Uncertainty-Quantified Multi-Output Deep Learning for Battery Degradation and Lifetime Prediction

Femi Okemakinde, Barancira Ted Doral, Youngmin Bae, Garam Yang, Jiwoong Kim, Jonghoon Kim*

*Chungnam National University

femiemmanuel067@gmail.com, *whdgns0422@cnu.ac.kr

Abstract

Accurate and interpretable prediction of lithium-ion battery (LiB) degradation is critical for ensuring system safety and reliability. This study presents a probabilistic deep learning framework for the joint estimation of state of health (SOH) and remaining useful life (RUL), leveraging Monte Carlo Dropout to quantify predictive uncertainty. The model is trained on engineered cycle-level features, and by framing the task as a multi-output regression problem, the model learns to infer degradation from both long-term trends and short-term fluctuations. The proposed approach reduces SOH RMSE to as low as 0.0098 and RUL RMSE to 4.5 cycles, outperforming a deterministic baseline across all test cases. The uncertainty estimates are well-calibrated, with prediction interval coverage probability exceeding 0.94 for RUL and reaching 1.00 for SOH, while maintaining narrow sharpness values.

Ⅰ. Introduction

Traditional state-of-health (SOH) and remaining useful life (RUL) estimation methods for LiBs rely on physics-based electrochemical and circuit models, which provide interpretability but require detailed internal parameters and high computational cost. To address these limitations, data-driven approaches leverage measurable signals like voltage, current, and temperature. Machine learning (ML) methods have shown strong performance, with hybrids further improving adaptability and accuracy [1]. Despite these advances, challenges remain in ML methods. Many models are deterministic, offering only point estimates without confidence measures. Generalization is also an issue, as models often perform well within a dataset but fail when tested on new batteries. Moreover, SOH and RUL are typically treated as separate tasks, leading to fragmented insights and reduced efficiency. While co-estimation methods are emerging, few integrate uncertainty quantification, leaving a gap in achieving robust and reliable predictions.

This study introduces a probabilistic deep learning framework using Monte Carlo Dropout-based feedforward neural network (FFNN) for joint SOH and RUL estimation. Trained on cycle-level data with engineered features, it delivers both predictions and calibrated uncertainties.

Ⅱ. Dataset Analysis and Preprocessing

Datasets were obtained from the CALCE [2] repository and contain cycle-level measurements of 1.1 Ah batteries. For SOH and RUL co-estimation, raw measurements of voltage, current, and capacity were engineered into features capturing long-term trends and local variability. Engineered features include delta_Q, which measures cycle-to-cycle capacity change, cycle_frac, the normalized cycle index, rolling_Q, a smoothed capacity measure, and short-term voltage and current volatility captured by V_std and I_std. Pearson correlation analysis was used to confirm their predictive value.

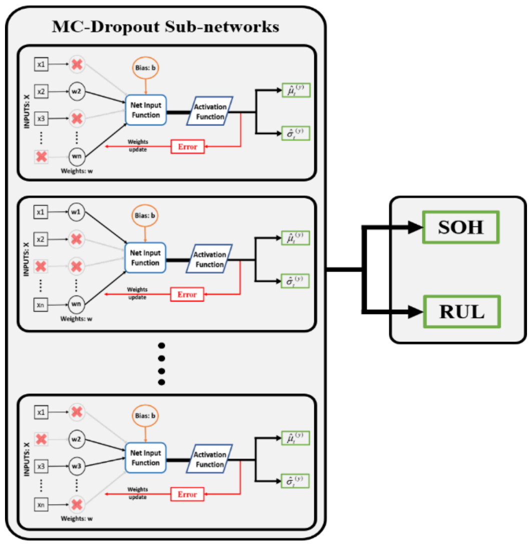

Fig. 1. Model architecture of the MC-Dropout FFNN for Probabilistic Co-Estimation.

Ⅲ. Methodology and Results

The FFNN in this study is a fully connected network that takes cycle-level inputs and outputs two scalars for SOH and RUL. It consists of an input layer, several hidden layers with ReLU activations, and a final linear layer. Training uses backpropagation with the Adam optimizer, where predictions are computed in a forward pass, loss is calculated, gradients are derived, and weights are updated until convergence [3]. The proposed model extends this baseline by adding dropout layers after each hidden layer, kept active during both training and testing. Fig. 1 shows the corresponding architecture of the proposed model. This Monte Carlo Dropout strategy approximates Bayesian inference by repeatedly sampling the network to generate a distribution of predictions. To evaluate the quality of the uncertainty estimates from MC-Dropout, two metrics are employed. Prediction Interval Coverage Probability (PICP), which measures how often true values fall within 95% prediction intervals, and Sharpness, which captures the average width of those intervals.

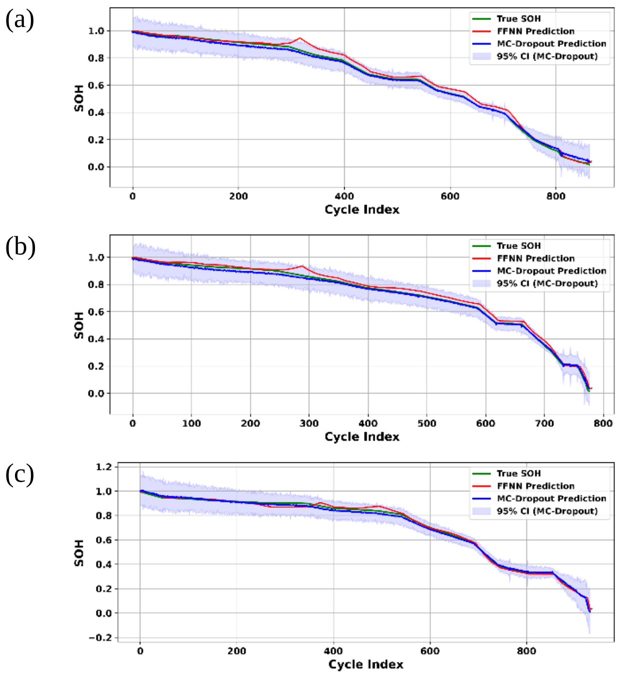

Fig. 2. SOH prediction with uncertainty; (a) Battery 1 (b) Battery 2 (c) Battery 3

The MC-Dropout model was evaluated against a baseline FFNN on three test batteries using MAE, RMSE, and R^2 for SOH and RUL. It consistently outperformed the baseline, reducing average SOH MAE from 0.0165 to 0.0108 and RUL MAE from 24.05 to 8.37 cycles, with R^2 values above 0.99 across all cases. Beyond accuracy, the model produced sharp and well-calibrated uncertainty estimates. SOH prediction intervals captured all true values with average widths below 0.17, while RUL intervals achieved PICP values of 0.94-1.00 and widened appropriately as batteries neared end-of-life. Fig. 2 shows the SOH estimation results, and Fig. 3 shows the RUL estimation results for the three test datasets.

IV. Conclusion

This study introduces a probabilistic deep learning approach for jointly estimating SOH and RUL of lithium-ion batteries using MC-Dropout feedforward neural networks. Formulated as a multi-output regression task, the model generates simultaneous predictions and quantifies uncertainty through Monte Carlo sampling. Cycle-level datasets were used with a cross-battery evaluation and engineered features captured degradation patterns. Compared with a baseline FFNN, the MC-Dropout model delivered substantial gains across three test batteries, lowering SOH RMSE and RUL RMSE significantly. It also produced well-calibrated uncertainty, with SOH PICP reaching 1.000 and RUL PICP ranging from 0.940 to 1.000 while maintaining sharpness below 131 cycles.

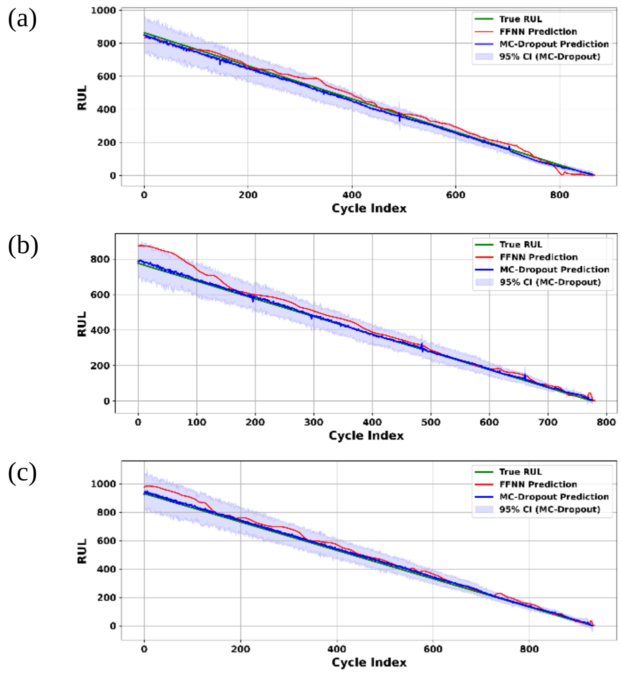

Fig. 3. RUL prediction with uncertainty; (a) Battery 1 (b) Battery 2 (c) Battery 3

ACKNOWLEDGMENT

This research was supported by Korea Agency for Infrastructure Technology Advancement(KAIA) through Research and Development on Safety Management Technology for EOL (End-of-Life) and Remanufactured Battery Project, funded by Korea Ministry of Land, Infrastructure and Transport(MOLIT)(RS-2025-02309323), and Korea Research Institute for defense Technology planning and advancement(KRIT) grant funded by the Korea government(DAPA(Defense Acquisition Program Administration))(No. 21-107-D00-009, Design and Development of a Seawater Secondary Battery-Based Module Pack and BMS, 2025).

REFERENCES

[1] R. Xiong et al. "A data-driven method for extracting aging features to accurately predict the battery health," Energy Storage Material, 57, pp. 460-470, 2023.

[2] Battery Data | Center for Advanced Life Cycle Engineering. (https://calce.umd.edu/battery-data).

[3] F. A. Vásquez et al. "Comparative study of methodologies for SOH diagnosis and forecast of LFP and NMC lithium batteries used in electric vehicles," J. Energy Storage, 105, 114725, 2025.