

Article

Early-Cycle Lifetime Prediction of Lithium-Ion Batteries with Ultra-Short Cycle Life Using Transferable Statistical Features

Yuxiang Kuang, Dongxu Guo *  and Yuejiu Zheng

School of Mechanical Engineering, University of Shanghai for Science and Technology, Shanghai 200093, China; 2335051616@st.usst.edu.cn (Y.K.)

* Correspondence: guodongxu@usst.edu.cn

Abstract

Early-cycle lifetime prediction of lithium-ion batteries is important for rapid cell screening, battery development, and manufacturing quality control. However, accurate prediction at the early stage remains difficult because capacity fade is usually very limited during the initial cycles, and the available degradation signals are weak. In this study, an early degradation voltage morphology (EDVM)-based framework is proposed for early cycle-life prediction. Two statistical features and one degradation mode voltage signature (DMVS) feature are extracted from the discharge capacity-difference profiles between the 10th and 3rd cycles and combined with an extreme gradient boosting (XGBoost) model. Validation on 138 commercial NCM811 cylindrical cells shows that the proposed framework achieves a mean absolute percentage error (MAPE) of 12.29% using only the first 10 cycles of data. In addition, the DMVS feature identifies three groups of early degradation behavior and provides physically interpretable information on degradation heterogeneity. These results indicate that the proposed method is an efficient and interpretable approach for early cycle-life prediction and has practical potential for battery evaluation and screening.

Keywords: lithium-ion battery; early-cycle prediction; early degradation voltage morphology (EDVM); degradation mode voltage signature (DMVS); extreme gradient boosting (XGBoost)

1. Introduction

Early cycle-life prediction has become increasingly important for lithium-ion batteries because it can support rapid cell screening, shorten evaluation time, and improve decision-making in battery development and manufacturing [1,2]. In practical settings, early identification of cells with poor durability is valuable for reducing testing cost and accelerating quality assessment [3,4]. However, this task remains challenging because the degradation information available in the initial cycles is limited [5]. During this stage, macroscopic capacity fade is usually small, while the underlying degradation process is often nonlinear and highly cell-dependent [6]. As a result, conventional bulk indicators provide limited ability to distinguish future cycle-life variation across cells, especially for batteries with relatively short service life [7].

Current approaches for cycle-life prediction can be broadly grouped into two categories [8]. The first category uses data-driven models to learn degradation patterns directly from capacity trajectories or other time-series signals [9]. Although these methods can achieve satisfactory performance under data-rich conditions, their effectiveness is often reduced when only a short observation window is available, because the early degradation



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signals remain weak and the sample size is limited [10]. The second category focuses on feature engineering by extracting health-related indicators from charge and discharge data [11–13]. This strategy is generally more suitable for early prediction, but many existing methods still depend on high-dimensional features that may introduce redundancy, reduce robustness, and provide limited physical insight into where the degradation develops along the voltage domain [12]. Therefore, there is still a need for compact and physically interpretable features that can support accurate early cycle-life prediction [14].

To address these limitations, this study develops a feature engineering framework based on early degradation voltage morphology (EDVM). The framework uses the voltage-domain capacity difference between selected early cycles to characterize early degradation behavior and support cycle-life prediction for short-lifespan batteries under limited-data conditions. The main contributions of this work are summarized as follows:

1. A degradation mode voltage signature (DMVS) feature is introduced to extend conventional differential capacity analysis. Unlike peak-tracking methods that are less sensitive before observable capacity fade, the DMVS feature captures early voltage-location shifts associated with kinetic degradation and enables the grouping of cells with different early degradation patterns.
2. The transferability of the extracted statistical features is examined across different degradation stages. Correlation analysis at the 10th and 100th cycles shows that the relationship between these features and cycle life evolves from an early nonlinear stage to a later approximately linear stage.
3. An EDVM-based predictive framework is established by combining three physically interpretable features with extreme gradient boosting (XGBoost). Using discharge data from only the first 10 cycles, the framework achieves a mean absolute percentage error (MAPE) of 12.29%, improves prediction accuracy relative to linear baselines, and reduces reliance on high-dimensional inputs.

Table 1 compares the proposed EDVM framework with representative existing approaches across different technical pathways in terms of physical interpretability, feature dimensionality, prediction window, and applicable scenario.

Table 1. Comparison of the proposed EDVM framework with representative existing methodologies across different technical pathways.

Method	Input Data	Feature Dimension	Physical Meaning	Prediction Window	Applicable Scenario
Deep learning sequence models [15,16]	Raw charge/discharge time-series matrices	High Raw data arrays	Learns latent temporal representations from raw sequential data.	Initial 30–100 cycles	Large datasets, extensive training samples, long-life batteries.
High-dimensional machine learning frameworks [17,18]	Multi-domain curves (Voltage, Current, Temp)	High >20 statistical scalars	Aggregates macroscopic multi-physics metrics from multiple signal domains.	Initial 30–100 cycles	Scenarios with sufficient early macroscopic degradation signals.
Early $\Delta Q(V)$ statistics [10]	Voltage-domain capacity difference $\Delta Q(V)$	Low Mean, Var, Min, Skewness, Kurtosis, Log(Min)	Quantifies capacity loss magnitude and overall shape variation in the voltage domain.	Initial 100 cycles	Fast charging, lithium iron phosphate/graphite, long-life batteries.
Incremental capacity/differential voltage (ICA/DVA) peak analysis [19,20]	dQ/dV or dV/dQ incremental curves	Medium Peak heights and positions	Tracks peak shifts associated with thermodynamic phase-transition behavior.	50–200 cycles	Conventional operational conditions, measurable kinetic shift.
EDVM (proposed)	Discharge capacity difference $\Delta Q_{10-3}(V)$	Low 3 scalars	Captures early kinetic polarization and identifies degradation voltage modes through the DMVS feature.	Initial 10 cycles	Early screening of short-lifespan batteries under limited-data conditions.

The remainder of this paper is organized as follows. Section 2 details the EDVM-based methodology, including profile construction, feature extraction, and the predictive

framework. Section 3 describes the data source, cell selection procedure, testing protocol, and early-cycle data characteristics. Section 4 presents the results and discussion. Section 5 summarizes the main conclusions and outlines directions for future work.

2. Methodology

To support early cycle-life prediction under limited-data conditions, this study develops a feature engineering framework based on EDVM. The framework is motivated by the observation that internal kinetic polarization and impedance growth can emerge in the early aging stage, even before clear macroscopic capacity loss becomes observable [21,22]. Building on this premise, a voltage-domain capacity-difference curve is constructed to capture subtle early degradation behavior along the discharge process. From this representation, two statistical descriptors together with the DMVS feature are extracted to characterize both the magnitude and location of degradation-related variation. These three interpretable features are then integrated with an XGBoost regression model to establish the complete predictive framework for cycle-life estimation.

2.1. Construction of EDVM

To capture voltage-dependent degradation features, the EDVM curve is defined as the differential capacity:

$$\Delta Q_{i-j}(V) = Q_i(V) - Q_j(V) \quad (1)$$

where $Q_i(V)$ and $Q_j(V)$ denote the cumulative discharge capacity up to voltage V at the i -th and j -th cycles, respectively. To ensure a consistent basis for comparison across cycles, a standardized voltage grid was established before constructing the EDVM curves. The raw discharge data were deduplicated and sorted monotonically by voltage. Subsequently, the capacity values were mapped onto 700 equidistant nodes spanning from 4.20 V to 2.75 V using piecewise cubic Hermite interpolating polynomials (PCHIPs). A sensitivity analysis was conducted to evaluate the robustness of the interpolation and smoothing parameters. The cross-validation mean absolute percentage error (MAPE) exhibited minimal variation, remaining between 12.2% and 12.6% across interpolation grids containing 400–1000 points, Savitzky–Golay filter window lengths of 11–51, and polynomial orders of 2–5. Relative to the baseline configuration of 700 interpolation points, a window length of 29, and a third-order polynomial, no statistically significant differences were detected, with p -values exceeding 0.05 and Cohen's d values remaining below 0.06. Therefore, the EDVM curves were smoothed using a 700-point interpolation grid and a Savitzky–Golay filter characterized by a window length of 29 and a third-order polynomial. This parameter combination ensured robust feature preservation while maintaining computational efficiency.

In the proposed framework, the reference baseline cycle and the observation cycle for EDVM construction are determined dynamically based on the dataset characteristics. After excluding the initial cycles corresponding to the formation stage, the cycle pair is selected within the early cycling window to optimize predictive performance. For the dataset evaluated in this study, Cycle 3 serves as the reference baseline, and Cycle 10 acts as the early observation point. This data-driven selection ensures that the differential calculation compares two states post-formation, providing a sufficient interval to detect degradation signals while mitigating potential accuracy loss from arbitrary cycle selection. The rationale for this configuration is further analyzed in Section 4.4, which presents the sensitivity analysis regarding the starting cycle position and the cycle interval.

2.2. Interpretable Feature Extraction

To quantify the degradation information embedded in the EDVM curves, three interpretable features were extracted based on the mechanistic characteristics of early

degradation reflected in the voltage domain, as shown in Table 2. Two low-dimensional statistical descriptors were used to characterize the overall magnitude and heterogeneity, while the proposed DMVS feature was introduced to capture the voltage-location dependence of the dominant degradation response. Together, these features describe both the severity and the spatial distribution of early degradation behavior along the voltage axis.

Table 2. Summary of the extracted EDVM features and corresponding units.

Feature	Unit
Mean(ΔQ)	Ah
Var(ΔQ)	Ah ²
$V_{(\Delta Q)_{\min}}$	V

2.2.1. Statistical Features Characterizing Degradation Magnitude and Heterogeneity

Two low dimensional statistical metrics were selected based on an analysis of how early degradation is manifested in the EDVM curves, together with evidence from prior early prediction studies [10]. Existing studies have shown that the distribution pattern, dispersion level, and extreme response of early cycle capacity differences can carry useful information about subsequent cycle life [23,24]. Following this insight, the present study uses these metrics to characterize degradation heterogeneity while avoiding the curse of dimensionality associated with high dimensional representations, thereby preserving computational efficiency for early-stage battery sorting in end-of-life (EOL) testing. The features are defined as follows:

1. Mean(ΔQ): the average value of the EDVM curve, reflecting the mean capacity loss per unit voltage interval. This quantity corresponds to the global magnitude of early degradation [25,26]. A larger absolute mean value indicates a faster overall degradation rate and a shorter expected lifespan.
2. Var(ΔQ): the variance of the EDVM curve, quantifying the heterogeneity of degradation along the voltage axis. A higher variance suggests that capacity loss is concentrated within specific voltage intervals, reflecting uneven localized deterioration. This aligns with observations reported in early prediction studies [10,27].

2.2.2. The Proposed DMVS Feature

To address the limitations of traditional differential capacity analysis in distinguishing degradation modes, the proposed DMVS is defined as the voltage coordinate of the minimum EDVM value, denoted by $V_{(\Delta Q)_{\min}}$:

$$V_{(\Delta Q)_{\min}} = \arg \min_V \Delta Q_{10-3}(V) \quad (2)$$

The purpose of introducing the DMVS is to complement magnitude-based statistical descriptors with a feature that preserves the voltage-location information of the dominant degradation response. In this way, the EDVM analysis is extended from quantifying only the magnitude of capacity loss to additionally identifying where the most pronounced degradation variation is located along the voltage axis. From an electrochemical perspective, the voltage coordinate of the EDVM minimum can be interpreted as a marker of the voltage region where degradation-induced kinetic variation is most strongly expressed [28,29]. Incremental capacity and differential voltage analyses reported for NCM/graphite systems further indicate that specific voltage regions are associated with distinct electrode reaction regimes and polarization sensitivities [20,30].

Unlike traditional differential capacity analyses such as dQ/dV , which can be sensitive to sampling frequency and measurement noise, the DMVS feature is comparatively robust.

By extracting the global minimum of the cumulative capacity–difference curve rather than relying on instantaneous derivatives, the influence of local high-frequency fluctuations on identifying this phase-transition signature is reduced.

2.3. XGBoost-Based Predictive Modeling

This study employed XGBoost as the regression model for cycle-life prediction [31]. Within the present framework, XGBoost is well suited to the extracted EDVM features because it can model nonlinear degradation behavior and feature interactions without requiring high-dimensional input representations. Its tree-based ensemble structure is also effective for structured tabular features under limited-data conditions, while the built-in regularization and subsampling mechanisms help reduce overfitting risk. In addition, Shapley additive explanations (SHAP) were adopted to quantify feature attribution and support the interpretability of the predictive framework [32].

The XGBoost hyperparameters were set as follows: 100 estimators, a maximum depth of 2, a learning rate of 0.05, a subsample ratio of 0.8, a colsample_bytree ratio of 0.7, an L2 regularization coefficient (λ) of 10.0, and a random state of 42. These parameters were selected based on explicit theoretical justifications. A very shallow tree depth combined with a moderate number of estimators restricts the model capacity, preventing it from memorizing noise in the training data. A high L2 regularization coefficient was employed to impose a strong penalty on leaf node weights, mitigating overfitting in scenarios with few input features. Furthermore, moderate subsample and colsample_bytree ratios introduce randomness during each iteration, forcing the model to avoid relying on a single feature or local sample subset for prediction, thereby improving generalization performance. A low learning rate paired with an L2 regularization term higher than the default value effectively suppresses the excessive growth of leaf node weights, which results in smoother and more stable predictions.

To evaluate model performance while precluding data leakage, a nested five-fold cross-validation strategy was implemented to obtain an unbiased assessment of generalization capability. The outer five folds were used to evaluate generalization error, while the inner five folds were used for hyperparameter tuning. The entire preprocessing workflow, including interpolation, filtering, and feature extraction, was executed independently solely on the training set after each outer split. This guarantees no information leakage between the training and testing data. Subsequently, a standard five-fold cross-validation was conducted on the complete dataset to search for the optimal hyperparameters for the final deployment model. The ultimate model was then trained on the entire dataset using these finalized parameters. Prediction accuracy was quantified using the mean absolute percentage error (MAPE) and the root mean square error (RMSE), defined as follows:

$$\text{MAPE} = \frac{1}{N} \sum_{i=1}^N \left| \frac{y_i - \hat{y}_i}{y_i} \right| \times 100\% \quad (3)$$

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

where N is the total number of tested cells, and y_i and $\hat{y}_i$ denote the true and predicted cycle life of cell i , respectively. These metrics were used jointly to assess both the relative prediction error and the absolute deviation in cycle life estimation.

3. Dataset and Testing Conditions

The dataset consists of 138 commercial high-energy-density 18650 NCM811 cylindrical batteries from the same manufacturing batch, providing a controlled basis for examining cell-to-cell variation in early degradation behavior. The discharge capacity at the 3rd cycle serves as the initial baseline for degradation analysis because the formation process and solid electrolyte interphase (SEI) stabilization are largely completed by this stage. The EOL criterion is defined as a reduction in capacity retention to 80% of the 1st-cycle capacity. All 138 cells in this dataset reached the EOL threshold, providing complete degradation trajectories and explicitly observed lifespans for supervised regression.

The 138 retained cells have a nominal capacity of 2.4 Ah and a nominal voltage of 3.6 V. Aging tests were conducted in a 25 °C environmental chamber so that the observed variation was primarily associated with intrinsic manufacturing heterogeneities and differences in early aging behavior.

The testing protocol employed a fast-charge and fast-discharge regime. Each cycle began with a 5.0 A constant-current charge, corresponding to 2.08 C, up to 4.2 V, followed by a constant-voltage charging step until the current decayed to 0.125 A. After a 5 min rest period, the cells underwent a 7.5 A constant-current discharge, corresponding to 3.13 C, down to 2.75 V, followed by another 5 min rest. This sequence was repeated until the capacity fell below the EOL threshold. Although this protocol differs from variable real-world electric-vehicle duty cycles, it provides an accelerated boundary condition for cell screening and early degradation evaluation. The test platform recorded timestamps, voltage, current, capacity, and surface temperature, thereby enabling the extraction of discharge profiles and the construction of EDVM curves.

Figure 1 summarizes the primary characteristics of the dataset evaluated in this study. By the tenth cycle, all batteries exhibited a consistent macroscopic capacity degradation of approximately 1.17%, with the deviation bounded within $\pm 0.05\%$. Following this initial uniform stage, Figure 1a illustrates the approximately linear capacity fade trajectories over the first 100 cycles. As depicted by the histogram in Figure 1b, all retained batteries demonstrated a cycle life below 200 cycles, yielding an average of 126.3 cycles, a median of 124 cycles, and a standard deviation of 22.3 cycles. The cycle life distribution presents a positive skewness of approximately 0.42. This right skew indicates a long-tail distribution where a small subset of batteries possesses extended lifespans, whereas the majority cluster within the lower to middle ranges. Consequently, this skewed distribution suggests that the predictive model may encounter higher uncertainty on samples with extreme longevity, necessitating targeted attention during model evaluation.

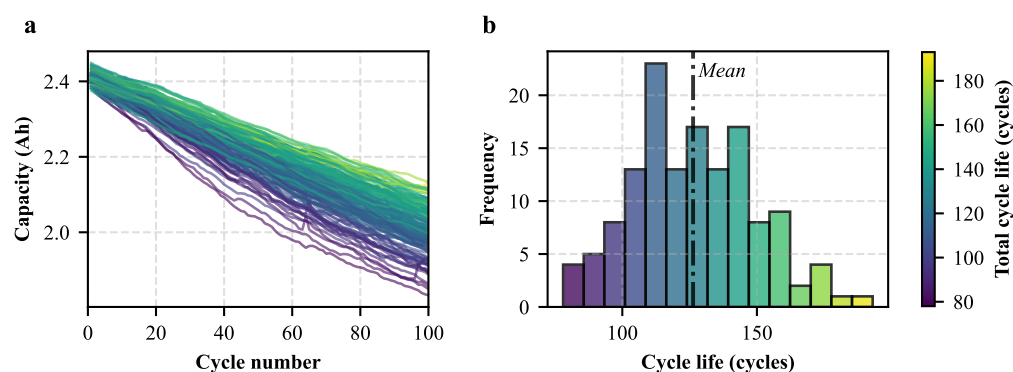


Figure 1. Overview of battery degradation trajectories and lifespan distribution. (a) Capacity degradation curves over the initial 100 cycles. (b) Histogram of the total cycle life distribution for the 138 evaluated cells.

Table 3 summarizes the evolution of macroscopic physical metrics across the first 10 cycles. After Cycle 1, the mean values of discharge capacity, Coulombic efficiency (CE), and average discharge voltage remain highly consistent, with relatively small standard deviations. This observation indicates that conventional macroscopic indicators provide limited discrimination among cells with different eventual lifespans during the very early stage [10].

Table 3. Evolution of macroscopic physical metrics during the initial 10 cycles.

Cycle	Capacity (Ah)	CE (%)	Energy (Wh)	Avg. Voltage (V)	Temp Rise (°C)
1	2.4088 ± 0.0151	97.03 ± 0.53	6.7741 ± 2.0390	2.8127 ± 0.8467	0.00 ± 0.00
2	2.4035 ± 0.0161	99.70 ± 0.14	8.2593 ± 0.0675	3.4363 ± 0.0081	0.00 ± 0.00
3	2.3983 ± 0.0169	99.74 ± 0.07	8.2388 ± 0.0713	3.4353 ± 0.0085	0.00 ± 0.00
4	2.3936 ± 0.0171	99.78 ± 0.05	8.2207 ± 0.0715	3.4344 ± 0.0084	0.00 ± 0.00
5	2.3893 ± 0.0175	99.79 ± 0.06	8.2048 ± 0.0728	3.4339 ± 0.0083	0.00 ± 0.00
6	2.3852 ± 0.0178	99.80 ± 0.06	8.1893 ± 0.0742	3.4333 ± 0.0084	0.00 ± 0.00
7	2.3811 ± 0.0181	99.80 ± 0.06	8.1743 ± 0.0756	3.4330 ± 0.0085	0.00 ± 0.00
8	2.3772 ± 0.0187	99.80 ± 0.29	8.1613 ± 0.0773	3.4332 ± 0.0084	0.00 ± 0.00
9	2.3743 ± 0.0195	99.85 ± 0.20	8.1522 ± 0.0808	3.4334 ± 0.0084	0.00 ± 0.00
10	2.3701 ± 0.0203	99.80 ± 0.07	8.1361 ± 0.0843	3.4327 ± 0.0088	0.00 ± 0.00

4. Results and Discussion

4.1. Predictive Performance Comparison and Feature Attribution Analysis

To evaluate the proposed XGBoost framework, its performance was compared against two baseline models: Elastic Net and Gaussian process regression (GPR), both of which are standard methods for structured low-dimensional regression tasks. A nested five-fold cross-validation strategy was implemented to ensure an unbiased assessment of generalization capability and to preclude data leakage. Under this rigorous nested evaluation protocol, the optimal three-feature XGBoost model achieved an unbiased generalization evaluation with a MAPE of 12.70% and an RMSE of 18.93 cycles. Subsequently, when utilizing a standard five-fold cross-validation to train and determine the parameters for the final deployment model, XGBoost achieved the lowest quantitative error on the complete dataset, with a 12.29% MAPE and an RMSE of 18.7 cycles. As demonstrated in Figure 2a, the XGBoost predictions exhibit the closest alignment with the diagonal reference line, indicating the minimal overall fitting deviation. In comparison, Elastic Net yielded a 13.41% MAPE and an RMSE of 20.3 cycles, while GPR produced a 13.46% MAPE and an RMSE of 20.1 cycles. The error distribution depicted in Figure 2b corroborates the overall accuracy trends. The prediction errors for XGBoost are densely clustered near zero, presenting a median error of −2.28% and an interquartile range (IQR) of 21.54%, which spans from −12.19% to 9.35%. Elastic Net exhibited a marginally narrower IQR of 21.12%, whereas GPR demonstrated a notably broader error dispersion of 23.55%. These results suggest that the XGBoost framework successfully captures the nonlinear feature response relationships embedded within the EDVM descriptors. It delivers the highest overall prediction accuracy while maintaining an error concentration comparable to the linear baseline, thereby significantly outperforming GPR.

All three models demonstrate a systematic tendency to underpredict the lifespan of long-life batteries and overpredict that of short-life ones. This phenomenon can be rationalized from two perspectives. Statistically, regression models optimized for mean squared error minimization naturally generate conservative predictions biased toward the population mean when evaluating extreme samples dominated by unmodeled factors. The persistent manifestation of this trend across all evaluated models implies that the deviation originates from the inherent informational limits of the dataset rather than algorithmic

deficiencies in any specific model. From an electrochemical perspective, the predictive features in this study are extracted from the third and tenth cycles. Although these features adequately capture the initial polarization states, the ultimate cycle life is concurrently governed by nonlinear degradation mechanisms that manifest only after extended cycling. These late-stage dynamics are not fully encapsulated by the macroscopic features of the initial ten cycles, thereby resulting in systematic predictive deviations for extreme individuals. Nevertheless, this characteristic residual distribution offers practical engineering utility. Specifically, a predicted short lifespan strongly indicates an elevated risk of premature degradation. Conversely, a predicted long lifespan should be interpreted as a relative indicator of superior durability rather than an absolute guarantee. This conceptualization provides a pragmatic foundation for establishing screening thresholds in battery production lines.

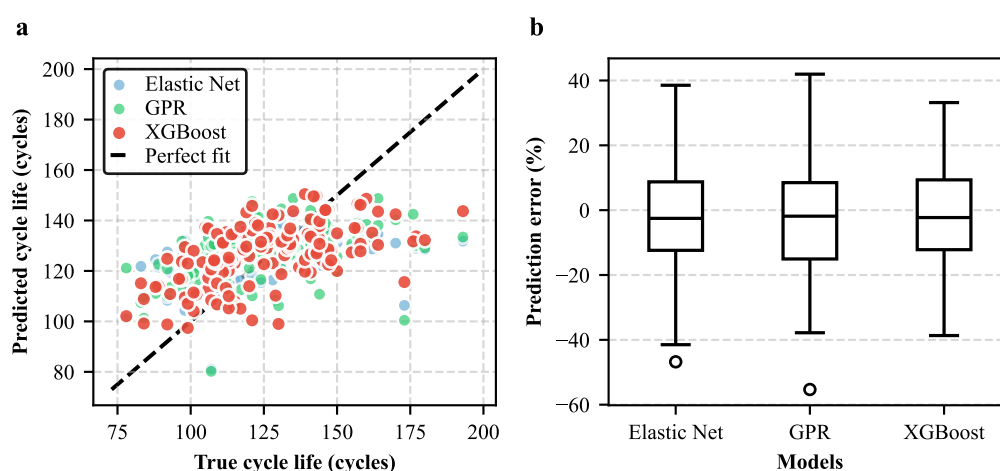


Figure 2. Predictive performance comparison among the XGBoost framework, GPR, and Elastic Net baselines. (a) Scatter plot of predicted versus true cycle life. (b) Prediction error distribution presented as box plots.

SHAP feature attribution analysis in Figure 3 indicates that $\text{Var}(\Delta Q)$ and $V_{(\Delta Q)_{\min}}$ acted as the primary contributors, accounting for a combined 72.29% of the model's predictive output. $\text{Var}(\Delta Q)$ ranked first, contributing 38.45%. High variance leads to negative model outputs and shorter predicted lifespans. This aligns with mechanisms where localized damage accelerates failure. The voltage coordinate $V_{(\Delta Q)_{\min}}$ acted as the second primary contributor at 33.84%, supporting the use of physical coordinates to identify distinct degradation modes.

The XGBoost model also captured the nonlinear interaction between $\text{Var}(\Delta Q)$ and $V_{(\Delta Q)_{\min}}$. Batteries grouped into different early degradation pathways exhibited varying sensitivities to the severity of early damage. For example, anode-dominant degradation near 3.12 V and cathode-dominant degradation near 3.54 V responded differently to variance. A high $\text{Var}(\Delta Q)$ at 3.12 V resulted in a greater reduction of predicted cycle life than an equivalent variance at 3.54 V, explaining the observed narrower and shorter lifespan distribution of the 3.12 V cohort. This interaction mechanism explains why XGBoost outperformed the linear baseline, which cannot model such coupled feature effects [31,32].

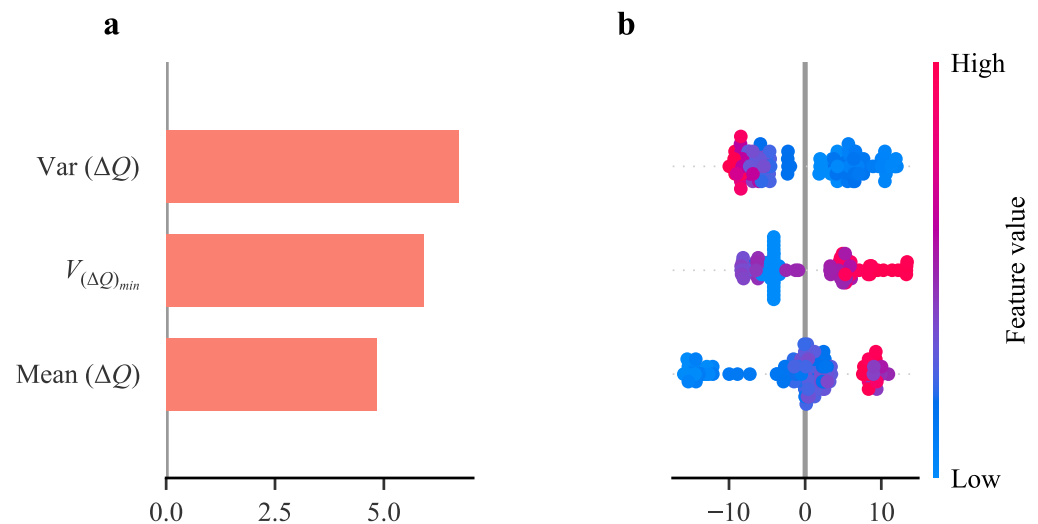


Figure 3. Feature attribution analysis utilizing the SHAP framework. (a) Global feature importance ranking based on mean absolute values. (b) Feature impact distribution on the model predictive output.

4.2. Degradation Mode Analysis Based on DMVS

4.2.1. Voltage Location Clustering and Lifespan Distributions

To determine the optimal number of clusters, a within-cluster sum of squares elbow analysis was conducted scanning K values from 1 to 10. The results show that the most significant marginal decrease occurred at $K = 3$ with an 84.89% drop, while $K = 4$ still exhibited a substantial reduction of 60.31%. Subsequent marginal decreases for $K = 5$ through $K = 10$ stabilized between 20% and 46%, with the within-cluster sum of squares curve showing a smooth decay and no further prominent elbow turning points. Considering both the significance of the marginal gain and the statistical robustness of the classification granularity, $K = 4$ was selected for this study.

Based on the $K = 4$ clustering, the DMVS centroid voltages for the four clusters, as shown in Figure 4a, were approximately 3.78 V, 3.54 V, 3.12 V, and 2.76 V, respectively. These centroids effectively cover the complete DMVS distribution space from the high-voltage phase transition region to the end of discharge. Each cluster possesses a narrow voltage range and clear separation from the others. The sample sizes for the four clusters were 5, 29, 69, and 35, respectively, reflecting the natural proportions of different degradation modes within the battery population.

To verify the statistical significance of these clusters, a Kruskal–Wallis H test was performed on the cycle life of the four battery groups. For this analysis, battery data within a $\pm 1\sigma$ boundary around the mean of each cluster were retained. The results demonstrate a statistically significant overall difference among the four groups, yielding an H value of 12.14 and a p -value of 0.007. The effect size is moderate with an η_H^2 of 0.086. As illustrated in Figure 4b, the average lifespans of the four groups were 114.5, 135.2, 119.8, and 130.4 cycles, respectively, exhibiting a regular gradient distribution along the DMVS voltage locations. This globally confirms the significant association between DMVS clustering and lifespan differentiation.

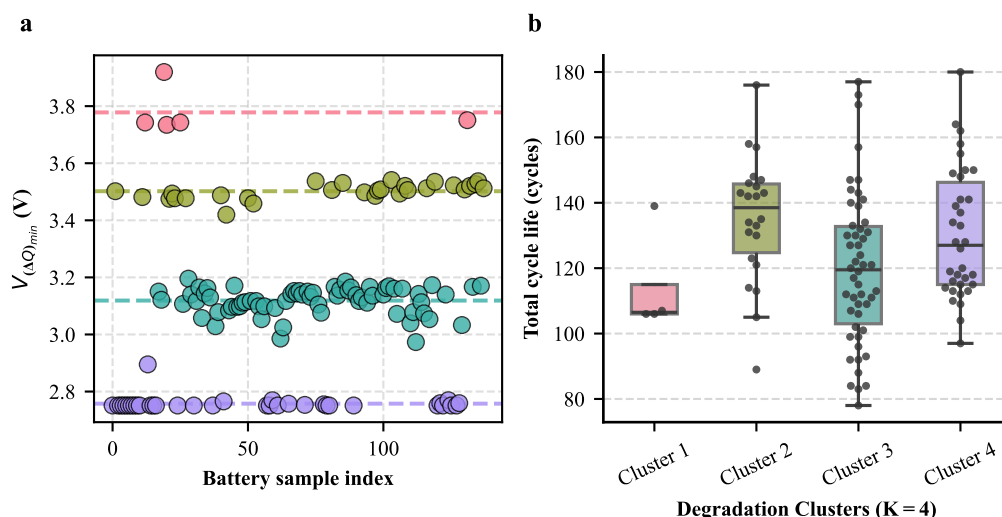


Figure 4. Clustering of DMVS locations and corresponding lifespan distributions. (a) Scatter plot of $V_{(\Delta Q)_{\min}}$ centroids identified via K-means clustering. (b) Total cycle life distribution across the voltage groups.

4.2.2. Thermodynamic Peak Stability and the Kinetic Sensitivity of DMVS

In the initial 10 cycles, the bulk phase structures of the NCM811 cathode and graphite anode remain stable without significant macroscopic degradation. Table 4 details the evolution of two primary thermodynamic peaks from Cycle 1 to Cycle 10. The peak positions exhibited maximum voltage shifts below 10 mV, and the peak heights showed minimal attenuation. The characteristic peaks in traditional dQ/dV profiles exhibited nearly identical positions and heights across all batteries [20], indicating that the characteristic phase transition potentials of both electrodes remain nearly unchanged during the early cycles.

These stable thermodynamic peaks correspond to specific electrochemical processes. Based on the phase transition characteristics of the NCM811 cathode and the graphite anode, the two peaks at approximately 3.5 V and 3.7 V correspond to the H1 to M and M to H2 host lattice phase transitions of the cathode, respectively. Within this voltage range, the graphite anode is in a distinct staged two-phase coexistence region, such as stage 1 to stage 2 or stage 2 to stage 3, maintaining a high lithium concentration. The third peak at approximately 3.1 V originates from a different physical mechanism. At this point, the cathode has completed its primary phase transitions, and this peak is mainly attributed to the graphite anode. According to the graphite lithium intercalation phase diagram established by Dahn and colleagues, as the discharge approaches the end and the lithium ion concentration in the graphite drops to an extremely low level where $x < 0.04$, the graphite exits the buffer of two-phase coexistence and enters a dilute stage 1 phase. This manifests as an independent characteristic peak on the dQ/dV curve. These three peaks mark three key stages of cathode structural evolution and anode lithium concentration states.

Although the positions and heights of these thermodynamic peaks are highly stable in early cycles, the degradation paths of all batteries are not entirely identical. The core question is whether this subtle thermodynamic drift has a statistically identifiable correlation with the final cycle life.

To examine this, a K-means clustering analysis was performed on the peak voltage shifts of the three main peaks between the 10th and 3rd cycle incremental capacity analysis curves, and the differences in cycle life among the resulting categories were evaluated. The results indicate that regardless of which incremental capacity analysis peak position is used for grouping, the cycle life among different clusters shows no statistically significant differences. All compared p -values are greater than 0.05, and the absolute values of

Cohen's d effect sizes are all less than 0.3. Consequently, during the early stage when thermodynamic peak positions remain highly stable, traditional peak tracking methods cannot effectively distinguish battery groups with different future lifespans. This quantitatively confirms the inherent limitations of relying solely on thermodynamic peak positions for early degradation diagnosis.

Table 4. Evolution of dQ/dV peak characteristics across the initial 10 cycles.

Cycle	Peak 1			Peak 2		
	Position (V)	Height (Ah/V)	Shift to C2 (mV)	Position (V)	Height (Ah/V)	Shift to C2 (mV)
1	3.4823 ± 0.0476	30.14 ± 15.70	-	3.1189 ± 0.0646	51.16 ± 24.86	-
2	3.5658 ± 0.0203	3.83 ± 0.05	Baseline	3.2157 ± 0.0105	2.42 ± 0.05	Baseline
3	3.5649 ± 0.0175	3.81 ± 0.05	7.2 ± 14.8	3.2140 ± 0.0112	2.42 ± 0.05	8.7 ± 6.2
4	3.5672 ± 0.0224	3.80 ± 0.05	7.1 ± 14.2	3.2137 ± 0.0118	2.42 ± 0.05	8.4 ± 7.3
5	3.5658 ± 0.0188	3.79 ± 0.05	7.6 ± 15.6	3.2127 ± 0.0120	2.42 ± 0.05	8.6 ± 6.3
6	3.5660 ± 0.0215	3.78 ± 0.05	6.5 ± 11.7	3.2126 ± 0.0120	2.41 ± 0.05	7.9 ± 6.7
7	3.5657 ± 0.0205	3.77 ± 0.05	8.7 ± 17.2	3.2131 ± 0.0116	2.41 ± 0.05	7.9 ± 5.9
8	3.5632 ± 0.0145	3.75 ± 0.05	9.1 ± 17.5	3.2132 ± 0.0110	2.40 ± 0.05	8.5 ± 6.5
9	3.5634 ± 0.0147	3.74 ± 0.05	8.5 ± 17.8	3.2120 ± 0.0124	2.41 ± 0.05	9.0 ± 7.1
10	3.5643 ± 0.0184	3.73 ± 0.05	9.8 ± 16.9	3.2120 ± 0.0118	2.40 ± 0.06	9.3 ± 6.7

In the early cycling stages, significant structural damage has not yet appeared inside the battery, but interfacial side reactions and local inhomogeneities can lead to a progressive increase in polarization. When the kinetic polarization of the battery increases, the traditional dQ/dV curve not only undergoes an overall voltage translation but also experiences morphological changes such as peak broadening and slope alterations. The minimum point of the EDVM is mathematically equivalent to the intersection of the incremental capacity analysis curves from two cycles. The voltage position of this intersection is determined not only by the overall translation of the curves but also by the local slopes and relative displacements of the two curves near the intersection. Translation moves the curves closer or further apart, while slope changes directly amplify or reduce the impact of translation on the intersection voltage. Therefore, incremental capacity analysis peak translation, peak height attenuation, and peak shape distortion caused by kinetic polarization are comprehensively encoded by the DMVS through changes in the intersection position. In contrast, traditional incremental capacity analysis peak tracking only captures the voltage movement of a single peak. It remains insensitive to peak shape changes, and the flat region near the peak further reduces positioning accuracy.

As illustrated in Figure 5, the EDVM minimum points at the three representative DMVS clustering voltages near 3.1 V, 3.5 V, and 3.7 V all exhibit obvious voltage offsets from their corresponding incremental capacity analysis peak apices. This visually demonstrates that the kinetic polarization information captured by DMVS cannot be reflected by traditional peak positions. This mechanistic difference fundamentally explains why DMVS can effectively capture the kinetic heterogeneity signals indicative of future lifespan divergence during the early stages when thermodynamic peak positions remain highly stable.

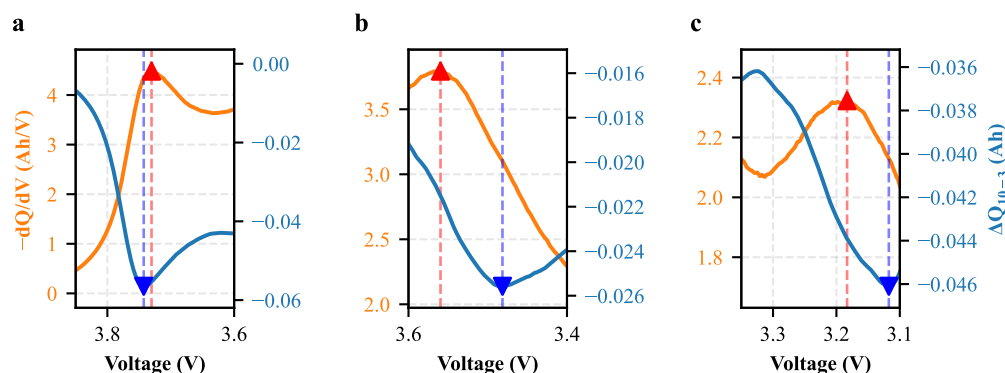


Figure 5. Voltage misalignment between thermodynamic peaks and degradation minimums. (a–c) Corresponding DMVS are located near 3.7 V, 3.5 V, and 3.1 V, respectively.

4.3. Cross-Scale Correlation Evolution

Pearson correlation analyses were conducted at the 10th and 100th cycles to evaluate the feature evolution. To ensure data integrity, 17 cells with a total lifespan below 100 cycles, accounting for 12.32% of the valid dataset, were excluded. This left a final cohort of 121 batteries for the comparative analysis.

Figure 6 shows the cross-scale evolution of the features. By the 100th cycle, the correlation coefficients for the Mean and Variance features reached $r = 0.754$ and -0.652 , respectively, both yielding a p -value of less than 0.001. These highly significant values demonstrate an explicit correlation with degradation. At the 10th cycle, the absolute coefficients for both features were below 0.3, with the Mean feature showing no statistical significance and the Variance feature exhibiting a weak but significant correlation, reflecting an implicit relationship.

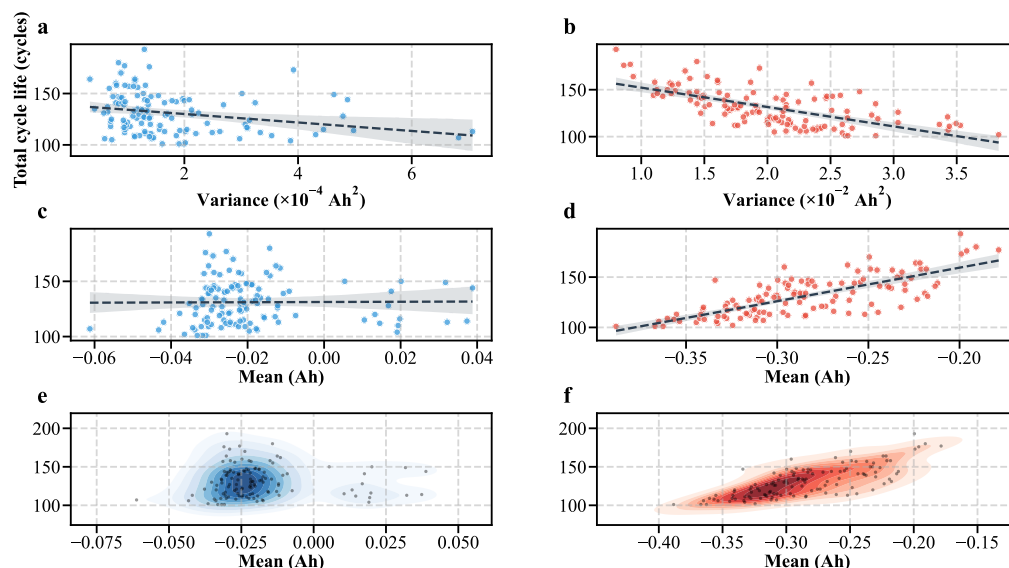


Figure 6. Cross-scale correlation analysis between transferable statistical features and cycle life. (a,c,e) Correlation plots of the two extracted features against cycle life at the Cycle 10. (b,d,f) Corresponding correlations at the Cycle 100.

This difference reflects the physical evolution of battery degradation. Early signals are affected by complex nonlinear kinetic processes, but the physical validity of these features remains stable and can be modeled by nonlinear frameworks such as XGBoost.

This evolution indicates that the EDVM features transition from an implicit state to an approximately linear state as degradation progresses.

4.4. Cycle Sensitivity Analysis

To systematically evaluate the impact of cycle pair selection on predictive performance, a sensitivity analysis was conducted from two dimensions. These dimensions are the starting position of the baseline cycle and the number of interval cycles between the baseline and observation cycles.

4.4.1. Selection of the Baseline Cycle

First, the predictive performance was compared using the first, second, third, and fifth cycles as the EDVM reference baseline. Table 5 summarizes the prediction results of the XGBoost model. When using the first cycle as the baseline, the prediction error was significantly higher than other baseline cycles, with a 14.25% MAPE and an RMSE of 21.4 cycles. The unsuitability of the first cycle as a baseline is directly supported by quantitative data from the macroscopic physical indicators of the first ten cycles shown in Table 3. The Coulombic efficiency of the first cycle was only 97.03%, which is significantly lower than the 99.70% of the second cycle and the stable level of 99.7% to 99.8% maintained in subsequent cycles. Furthermore, its average discharge voltage standard deviation reached a high of 0.8467 V, whereas the standard deviations for the second through tenth cycles were all below 0.009 V. The abnormally low Coulombic efficiency combined with the massive dispersion in average voltage indicates that the first cycle remains in an unstable interfacial evolution period, making it unsuitable as a unified benchmark.

Starting from the second cycle, all indicators stabilized, leading to a noticeable improvement in predictive performance. When using the second through fifth cycles as baselines, the MAPE fluctuation range was only about one percentage point, spanning from 12.29% to 13.01%. Among these, the third cycle achieved the lowest prediction error, yielding a 12.29% MAPE and an RMSE of 18.7 cycles.

Table 5. Predictive performance of XGBoost using different early baseline cycles for EDVM feature extraction.

Baseline Cycle	MAPE (%)	RMSE (Cycles)
Cycle 1	14.25	21.4
Cycle 2	12.97	20.0
Cycle 3	12.29	18.7
Cycle 5	13.01	20.6

4.4.2. Selection of the Cycle Interval

Using the third cycle as the fixed baseline, the predictive performance was evaluated across cycle intervals ranging from 2 to 17 cycles, corresponding to observation windows from the 5th to the 20th cycle. The overall evolution trends of MAPE and RMSE are illustrated in Figure 7. In the very early stage with short intervals, the prediction error remained high and exhibited noticeable fluctuation. The MAPE dropped sharply from 14.87% at an interval of 2 cycles to 12.94% at an interval of 4 cycles, i.e., the 7th cycle, marking the first significant inflection point of accuracy improvement. Subsequently, the prediction accuracy rebounded slightly under shorter intervals, reflecting the inherent instability when degradation signals are insufficiently accumulated. As the interval expanded to 7 cycles, corresponding to the 10th cycle, the MAPE further decreased to 12.29%, forming the second critical inflection point where the predictive performance entered a stable and reliable range.

As the cycle interval continued to increase, the MAPE declined gradually, with the accuracy gain slowing down significantly and exhibiting a clear marginal diminishing characteristic.

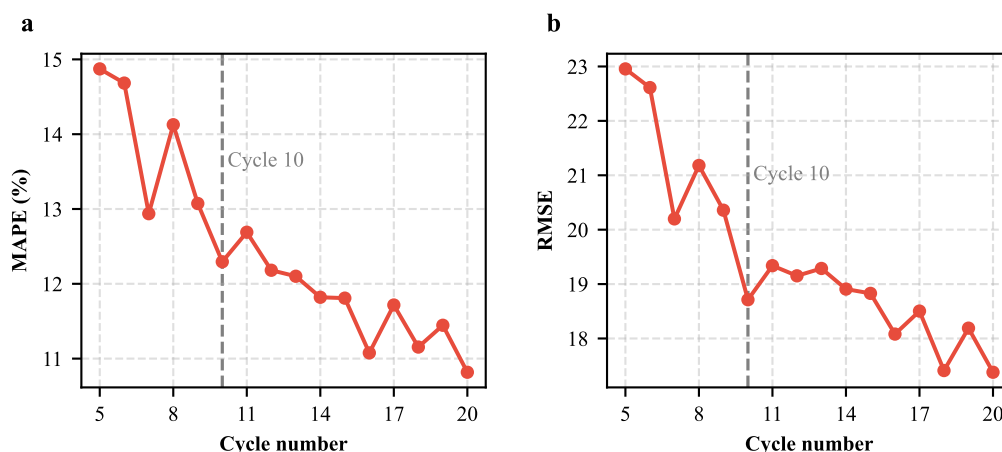


Figure 7. Cycle-wise sensitivity analysis. (a) Evolution of MAPE. (b) Evolution of RMSE.

4.4.3. Engineering Trade-Off and Recommended Cycle Pair

To evaluate the significance of these differences, a two-way analysis of variance was conducted using the starting cycles of 2, 3, and 4, along with cycle intervals of 5, 7, 10, and 15 as factors. The results indicate that the main effect of the starting cycle is negligible, yielding a p -value of 0.769 and a partial η^2 of 0.001. Although the cycle interval exhibits a statistically significant main effect with $p < 0.001$, the full-range MAPE fluctuation remains tightly controlled within a narrow band of 10.4% to 14.0%. Furthermore, a Tukey honestly significant difference post hoc test reveals no significant discrepancy in predictive performance between the seven-cycle and ten-cycle intervals, as supported by a p -value exceeding 0.05. This finding demonstrates that predictive accuracy reaches a plateau region around the tenth cycle.

The aforementioned analysis highlights a clear engineering trade-off. An overly short cycle interval fails to accumulate sufficient degradation signals, leading to suboptimal prediction accuracy. Conversely, an excessively long interval only marginally enhances accuracy at the severe expense of early warning lead time. The tenth cycle, corresponding to a seven-cycle interval, provides a practical balance between prediction accuracy and early-warning timeliness. This configuration allows the prediction accuracy to enter a stable and reliable range while maximizing early-warning timeliness. Concurrently, variations of the starting cycle within the early stable window—specifically from the second to the fifth cycle—exert no significant impact on predictive performance. This evidence substantiates the robust nature of the proposed framework regarding cycle pair selection. Consequently, establishing the third cycle as the baseline is not the exclusive optimal solution, but rather a highly pragmatic recommendation that elegantly balances predictive precision with engineering convenience.

To further evaluate the robustness of the selected cycle pair, the cycle-pair sensitivity analysis was expanded by considering baseline cycles from C2 to C5 and observation cycles from C5 to C20. The corresponding MAPE values are summarized in Table 6. For all baseline cycles, the MAPE generally decreases as the observation cycle increases, indicating that the EDVM features become progressively more informative with the accumulation of early degradation signals. For the C3 baseline, the MAPE decreases from 14.87% at C5 and 14.68% at C6 to 12.94% at C7 and 12.29% at C10, while longer observation windows further reduce the error at the cost of early-warning timeliness. Overall, Cycle 3 provides a stable

post-formation baseline for the present dataset, and the C3–C10 configuration is retained as a practical accuracy–timeliness trade-off in the proposed framework.

Table 6. Expanded cycle-pair sensitivity analysis. Values denote MAPE (%).

Baseline Cycle	Observation Cycle									
	C5	C6	C7	C8	C9	C10	C11	C12	C15	C20
C2	15.22	14.98	13.22	14.38	13.29	12.47	12.87	12.33	11.96	10.94
C3	14.87	14.68	12.94	14.13	13.07	12.29	12.69	12.18	11.81	10.82
C4	–	14.90	13.14	14.31	13.22	12.43	12.82	12.30	11.93	10.92
C5	–	–	13.20	14.36	13.27	12.47	12.86	12.33	11.95	10.94

4.5. Feature Ablation Study and Contribution Analysis

To evaluate the contributions of the three features, 7 subsets were tested using Elastic Net, GPR, and XGBoost via a five-fold cross-validation strategy. Table 7 presents the MAPE and RMSE results.

When using single-feature inputs for XGBoost, DMVS and Mean(ΔQ) yielded the lowest MAPEs of 13.90% and 14.16%, respectively. The subset excluding DMVS, comprising Mean(ΔQ) and Var(ΔQ), yielded a 13.68% MAPE in XGBoost. Integrating the DMVS feature further reduced the prediction error.

For the baseline models, the linear Elastic Net exhibited limited sensitivity to feature combinations, achieving its lowest MAPE of 13.41% with the complete three-feature set comprising Mean(ΔQ), Var(ΔQ), and DMVS, while GPR reached a 13.32% MAPE with the dual-feature combination of Mean(ΔQ) and DMVS, its error increased to 13.46% when utilizing the full three-feature set, exhibiting an anomalous performance degradation after feature addition. In contrast, XGBoost effectively utilized the information of the complete feature set, achieving the lowest overall prediction error by modeling the nonlinear interactions among features: a 12.29% MAPE and an RMSE of 18.7 cycles. XGBoost outperformed GPR and Elastic Net across most feature subsets, validating the applicability of tree-based ensemble learning [17]. Therefore, this study ultimately adopted the XGBoost model utilizing the complete three-feature EDVM framework for early cycle life prediction.

Table 7. Ablation Study of Extracted Features on Cycle Life Prediction (Cycle 10 vs. Cycle 3).

Features	Elastic Net		GPR		XGBoost	
	MAPE (%)	RMSE (Cycles)	MAPE (%)	RMSE (Cycles)	MAPE (%)	RMSE (Cycles)
F_1	15.40	22.9	14.93	22.1	14.16	21.3
F_2	14.26	21.5	15.03	22.4	14.49	22.0
F_3	15.32	22.9	13.79	20.9	13.90	21.0
$F_1 + F_2$	13.87	20.9	14.50	21.6	13.68	20.7
$F_1 + F_3$	15.05	22.6	13.32	19.5	12.72	19.2
$F_2 + F_3$	14.20	21.5	14.12	20.7	13.45	20.2
$F_1 + F_2 + F_3$	13.41	20.3	13.46	20.1	12.29	18.7

Note: F_1 : Mean(ΔQ), F_2 : Var(ΔQ), F_3 : $V_{(\Delta Q)\min}$.

5. Conclusions

This study develops an early cycle-life prediction framework based on early degradation voltage morphology (EDVM) for short-lifespan NCM811 batteries. By extracting three physically interpretable features, including the degradation mode voltage signature (DMVS), and combining them with the XGBoost algorithm, the framework achieves a

mean absolute percentage error (MAPE) of 12.29% using only the first 10 cycles of data. Compared with data-intensive deep learning methods and high-dimensional feature engineering approaches, the proposed framework reduces feature dimensionality, maintains physical interpretability, and improves the timeliness of early prediction. In addition, the cross-scale correlation analysis indicates that the relationship between the extracted features and cycle life evolves from an early nonlinear stage to a later approximately linear stage. Overall, the proposed method provides an efficient and interpretable engineering approach for early battery evaluation and cell screening.

Using only the initial 10 cycles makes the framework attractive for practical deployment in formation lines, laboratory screening, and other early diagnostic settings. The proposed feature set may also support rapid cell sorting for second-life applications; however, the present validation is limited to fresh cells tested under an accelerated aging protocol. Future work should therefore examine the generalization of this methodology on retired battery datasets with different state-of-health levels, cell-to-cell inconsistencies, and usage histories, as well as under broader temperature conditions and charging protocols. Further reductions in diagnostic time may be achieved by using partial discharge segments instead of full discharge cycles. In addition, in situ characterization methods, such as three-electrode electrochemical impedance spectroscopy and in situ X-ray diffraction, could help clarify the kinetic mechanisms associated with the DMVS.

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Abbreviations

The following abbreviations are used in this manuscript:

CE	Coulombic efficiency
DMVS	Degradation mode voltage signature
DVA	Differential voltage analysis
EDVM	Early degradation voltage morphology
EOL	End of life
GPR	Gaussian process regression
ICA	Incremental capacity analysis
MAPE	Mean absolute percentage error
NCM	Nickel–cobalt–manganese
OCV	Open-circuit voltage
RMSE	Root mean square error
SEI	Solid electrolyte interphase
SHAP	Shapley additive explanations

XGBoost Extreme gradient boosting

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