilistic predictions and ability to handle data variability, and FNN excels in capturing complex nonlinear relationships, our novel contribution lies in combining these methods. This hybrid approach benefits from GPR's uncertainty quantification and FNN's predictive power, enabling efficient and accurate SOH estimation.

Our proposed model achieves more accurate SOH estimation using only 10 seconds of voltage data from the Oxford Battery Dataset. It outperforms a data-driven SOH estimation method based on voltage variation curves, which requires approximately 6000 seconds of data from both discharge and charge cycles [3], in terms of accuracy. Additionally, by reconstructing the database to exclude poorly performing cells, we enhance the model's reliability and provide insights into cell balancing challenges. This dual focus on rapid estimation and database optimization addresses critical gaps in the state-of-the-art and establishes a robust framework for battery health monitoring.

The initial step involves importing data from the Oxford Battery Dataset [12], which provides essential measurements such as battery charge and discharge voltages. The dataset includes high-resolution data from eight Kokam lithium-ion pouch cells tested under specific conditions represented in Table 1.

Table 1. Characteristics of the Oxford Battery Dataset Characteristics of the Oxford Battery Dataset

Characteristic	Details
Anode Material	Graphite
Cathode Material	$LiCoO2/LiNiMnCoO2$
Testing Temperature	40°C
Charging Protocol	1C-CC
Discharge Protocol	Artemis driving cycle, 2.7V cutoff
Data Sample Rate	1 second

The performance of the batteries in the dataset varies significantly, as illustrated in Figure 1. Cells 2, 5, and 6 exhibit early degradation and the capacity curve drops sharply [11]. This observation will guide our analysis and methodology moving forward. This variability underscores the need for a targeted strategy to identify poorly performing cells. By analyzing performance data, we can develop a method to detect cells with rapid degradation. Combining this approach with fast SOH estimation techniques enables us to address cell balancing challenges effectively. The objective is to establish a strategy that efficiently identifies underperforming cells while facilitating effective balancing, ultimately improving the overall performance and longevity of battery systems.

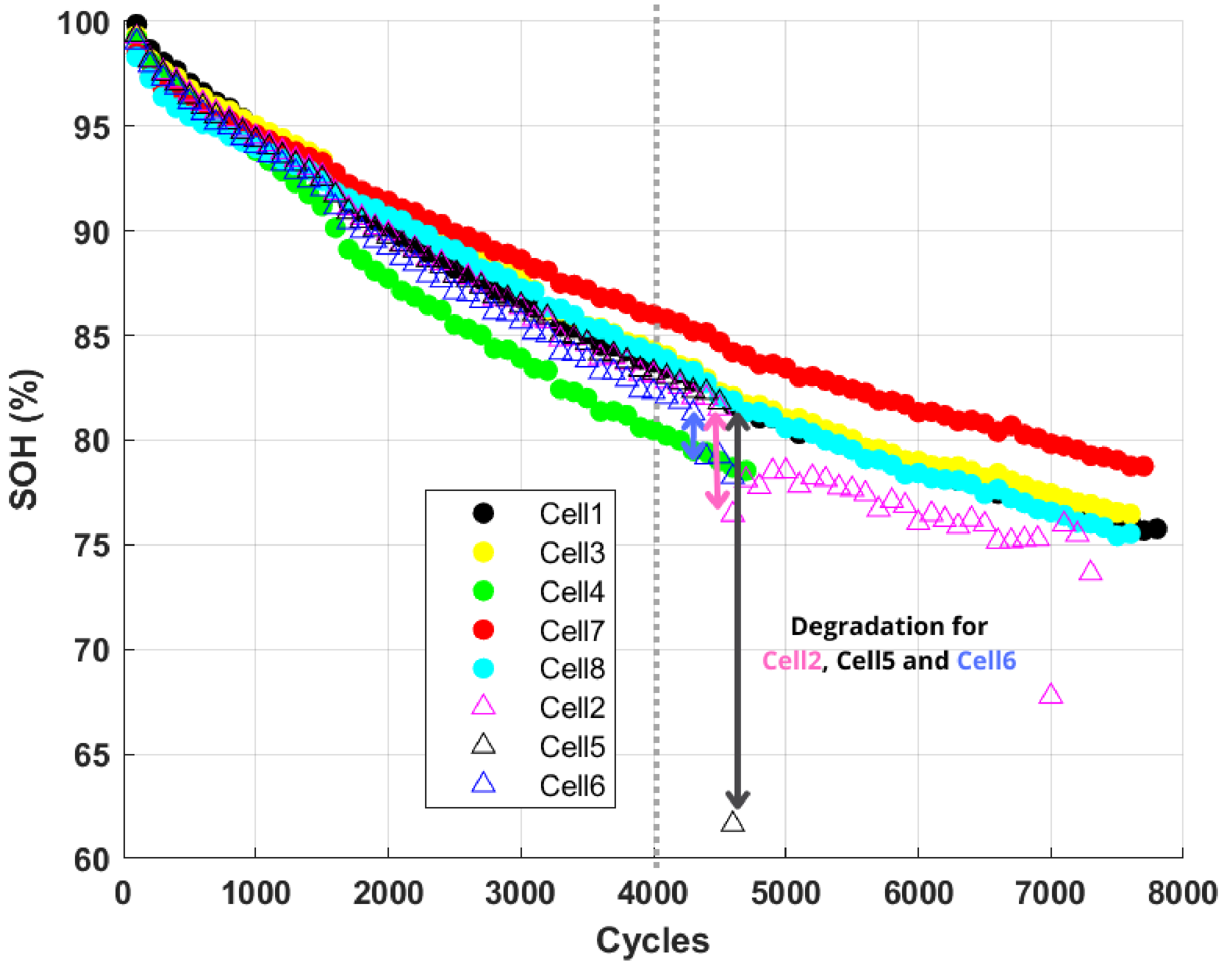

Figure 1 : SOH evolution across cycles for individual cells.

3. Features extractions and methodology

To enable rapid SOH estimation, we concentrate on analyzing the first 10 seconds of charge voltage data from each cycle. For feature extraction, we calculate the area under the charge voltage curve and apply a fifth-degree polynomial regression, extracting all resulting coefficients. This approach was selected for its ability to effectively capture the performance characteristics of the charging voltage curve, providing valuable information for AI models. It was also validated in our previous research during the full discharge phase, demonstrating high correlation and effectiveness [10].

The regression equation can be expressed as follows:

$$V(t) = \sum_{i=0}^{5} a_i t^i \qquad (2)$$

where V(t) represents the voltage at time t, and a_i are the coefficients obtained from the polynomial regression of degree 5.

To compute the area under the charge curve, we integrate the polynomial function from the initial time: 1 second to the final time: 10 seconds.

$$Area = \int_1^{10} V(t)\,dt \qquad (3)$$

Consequently, the input features for both algorithms include the area under the curve, which demonstrates a strong correlation with SOH, as detailed in Table 2, the absolute correlation exceeds 90%, indicating that extracting data from just the first 10 seconds provides a substantial amount of information. The performance of polynomial regression of degree 5 and degree 6 is similar in terms of fitting accuracy as represented in Figure 2. However, the coefficients from the degree 5 polynomial demonstrate better correlation with SOH. For instance, the coefficient a_2 from the degree 5 polynomial has an absolute correlation of 0.47 with SOH, compared to 0.38 for the degree 6 polynomial. This stronger correlation is valuable for capturing non-linear relationships and enhances the performance of the FNN and GPR models. Thus, polynomial regression of degree 5 is preferred for its superior correlation with SOH.

Table 2. Correlation of SOH with the Area of the First 10 Seconds of Charging Voltage.

Cell	Absolute Correlation
C1	0.95
C2	0.94
C3	0.92
C4	0.93
C5	0.94
C6	0.91
C7	0.91
C8	0.94

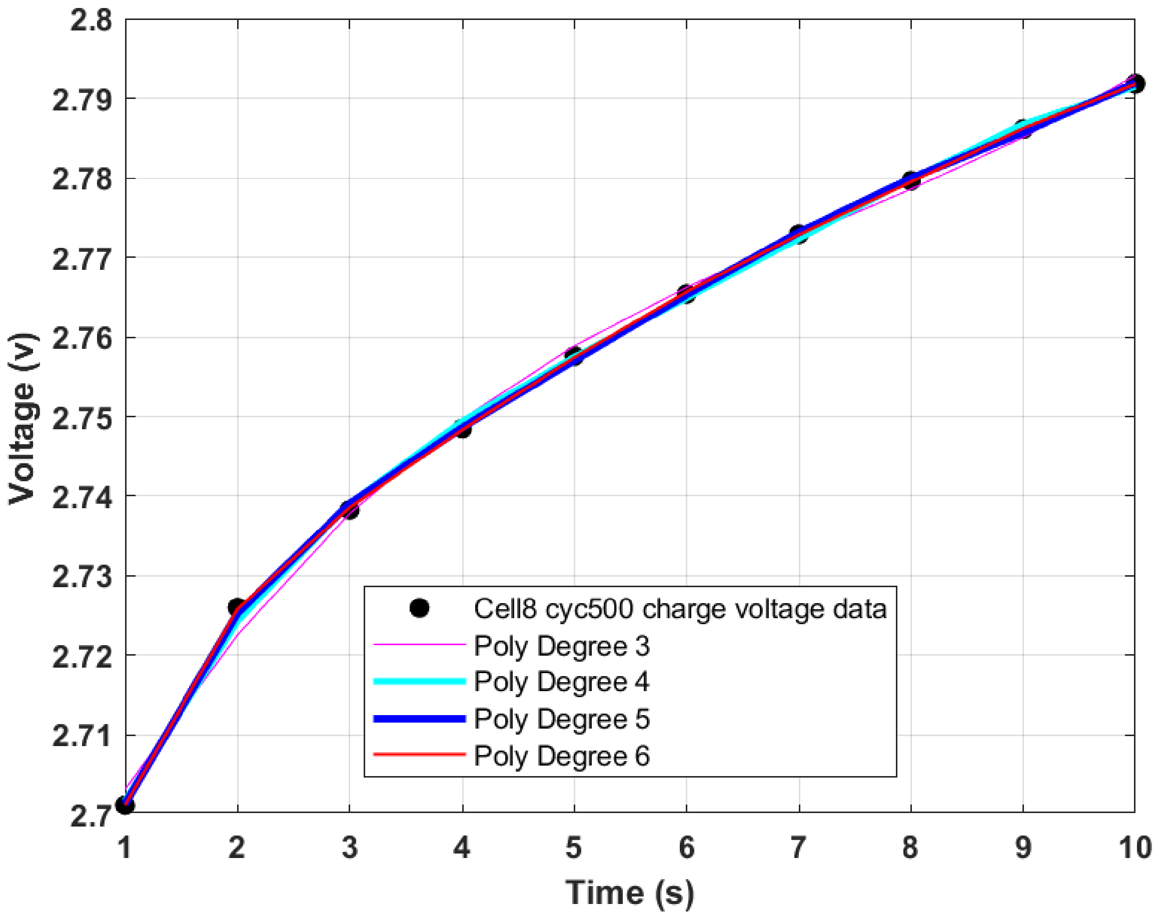

Figure 2: Polynomial Fittings of Voltage Data Across Different Degrees.

To determine the most effective modeling approach, this study will evaluate two machine learning techniques: GPR and FNN with 5 hidden layers, the optimal FNN model was determined through extensive testing with different configurations, and it was found that using five hidden layers for the FNN yielded the best performance. The evaluation process will employ rigorous cross-validation methods to assess key performance metrics, including Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and Maximum Absolute Error (MaxAE). Based on these metrics, an optimal model for SOH prediction will be identified, leading to the development of a hybrid FNN-GPR model. Following the selection of the optimal model, an in-depth statistical analysis will be conducted to further refine its performance.

Additionally, this approach aims to develop a novel strategy for fast detecting poorly performing cells due to early degradation, which could significantly benefit battery cell balancing and management.

The Leave-One-Out Cross-Validation (LOOCV) will be applied and this procedure involves systematically testing one cell while training the model on all other cells. This method provides a robust assessment of the model to generalize across different battery conditions, highlighting its performance and identifying potential issues related to overfitting or underfitting. By applying this approach, the plan offers a thorough and systematic strategy for battery diagnostics using machine learning, covering data preparation, model selection, evaluation, and integration, which is essential for practical applications in battery management and optimization.

The comparative study of these models involves a thorough evaluation using established metrics:

• RMSE for comprehensive error assessment, calculated using the equation:

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

• MAE for average prediction error, calculated using the equation:

$$\frac{1}{n}\sum_{i=1}^{n}|y_i-\hat{y}_i|. \quad (5)$$

• MaxAE for assessing the maximum absolute error, calculated using the equation:

$$\max_i |y_i-\hat{y}_i| \quad (6)$$

These metrics ensure a rigorous scientific analysis of model performance and applicability.

4. Application and model validation

To assess the performance of both GPR and FNN algorithms, a leave one-out cross-validation (LOOCV) technique will be used. This approach provides a rigorous evaluation of the models across varying battery behaviors, simulating real-world conditions. The first LOOCV test will encompass all battery cycles, and as shown in Tables 3 and 4, the GPR model consistently outperforms FNN across all cycles in 7 out of 8 tests, achieving superior results in at least two error metrics compared to the FNN model.

Table 3. FNN Performance Metrics.

Cell	RMSE	MAE	MaxAE
C1	1.09	0.83	2.57
C2	1.47	2.22	19.92
C3	1.07	0.85	3.25
C4	1.01	0.87	2.16
C5	1.98	0.73	12.92
C6	1.98	0.98	2.58
C7	0.76	0.63	1.62
C8	0.55	0.43	1.50

Table 4. GPR Performance Metrics.

Cell	RMSE	MAE	MaxAE
C1	0.71	0.57	1.42
C2	2.10	1.46	8.78
C3	1.06	0.95	1.86
C4	0.66	0.50	1.64
C5	1.00	0.54	5.77

C6	0.70	0.58	1.62
C7	**0.80**	**0.67**	**1.84**
C8	0.53	0.44	1.41

After analyzing the battery performance in Figure 1, it is evident that during the first 4000 cycles, the batteries exhibit similar behavior. Applying LOOCV within this range reveals that the FNN model outperforms the GPR model in 7 tests out of 8, as demonstrated in the corresponding Tables 5 and 6.

Table 5. FNN Performance Metrics for the First 4000 Cycles.

Cell	RMSE	MAE	MaxAE
C1	0.55	0.44	1.36
C2	0.56	0.49	1.18
C3	0.71	0.61	1.41
C4	0.49	0.38	1.31
C5	0.56	0.47	1.21
C6	0.53	0.45	1.05
C7	**0.75**	**0.65**	**1.30**
C8	0.46	0.37	0.93

Table 6. GPR Performance Metrics for the First 4000 Cycles.

Cell	RMSE	MAE	MaxAE
C1	0.56	0.68	1.57
C2	0.59	0.53	1.37
C3	1.14	0.94	4.33
C4	1.40	0.84	5.53
C5	0.62	0.44	2.17
C6	0.61	0.49	1.40
C7	0.65	0.54	1.48
C8	0.65	0.54	1.27

Based on the results, it is evident that the FNN algorithm outperforms GPR in terms of RMSE, MAE, and MaxAE when applied to the first 4000 cycles. Conversely, the GPR model demonstrates superior performance across all cycles. To leverage the strengths of both models, we developed a hybrid approach combining FNN and GPR using average modeling. This hybrid model combines the strengths of both techniques to improve overall accuracy. For instance, compared to reference [3], which uses approximately 6000 seconds of charge and discharge voltage data, our model achieves superior performance on cell C8, with a lower MAE of 0.52% and RMSE of 0.42%, outperforming the best results reported in [3], which are 0.88% and 0.92%, respectively. Subsequently, we employed this combined model to effectively identify poorly performing cells. Specifically, Cells 2, 5, and 6 were detected as underperforming due to their MaxAE values exceeding 2%, indicating significant degradation as represented in Table 7.

Table 7. Performance Metrics for Hybrid GPR+FNN Model.

Cell	RMSE	MAE	MaxAE
C1	0.86	0.68	1.94
C2	2.79	1.82	**11.85**
C3	0.84	0.72	1.86
C4	0.68	0.54	1.48
C5	1.47	0.62	**9.35**
C6	0.88	0.73	**2.10**

C7	0.70	0.58	1.63
C8	0.52	0.42	1.20

To justify the use of average modeling, we observed that it consistently outperforms both individual models in various configurations. For instance, in testing on Cell 8, the average modeling approach achieved an RMSE of 0.52, which is superior to the RMSE of 0.73 for a model with 70% FNN and 30% GPR, and 0.61 for a model with 70% GPR and 30% FNN. This performance demonstrates that average modeling effectively leverages the strengths of both GPR and FNN, providing more accurate predictions.

After identifying the poorly performing cells, we excluded them to create a refined dataset. This new dataset was then utilized to train the hybrid model, with the goal of improving the estimation accuracy for high-performing cells and enhancing the detection of degraded cells.

The hybrid model consistently outperforms both the FNN and GPR models, after applying 5 LOOCV tests on the cells 1, 3, 4, 7 and 8, achieving superior results in at least two error metrics and displaying a better overall average across all three errors, as shown by the error metrics in Figure 3.

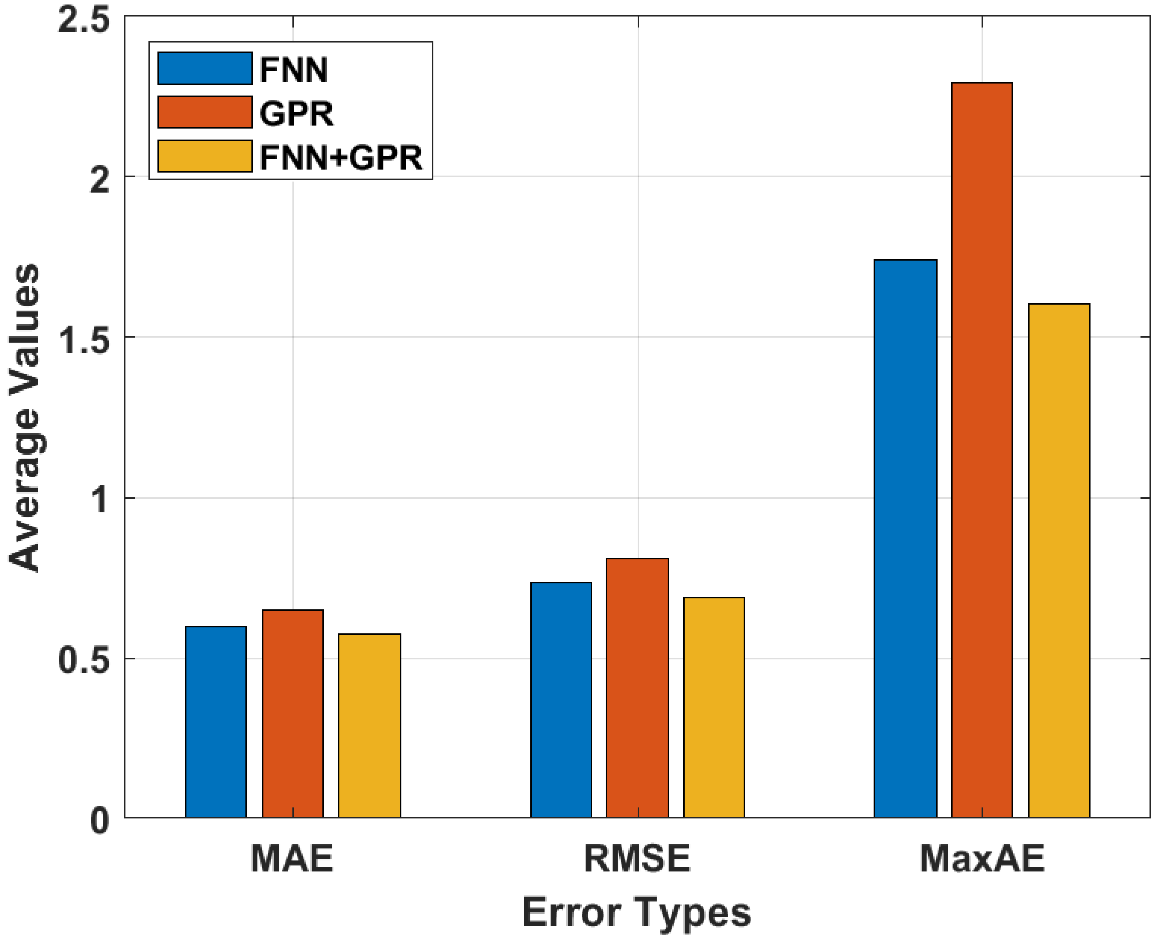

Figure 3: Comparison of FNN, GPR, and FNN+GPR average errors across categories.

To underscore the importance of the hybrid model, it is crucial to note that the estimation accuracy for high-performing cells improves as more data is incorporated. For instance, as illustrated in Table 8, the RMSE for Cell 8 decreases with the inclusion of additional training cells.

Table 8. RMSE for Cell 8 with Varying Training Sets.

Test Cell	Training Cells	RMSE
C8	C1	0.90
C8	C1, C3	0.615
C8	C1, C3, C4	0.612

C8	C1, C3, C4, C7	0.52

This trend illustrates that the accuracy of SOH estimation for well-performing cells, such as Cell 8, improves significantly with the inclusion of more data, validating the efficacy of the hybrid model in leveraging comprehensive datasets to enhance predictive performance.

To validate the degraded performance of Cells 2, and 5, the hybrid model will be applied to the refined database. This approach aims to identify whether these cells exhibit an absolute error exceeding 2%, confirming their status as poorly performing. The refined dataset, which excludes previously identified poorly performing cells, provides a more accurate assessment of these cells' degradation. By evaluating the MaxAE on this refined dataset, we can effectively confirm the degraded condition of Cells 2 and 5 and ensure they meet the criteria for poor performance as shown in Figure 4 and Figure 5.

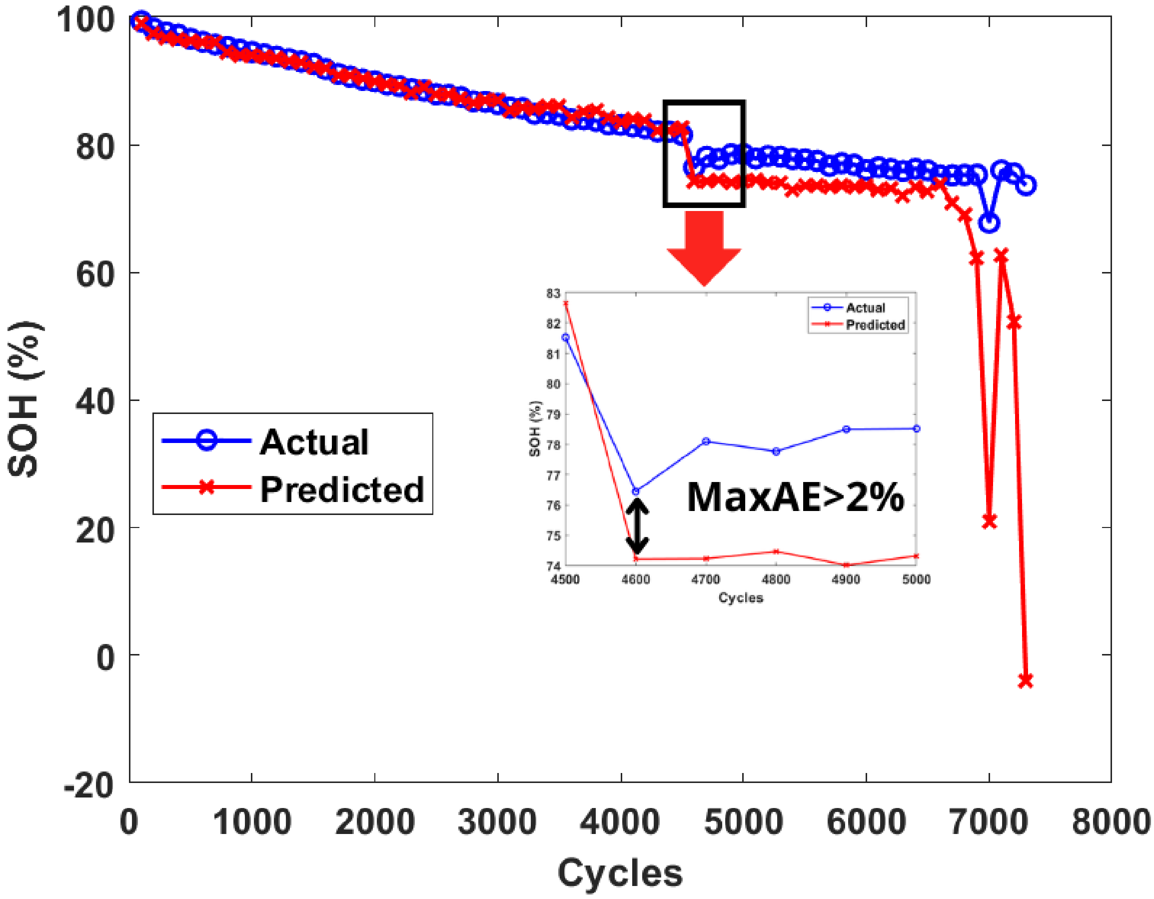

Figure 4: Comparison of Actual vs. Predicted SOH values: detection of errors greater than 2% for cells 2.

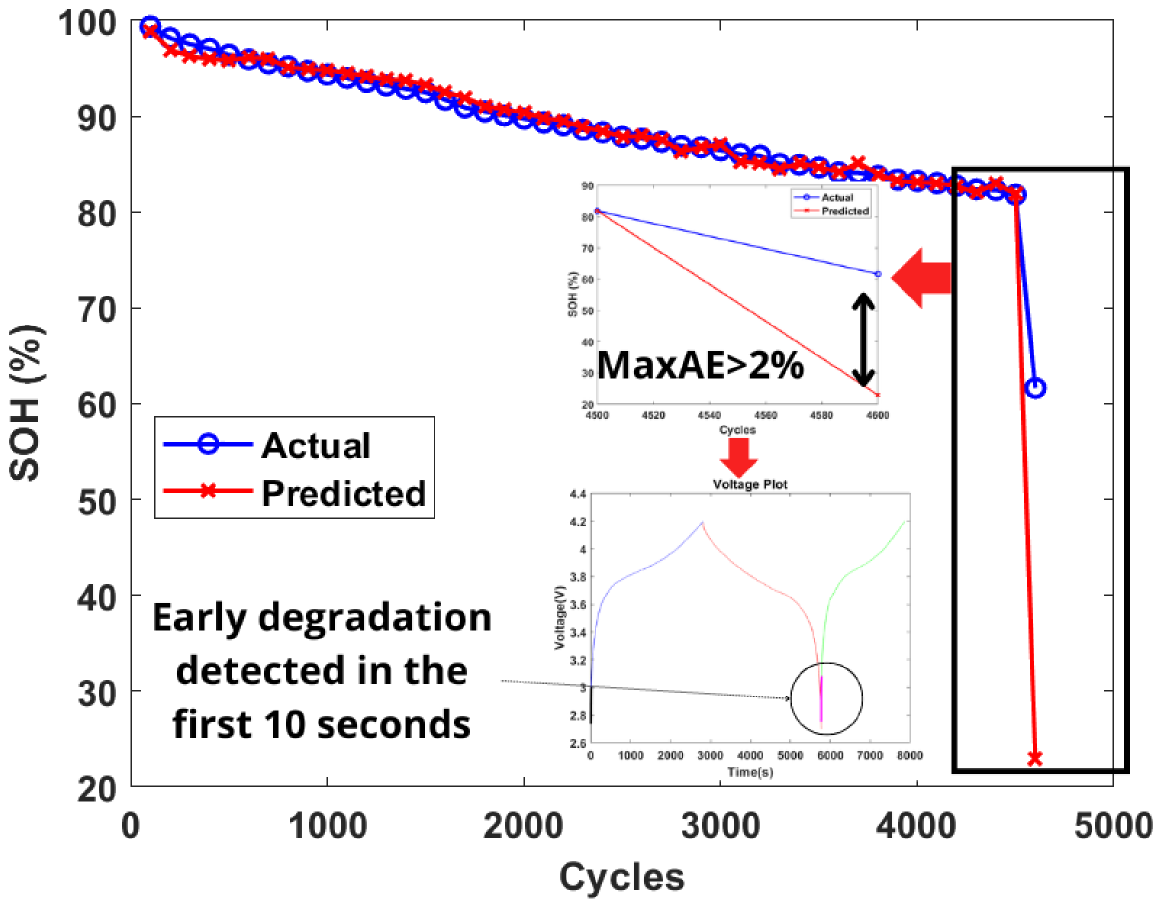

Figure 5: Comparison of Actual vs. Predicted SOH values: detection of errors greater than 2% for cells 5.

Cell 6 did not meet the criterion of a MaxAE greater than 2% as shown in Figure 6. The lower MaxAE for Cell 6 can be attributed to its minimal degradation and limited data, as it exhibited only minor degradation with just three cycles after the observed degradation point. In contrast, Cell 2 experienced medium degradation followed by over ten cycles and a subsequent significant degradation, while Cell 5 underwent substantial degradation. This nuanced analysis underscores the necessity of evaluating cells within the context of their operational history and the characteristics of the dataset and highlights the need for additional data to better understand and detect subtle degradation patterns.

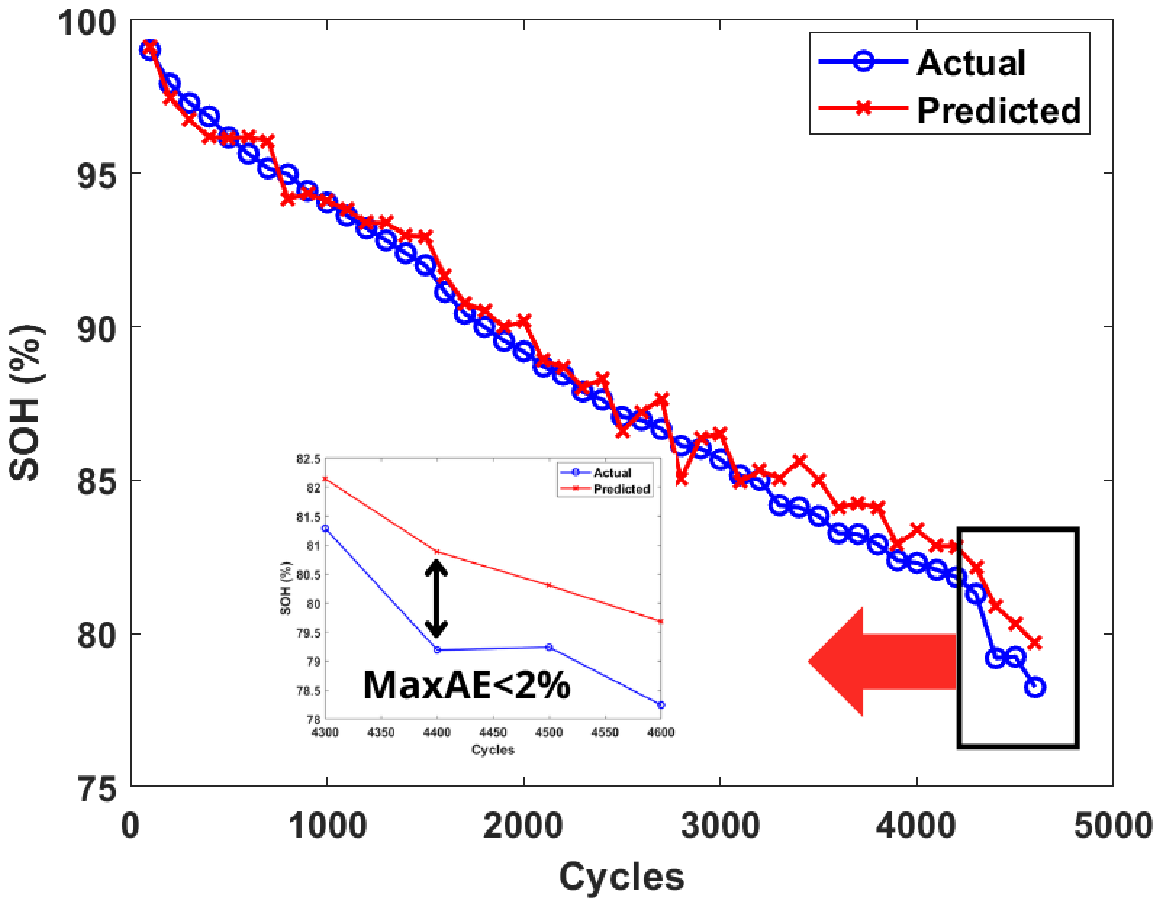

Figure 6: Comparison of Actual vs. Predicted SOH values: detection of errors less than 2% after degradation for cells 6.

The significance of this strategy lies in its ability to detect poorly performing cells by estimating SOH directly after degradation, using an error threshold greater than 2%. As demonstrated for Cell 2 and Cell 5, this fast SOH estimation—based on only 10 seconds of charge voltage data—proves crucial for cell balancing techniques. By identifying degraded cells swiftly, this approach supports more effective cell balancing, ensuring better overall battery performance and longevity.

5. Conclusion

This study introduced a hybrid model combining GPR and FNN for estimating the SOH of lithium-ion batteries. By applying LOOCV, we found that while GPR was superior across all cycles, FNN excelled in the first 4000 cycles, justifying the use of a hybrid approach. The refined model, after excluding poorly performing cells, demonstrated improved accuracy in estimating SOH and detecting degradation.

After refining the training dataset by excluding poorly performing cells, the hybrid model's accuracy in estimating SOH improved significantly. This enhancement led to superior performance metrics compared to individual algorithms, highlighting the hybrid model's effectiveness in rapid SOH estimation, especially for detecting degraded cells.

Our approach, utilizing just 10 seconds of charge voltage data, proved effective in identifying degraded cells and enhancing battery management. This method is crucial for cell balancing, ensuring better battery performance and longevity through timely and precise interventions.

However, the performance of Cell 6, which did not meet the criterion for high MaxAE, underscores the need for additional data. Further research and data collection are essential to enhance the detection of subtle degradation patterns and refine the effectiveness of the model in various scenarios.

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