Machine Learning Approaches for Battery State of Health Assessment and Remaining Useful Life Prediction: A Mathematical Framework for Sustainable Energy Storage

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Abstract

Distinguished colleagues, today I present a comprehensive mathematical framework for battery prognostics that addresses one of the most pressing challenges in sustainable energy systems: accurately predicting the State of Health (SOH) and Remaining Useful Life (RUL) of lithium-ion batteries to enable circular economy principles and reduce electronic waste.

1 Introduction: The Mathematical Foundation of Battery Degradation

The degradation of lithium-ion batteries represents a complex, multiphysics phenomenon that can be mathematically modeled through careful feature engineering and machine learning approaches. Our fundamental challenge lies in mapping observable parameters to unobservable degradation states.

Let us define our State of Health mathematically:

$$SOH(t) = \frac{Q_{max}(t)}{Q_{nominal}} \times 100\% \tag{1}$$

where $Q_{max}(t)$ represents the maximum dischargeable capacity at cycle t, and $Q_{nominal} =$ 740 mAh represents the nominal capacity of our Kokam cells.

2 Feature Engineering: Translating Physics to Mathematics

Our machine learning approach relies on three carefully engineered features that serve as proxies for underlying degradation mechanisms:

2.1 Feature 1: Internal Resistance Approximation

The Direct Current Internal Resistance (DCIR) serves as a powerful health indicator, calculated using Ohm's law from pseudo-OCV test data:

$$R_{int} \approx \frac{\Delta V}{I} = \frac{V(t_0) - V(t_0 + \Delta t)}{I} \tag{2}$$

where $I = 0.040$ A represents our constant test current, and ΔV represents the voltage drop over a short interval.

Example Calculation: For Cell 5 at cycle 200, we observe:

$$\Delta V = 0.040 \text{ A} \times 0.065 \ = 0.0026 \text{ V} = 2.6 \text{ mV} \tag{3}$$

$$R_{int} = 0.065 \tag{4}$$

At cycle 7000, degradation increases the resistance:

$$\Delta V = 0.040\ \text{A} \times 0.110\ \ = 0.0044\ \text{V} = 4.4\ \text{mV} \tag{5}$$

$$R_{int} = 0.110 \tag{6}$$

This 69% increase in internal resistance demonstrates the strong correlation between impedance growth and degradation.

2.2 Feature Vector Construction

Our complete feature vector becomes:

$$\mathbf{x} = \begin{bmatrix} \text{Cycle Number} \\ \text{Average Temperature (°C)} \\ \text{Internal Resistance ()} \end{bmatrix} \in \mathbb{R}^3 \tag{7}$$

3 Multi-Layer Perceptron Architecture and Training

3.1 Network Architecture

Our MLP implements a feed-forward neural network with the following mathematical structure:

$$\hat{y} = f_{MLP}(\mathbf{x}) = \sigma_3(\mathbf{W}_3\sigma_2(\mathbf{W}_2\sigma_1(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2) + \mathbf{b}_3) \tag{8}$$

where:

- Layer 1: Input layer with 3 neurons
- Layer 2: Hidden layer with 20 neurons
- Layer 3: Hidden layer with 10 neurons

- Layer 4: Output layer with 1 neuron
- σ represents the activation function (typically sigmoid or ReLU)
- $\mathbf{W}_i$ and $\mathbf{b}_i$ represent weights and biases for layer i

3.2 Loss Function and Optimization

The network minimizes the Mean Squared Error (MSE) loss function:

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

where θ represents all trainable parameters, y_i represents true SOH values, and $\hat{y}_i$ represents predicted values.

Our implementation uses the Levenberg-Marquardt optimization algorithm, which combines the advantages of Gauss-Newton and gradient descent methods:

$$\theta_{k+1} = \theta_k - (\mathbf{J}^T \mathbf{J} + \lambda \mathbf{I})^{-1} \mathbf{J}^T \mathbf{r} \tag{10}$$

where $\mathbf{J}$ is the Jacobian matrix, λ is the damping parameter, and $\mathbf{r}$ is the residual vector.

3.3 Performance Analysis: Quantitative Results

Our trained model achieved exceptional performance metrics:

$$RMSE = \sqrt{\frac{1}{n_{test}} \sum_{i=1}^{n_{test}} (y_i - \hat{y}_i)^2} = 0.0130 \tag{11}$$

This translates to an average prediction error of only 1.30% in SOH estimation, with a correlation coefficient of $R = 0.98247$, indicating strong predictive capability.

4 Remaining Useful Life Prediction: The Prognostic Challenge

4.1 The RUL Mathematical Framework

Remaining Useful Life prediction requires extrapolation beyond the training domain, presenting unique mathematical challenges. We define RUL as:

$$RUL(t) = \min\{t_{future} | t_{future} > t, SOH(t_{future}) \leq SOH_{threshold}\} \tag{12}$$

where $SOH_{threshold} = 60\%$ represents our end-of-second-life criterion.

4.2 Hybrid Prognostic Model

Recognizing the limitations of neural networks in long-term extrapolation, we developed a hybrid approach that combines MLP accuracy with mathematical stability:

4.2.1 Degradation Modeling

We model internal resistance evolution using a linear degradation model derived from historical data:

$$R_{int}(t) = R_{int}(t_0) + \alpha \cdot (t - t_0) \tag{13}$$

where α represents the degradation slope obtained through polynomial fitting:

$$\alpha = \frac{\sum_{i=1}^{n}(t_i - \bar{t})(R_i - \bar{R})}{\sum_{i=1}^{n}(t_i - \bar{t})^2} \tag{14}$$

4.2.2 Scenario-Based Projections

Our framework generates multiple usage scenarios:

Normal Use Scenario:

$$R_{int,normal}(t) = R_{int}(t_0) + \alpha \cdot (t - t_0) \tag{15}$$

Gentle Use Scenario (70% degradation rate):

$$R_{int,gentle}(t) = R_{int}(t_0) + 0.7\alpha \cdot (t - t_0) \tag{16}$$

Harsh Use Scenario (130% degradation rate):

$$R_{int,harsh}(t) = R_{int}(t_0) + 1.3\alpha \cdot (t - t_0) \tag{17}$$

5 Practical Example: Complete Mathematical Solution

Let me demonstrate our framework with a real example from Cell 2 at cycle 7500.

5.1 Input Parameters and Feature Extraction

Given data point:

$$\text{Cycle Number} = 7500 \tag{18}$$

$$\text{Average Temperature} = 40.7C \tag{19}$$

$$\text{Internal Resistance} = 0.1012 \tag{20}$$

5.2 SOH Prediction via MLP

The input vector undergoes normalization:

$$\mathbf{x}_{norm} = \text{mapminmax}(\mathbf{x}, [-1, 1]) \tag{21}$$

The MLP produces:

$$SOH_{predicted} = f_{MLP}(\mathbf{x}_{norm}) \times 100\% = 76.58\% \tag{22}$$

5.3 RUL Calculation

Using our prognostic model with quadratic degradation:

$$S\hat{O}H(t) = at^2 + bt + c \tag{23}$$

where coefficients are calibrated to match the MLP prediction at $t = 7500$:

$$a = -3 \times 10^{-7} \tag{24}$$

$$b = -0.002 \tag{25}$$

$$c = 76.58/100 - (a \times 7500^2 + b \times 7500) \tag{26}$$

Solving for the end-of-life cycle:

$$t_{EOL} = \min\{t | t > 7500, S\hat{O}H(t) \leq 60\%\} = 7600 \tag{27}$$

Therefore:

$$RUL = t_{EOL} - t_{current} = 7600 - 7500 = 100 \text{ cycles} \tag{28}$$

6 Economic and Environmental Impact Quantification

6.1 Market Value Assessment

The remaining energy capacity:

$$E_{rem} = \frac{Q_{nom} \times V_{nom}}{1000} \times \frac{SOH}{100} \tag{29}$$

$$E_{rem} = \frac{0.740 \text{ Ah} \times 3.7 \text{ V}}{1000} \times \frac{76.58}{100} = 0.002097 \text{ kWh} \tag{30}$$

Market value calculation:

$$\text{Value} = E_{rem} \times \text{Price}_{used} = 0.002097 \times \$50/\text{kWh} = \$0.10 \tag{31}$$

6.2 Environmental Impact

CO emissions saved through second-life applications:

$$\text{CO}_2 \text{ Saved} = E_{rem} \times \text{CO}_2 \text{ Factor} = 0.002097 \times 150 = 0.3 \text{ kg CO}_2 \tag{32}$$

7 Model Validation and Performance Metrics

7.1 Statistical Performance Analysis

Our model demonstrates excellent statistical performance across multiple metrics:

Root Mean Squared Error:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} = 1.30\% \tag{33}$$

Coefficient of Determination:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} = 0.965 \tag{34}$$

Mean Absolute Error:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| = 0.98\% \tag{35}$$

8 Limitations and Future Directions

While our framework demonstrates strong performance, several mathematical and methodological limitations warrant discussion:

8.1 Uncertainty Quantification

Current predictions are deterministic. Future work should implement Bayesian neural networks to provide confidence intervals:

$$P(SOH|\mathbf{x}, \mathcal{D}) = \int P(SOH|\mathbf{x}, \theta)P(\theta|\mathcal{D})d\theta \tag{36}$$

where $\mathcal{D}$ represents the training dataset and θ represents model parameters.

8.2 Physics-Informed Machine Learning

Integration of physical constraints into the loss function could improve extrapolation capability:

$$L_{total} = L_{data} + \lambda L_{physics} \tag{37}$$

where $L_{physics}$ enforces monotonic capacity fade and thermodynamic constraints.

9 Conclusion

Our mathematical framework successfully bridges the gap between complex electrochemical phenomena and practical decision-making tools. The Multi-Layer Perceptron achieves 1.30% RMSE in SOH prediction, while the hybrid prognostic model provides stable RUL estimates across multiple usage scenarios.

The quantitative nature of our approach enables automated battery grading, economic valuation, and environmental impact assessment, directly supporting circular economy principles. With 519 training samples and rigorous validation, our model demonstrates the power of data-driven approaches in addressing real-world sustainability challenges.

The mathematical rigor presented today - from fundamental feature engineering through advanced neural network architectures to hybrid prognostic modeling - provides a solid foundation for scaling battery health management across the rapidly expanding electric vehicle ecosystem. Each equation, each calculation, represents a step toward transforming potential electronic waste into valuable, reusable assets.

Thank you for your attention to these mathematical foundations that enable practical environmental solutions.