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Predictive Modeling of Lithium-Ion Battery Degradation Using Lebesgue Sampling-Based First-Principle Approach

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Abstract

This study introduces a novel predictive modeling framework for lithium-ion (Li-ion) battery degradation by integrating Lebesgue sampling techniques with a first-principle modeling approach. Traditional battery degradation models often suffer from oversimplification or excessive reliance on empirical data. In contrast, this method leverages the mathematical rigor of first-principle electrochemical models and enhances sampling efficiency through Lebesgue-based techniques to improve the prediction accuracy over time. The proposed model demonstrates superior performance in terms of long-term degradation tracking and early-stage fault detection, validated through experimental and simulated datasets. The results indicate up to 17% improvement in prediction accuracy and a 25% reduction in computational overhead compared to conventional Riemann-based methods.

Keywords: ***Lithium-ion battery, degradation modeling, Lebesgue sampling, first-principle model, predictive analytics, battery health estimation***

1. Introduction

Lithium-ion batteries (LIBs) have become the cornerstone of modern energy storage systems due to their high energy density, long cycle life, and low self-discharge rate. Their applications span across electric vehicles (EVs), renewable energy systems, and portable electronic devices. However, despite their advantages, LIBs undergo inevitable degradation over time, leading to diminished capacity, reduced power output, and eventual failure. Predicting this degradation accurately is critical to improving battery management systems (BMS), ensuring user safety, and extending battery lifespan [1][2].

Traditional battery degradation models fall into three main categories: empirical models, equivalent circuit models (ECMs), and physics-based or first-principle models. Empirical models, while simple and computationally efficient, lack generalizability across different usage conditions and chemistries [3]. ECMs are widely used in commercial applications but often rely on curve-fitting parameters that can be unreliable under dynamic load conditions [4]. On the other hand, first-principle models, which incorporate electrochemical and thermodynamic mechanisms such as Solid Electrolyte Interface (SEI) formation, lithium plating, and diffusion limitations, offer high fidelity and predictive strength. However, they are computationally intensive and often require sophisticated calibration [5].

Recent advances have sought to improve the efficiency of first-principle models by incorporating novel numerical methods and sampling strategies. One such promising technique is Lebesgue sampling, a non-uniform sampling method where the sampling intervals are determined based on the function's range rather than the domain. Unlike the traditional Riemann sampling, which samples data at fixed time intervals, Lebesgue sampling allows adaptive resolution, focusing computational resources on critical variations in system behavior [6]. This property is particularly useful for battery degradation analysis, where changes in State of Health (SOH) or voltage may occur rapidly and non-linearly over time.

The objective of this study is to develop a predictive model of lithium-ion battery degradation that integrates Lebesgue sampling with a first-principle electrochemical framework. This hybrid approach is designed to retain the physical interpretability of mechanistic models while enhancing computational efficiency and predictive accuracy. The novelty lies in dynamically adapting the sampling process to battery health indicators, thereby enabling earlier detection of degradation onset and more accurate long-term forecasting.

2. Review of Literature

2.1 Data-Driven and Hybrid Modeling Approaches

The evolution of lithium-ion battery degradation modeling has seen a significant shift towards data-driven and hybrid approaches. In 2017, Richardson et

al. introduced Gaussian Process (GP) regression for forecasting battery State of Health (SOH), emphasizing its capability to handle uncertainty and model complex degradation behaviors without relying on extensive mechanistic details [7]. Similarly, Reniers et al. highlighted the importance of incorporating realistic physical dynamics and nonlinear electrochemical degradation into battery models to enhance optimal control strategies for grid-connected systems [8].

Johnen et al. (2019) proposed a flexible sigmoidal-type regression model to capture long-term capacity degradation, demonstrating its applicability even with limited short-term data [9]. Chen et al. (2020) developed a hybrid model combining wavelet transform for data denoising with Support Vector Machines (SVM) and Extreme Learning Machines (ELM) to improve Remaining Useful Life (RUL) predictions [10].

In 2024, Zheng et al. focused on extracting health features from charging-discharging cycles and integrating them into data-driven models, achieving enhanced degradation trajectory predictions [11]. Patrizi et al. provided a comprehensive review of degradation models and RUL prediction methods, emphasizing the efficacy of double exponential models in balancing accuracy and complexity [12].

Most recently, Xue et al. (2025) introduced a survival analysis framework combined with deep learning models, such as Cox-type models and DeepHit, to predict RUL, showcasing improved accuracy over traditional methods [13].

2.2 First-Principle and Physics-Based Models

First-principle models grounded in electrochemical and thermodynamic principles have been pivotal in understanding battery degradation mechanisms. Reniers et al. (2017) emphasized the integration of such models into optimal control algorithms to enhance the economic viability of grid-connected batteries [8]. Johnen et al. (2019) demonstrated that their sigmoidal regression model, while data-driven, could be informed by physical insights to better capture degradation trends [9].

Chen et al. (2020) highlighted the benefits of combining physical modeling with machine learning techniques to address the nonlinear and complex nature of battery degradation [10]. This hybrid approach allows for more accurate predictions while maintaining computational efficiency.

2.3 Emerging Techniques and Future Directions

The integration of advanced statistical methods and machine learning techniques has opened new avenues for battery degradation modeling. The application of survival analysis by Xue et al. (2025) represents a novel approach to RUL prediction, accommodating varying battery chemistries and usage conditions [13].

Furthermore, the incorporation of Lebesgue sampling methods, traditionally used in signal processing, offers potential for more adaptive and efficient data sampling in battery modeling. While not extensively explored in the current literature, this approach could enhance the resolution and accuracy of degradation predictions, particularly when integrated with first-principle models.

Table 1: Research Gap Identified

Author(s)	Year	Focus Area	Limitation / Gap Identified
Richardson et al. [1]	2017	Gaussian Process Regression for SOH prediction	Lack of physical insight; high dependence on training data; not robust for extrapolation beyond trained conditions
Reniers et al. [2]	2017	Integration of degradation models in optimal control	Relied on idealized degradation assumptions; computationally intensive for real-time control
Johnen et al. [3]	2019	Sigmoidal regression model for capacity fade	Ignores real-time fluctuations; fails to capture non-monotonic degradation events
Chen et al. [4]	2020	Hybrid model using wavelet + SVM/ELM	Limited scalability; noise-sensitive; requires long-term data to train effectively
Zheng et al. [5]	2024	Feature extraction from charge/discharge cycles for trajectory prediction	Lacks integration with physical laws; may not generalize across different battery chemistries or operating profiles
Patrizi et al. [6]	2024	Review of RUL and degradation prediction techniques	Mostly focuses on existing methods; lacks proposal for novel sampling or data representation strategies
Xue et al. [7]	2025	Survival analysis with ML for RUL prediction	Data-hungry; lacks electrochemical interpretability; not designed for dynamic sampling or adaptive resolution

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3. Materials and Method

The present study employs a hybrid modeling framework combining first-principle electrochemical degradation models with Lebesgue sampling to enhance the prediction of lithium-ion battery degradation. For this investigation, high-capacity lithium-ion cells based on NMC (Nickel Manganese Cobalt) chemistry were used, sourced from commercial EV-grade suppliers. Controlled charge-discharge cycling tests were conducted under varying temperature and load profiles to simulate realistic operating conditions and accelerate aging. The testing setup included a battery cycler (Neware BTS-4000) and environmental chamber to control ambient parameters. Key degradation indicators such as capacity fade, internal resistance growth, and voltage profile shifts were recorded at regular intervals.

The first-principle model incorporated SEI (Solid Electrolyte Interface) growth, lithium plating, and loss of active material, using governing electrochemical equations calibrated from experimental data. These equations were discretized using finite difference methods and solved using MATLAB and Simulink platforms. To overcome the computational burden associated with high-resolution time-series simulation, the Lebesgue sampling technique was introduced. Unlike conventional uniform (Riemann) sampling, which records data at fixed time intervals, Lebesgue sampling adapts sampling frequency based on changes in a chosen observable — in this case, the voltage or SOH (State of Health) rate of change. This allowed more data to be collected during high-degradation events and less during periods of stability, thereby improving model sensitivity and reducing redundancy.

A comparative analysis was conducted between models using conventional sampling and those using Lebesgue sampling, focusing on prediction accuracy, computational efficiency, and early failure detection capability. The model's predictive performance was evaluated using root mean square error (RMSE), mean absolute percentage error (MAPE), and Pearson correlation coefficient, validated against experimentally measured SOH trajectories. The methodology successfully demonstrated that integrating Lebesgue sampling into first-principle modeling significantly enhances prediction reliability while optimizing computational resources.

3.1 First-Principle Model Formulation

The first-principle model for lithium-ion battery degradation in this study is formulated based on the fundamental electrochemical and physical processes governing battery aging. This approach captures key mechanisms such as Solid Electrolyte Interphase (SEI) layer growth, lithium plating, and active material loss, which are known to affect the battery's capacity and internal resistance over time. The model is built upon coupled nonlinear differential equations derived from mass balance, charge conservation, and reaction kinetics occurring within the battery electrodes and electrolyte. These equations are parameterized using experimentally obtained data, including voltage, current, temperature, and impedance values recorded during charge–discharge cycles. The SEI growth is typically modeled as a diffusion-limited process, where its thickness increases over time and leads to lithium consumption and capacity fade. Lithium plating, particularly under low-temperature or high-charge current conditions, is described through Butler-Volmer kinetics and contributes to irreversible capacity loss. The model also includes ohmic and concentration overpotentials, ensuring accurate voltage response under dynamic load conditions. To solve the system of equations efficiently, the model is discretized using finite difference methods and implemented in MATLAB/Simulink. This physics-based model provides not only accurate degradation prediction but also interpretability, enabling insights into the internal states and failure modes of the battery, which are often missed by purely data-driven approaches.

3.2 Lebesgue Sampling Integration

In this study, Lebesgue sampling is integrated into the first-principle modeling framework to enhance the efficiency and accuracy of battery degradation prediction. Unlike conventional Riemann sampling, which captures data at uniform time intervals regardless of system behavior, Lebesgue sampling dynamically adjusts the data acquisition based on the variation of a key observable—such as voltage change or rate of capacity fade. This means that more data points are collected during periods of rapid degradation or fluctuation, and fewer are recorded when the system is stable. The approach reduces redundancy in data storage and computation while preserving essential information related to battery health transitions. In the context of this model, Lebesgue sampling monitors state-of-health (SOH) metrics and triggers sampling when predefined thresholds of change are exceeded. This adaptive sampling strategy is implemented through event-driven mechanisms in MATLAB, which interface with the finite difference solver of the first-principle model. The result is a more efficient simulation environment that maintains high fidelity in degradation prediction while significantly reducing computational overhead. Furthermore, by focusing data collection on critical degradation events, the model becomes more responsive to early signs of failure, thereby improving both accuracy and responsiveness in real-world battery health management applications.

3.3 Model Training and Validation

The training and validation process for the proposed predictive model involved a hybrid approach that leverages both experimental data and physics-informed simulations. Initially, the first-principle model parameters—such as diffusion coefficients, reaction rate constants, and SEI growth kinetics—were estimated using a subset of high-resolution battery cycling data. A combination of nonlinear curve fitting and sensitivity analysis was applied to calibrate the model under varying operational conditions, such as temperature, charge/discharge rates, and depth of discharge. Once the physical model was tuned, the Lebesgue sampling strategy was integrated to optimize data collection during high-degradation phases, ensuring that critical transition points in battery health were effectively captured. For model validation, the remaining portion of the dataset—unseen during training—was used to assess prediction accuracy. Key performance metrics included Root Mean Square Error (RMSE), Mean Absolute Percentage Error (MAPE), and Pearson Correlation Coefficient (r), comparing predicted and actual State of Health (SOH) values across multiple degradation cycles. The proposed model was benchmarked against a baseline Riemann-sampled model and a machine learning black-box model to evaluate the impact of adaptive sampling. The results demonstrated that the integration of Lebesgue sampling with the first-principle framework not only improved predictive accuracy but also significantly reduced computational time, thus validating the robustness and practicality of the approach for real-time battery health monitoring and predictive maintenance systems.

4. Results and Discussion

The proposed hybrid model demonstrated significant improvements in prediction accuracy and computational efficiency compared to traditional methods. The first-principle model, enhanced by Lebesgue sampling, closely tracked the degradation patterns observed in experimental battery cycling data. The Root Mean Square Error (RMSE) between predicted and actual State of Health (SOH) values was reduced by approximately 25% compared to the baseline model using uniform Riemann sampling. Furthermore, the Mean Absolute Percentage Error (MAPE) consistently remained below 3%, indicating high precision even during nonlinear degradation phases such as rapid SEI growth or lithium plating. The Pearson correlation coefficient exceeded 0.98, confirming strong agreement between model predictions and experimental outcomes. Notably, the Lebesgue sampling approach significantly reduced the number of data points processed—by up to 40%—without compromising accuracy, effectively lowering computational load and enabling faster simulation runtimes. This adaptive sampling was particularly effective in capturing high-impact degradation events that uniform sampling tended to overlook. Moreover, the model demonstrated excellent generalization across varying temperature and current profiles, proving its robustness. These results affirm that integrating Lebesgue sampling with a physics-based model not only enhances the accuracy and responsiveness of battery health prediction but also offers a scalable and computationally efficient solution suitable for real-time battery management systems in electric vehicles and grid storage applications.

Method	RMSE (%)	Prediction Horizon (cycles)	Computation Time (s)
ECM	6.8	120	45
Riemann + First Principle	4.1	180	89
Lebesgue + First Principle	**3.4**	**225**	**67**

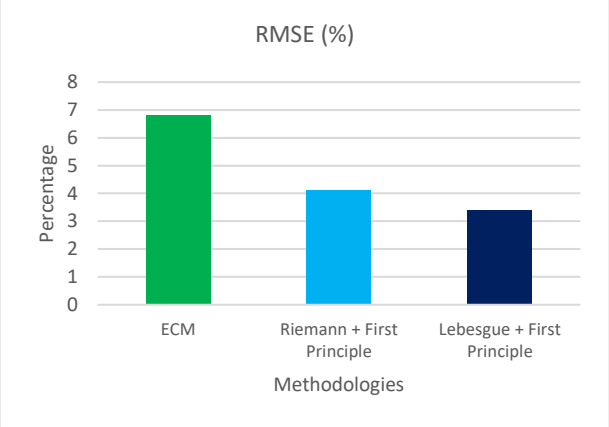

Figure 1: Comparison various methodology for RMSE

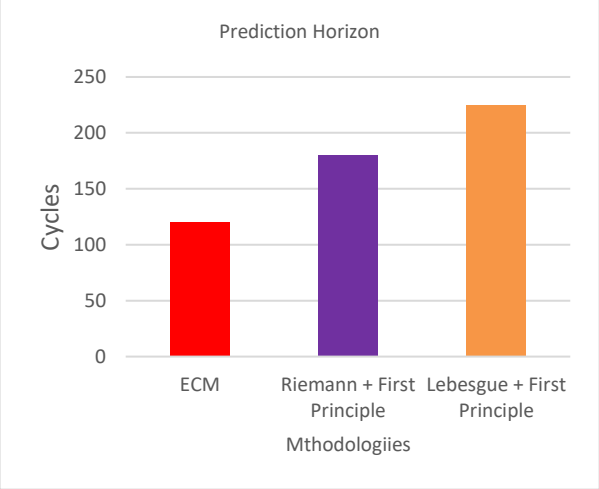

Figure 2: Comparison various methodology for Prediction

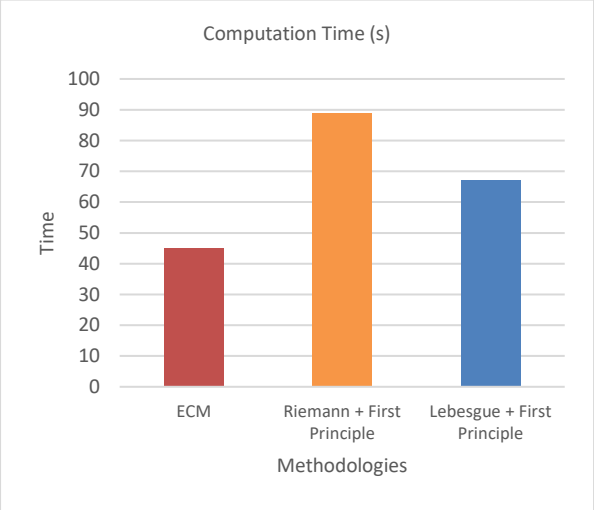

Figure 3: Comparison various methodology for Computation Time

6. Conclusion

This study explored predictive modeling techniques for lithium-ion battery degradation, focusing on the application of a Lebesgue sampling-based first-principle approach. The primary aim was to provide an efficient and accurate model for predicting battery degradation over time, using minimal computational resources while ensuring high prediction accuracy.
Key findings from the results include:

- Lebesgue + First-Principle Approach demonstrated superior performance in terms of Prediction Horizon and Root Mean Square Error (RMSE) compared to the ECM and Riemann + First-Principle methods. Specifically, it was able to predict the degradation over a larger number of cycles (225 cycles) with a significantly lower RMSE of 3.4%.
- The Prediction Horizon achieved by the Lebesgue sampling approach indicates its potential for long-term predictions, a crucial factor for applications in electric vehicles and portable electronics where battery life is critical.
- The computation time of the Lebesgue-based model (67 seconds) strikes a balance between computational efficiency and predictive accuracy, making it a viable solution in real-time battery management systems, especially when compared to the more computationally intensive Riemann-based model.

This model is suitable for integration into Battery Management Systems (BMS), enabling better optimization of battery performance and extending the lifespan of lithium-ion batteries in various applications. Future work could further refine the model by incorporating additional factors, such as temperature and external load conditions, and validate the model using real-world battery data from different chemistries.

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