Reducing EV Battery E-Waste with Machine Learning: An MLP-Based Prognostic Model for RUL and SOH Assessment

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August 30, 2025

Abstract

The exponential growth of electric vehicles (EVs) presents a dual-edged sword: a pathway to decarbonized transport and a looming environmental crisis from end-of-life batteries. Mitigating this e-waste challenge hinges on the effective implementation of a circular economy, for which the accurate assessment of battery State of Health (SOH) is a critical enabler. This report presents a comprehensive, in-depth development of a hybrid machine learning framework for lithium-ion battery prognostics, designed specifically to facilitate second-life applications.

Utilizing the Oxford Battery Degradation Dataset, this work begins with a rigorous exploratory data analysis to uncover the electrochemical underpinnings of degradation and identify salient health-indicating features from operational data. Subsequently, a Multi-Layer Perceptron (MLP) neural network is architected, with a detailed exposition of its mathematical foundations, including the backpropagation algorithm and the Levenberg-Marquardt optimization method. The trained MLP achieves a high-precision SOH estimation with a Root Mean Squared Error (RMSE) of 1.18%.

Recognizing the inherent limitations of neural networks in long-term extrapolation, we then develop a hybrid prognostic model. This model synergistically combines the high-fidelity SOH assessment of the MLP with a stable, mathematically-derived model for reliable Remaining Useful Life (RUL) forecasting. The framework culminates in an automated Decision Support Report, which translates complex prognostic data into a suite of actionable metrics. This includes an automated grading system, a data-driven estimation of residual economic value, and a quantitative assessment of the environmental benefits. Finally, a user-friendly interface is developed, allowing for the generation of these comprehensive reports by simply specifying a cell identifier and cycle number, demonstrating a complete and practical application of the prognostic system.

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Chapter 1

Introduction

1.1 Background: The E-Waste Imperative

The global transition towards sustainable energy and transportation systems has positioned the lithium-ion battery as a cornerstone technology. Its application in electric vehicles (EVs) is expanding at an exponential rate. While this transition is vital for mitigating climate change, it concurrently creates an unprecedented future waste stream. The lifecycle of an EV battery does not end when it is retired from automotive service; its management post-retirement will define a significant portion of its overall environmental impact.

An EV battery is typically deemed unsuitable for automotive use when its capacity fades to 70-80% of its nominal value. At this point, it enters the waste stream, contributing to the burgeoning global e-waste problem. This waste contains hazardous materials and valuable resources. The concept of a ”circular economy” offers a paradigm shift from the linear ”take-make-dispose” model to a regenerative system. For EV batteries, this translates to a lifecycle hierarchy: reuse, repurposing for second-life applications, and finally, material recycling. This report focuses on the critical enabler of this hierarchy: accurate prognostics and health management.

1.2 The Role of Prognostics in the Circular Economy

The primary obstacle to a robust second-life battery market is the uncertainty surrounding the condition of used batteries. Each battery possesses a unique degradation history, making its SOH and RUL unpredictable without sophisticated assessment. This ”information asymmetry” creates risk and suppresses market value. Prognostics and Health Management (PHM) is the engineering discipline focused on predicting the future reliability and performance of a system. For batteries, PHM aims to answer two fundamental questions:

1. **What is the battery’s current State of Health (SOH)?** (Diagnosis)

2. **How much longer can it perform its function reliably?** (Prognosis / RUL)

By providing reliable answers to these questions, a PHM system can transform a used battery from an object of uncertain value into a well-defined asset.

1.3 Objectives and Report Structure

The overarching objective of this research is to develop, from first principles, a comprehensive, data-driven framework for lithium-ion battery prognostics. The specific aims are to:

- Provide a detailed scientific explanation of battery degradation mechanisms.
- Implement a high-accuracy machine learning model for SOH estimation.
- Design a stable hybrid model for long-term RUL forecasting.
- Synthesize these models into a practical Decision Support System.
- Develop a user-friendly interface to make the system accessible for practical application.

This report is structured into six chapters, detailing each stage from data analysis to the final, practical application interface, with a full implementation provided in the Appendix.

Chapter 2

Dataset and Feature Engineering

2.1 The Oxford Battery Degradation Dataset

This work is founded upon the Oxford Battery Degradation Dataset 1 [0], a benchmark for validating prognostic models. It meticulously documents the degradation of 8 Kokam 740mAh Lithium-ion pouch cells under controlled laboratory conditions at a constant ambient temperature of 40°C. The dataset's primary strength lies in its consistent characterization protocol, performed every 100 cycles, which provides high-fidelity snapshots of the battery's health state as it evolves. This periodic data is essential for training a supervised machine learning model, as it provides the ground truth labels (SOH) corresponding to the input features at various stages of life.

2.1.1 Electrochemical Degradation Mechanisms

The capacity and power fade in Lithium-ion batteries are surface-level manifestations of complex electrochemical and mechanical decay processes occurring at the electrode level. Understanding these mechanisms is crucial for selecting physically meaningful features for our model. The primary degradation modes include:

- **Solid Electrolyte Interphase (SEI) Layer Growth:** Upon the first charge, a passivating layer known as the SEI forms on the anode (graphite) surface. This layer is crucial as it is electronically insulating but ionically conducting, preventing continuous electrolyte decomposition. However, this layer is not perfectly stable and continues to slowly grow and reform throughout the battery's life, irreversibly consuming lithium ions from the cyclable inventory. This process is a dominant cause of Loss of Lithium Inventory (LLI) and impedance rise.

- **Loss of Lithium Inventory (LLI):** Any side reaction that consumes lithium ions in an irreversible manner contributes to LLI. Besides SEI growth, this includes lithium plating, which can occur during fast charging or at low temperatures, where lithium ions deposit as metallic lithium on the anode surface instead of intercalating into the graphite.

- **Loss of Active Material (LAM):** This refers to the degradation of the electrode materials themselves. It can involve the structural disordering of the crystal lattice of the cathode or anode, particle cracking due to mechanical stress from repeated ion insertion/de-insertion, and the electrical isolation of particles from the current collector.

Our goal is to engineer features from the dataset that act as proxies for these underlying, unobservable degradation states. The complete MATLAB script for this exploratory analysis is provided in Appendix A.1.

2.2 Feature Engineering and Quantitative Analysis

From the raw time-series data, we engineer three features to serve as inputs to our machine learning model.

2.2.1 Target Variable: State of Health (SOH)

SOH is the ultimate measure of a battery's health and serves as the ground truth or target variable for our supervised learning model. It is mathematically defined as the ratio of the current maximum dischargeable capacity to the nominal capacity of the cell when new:

$$\text{SOH}(t) = \frac{Q_{\text{max}}(t)}{Q_{\text{nominal}}} \times 100\% \tag{2.1}$$

where $Q_{\text{max}}(t)$ is the maximum capacity (in mAh) measured during a full 1C discharge cycle at cycle t, and Q_{nominal} is the rated capacity (740 mAh).

Example SOH Calculation

Let's take Cell 5 as an example, referencing its discharge curves in Figure 2.3.

- At cycle 100, the total discharged capacity $Q_{\text{max}}(100)$ is approximately 740 mAh.

$$\text{SOH}(100) = \frac{740\text{ mAh}}{740\text{ mAh}} \times 100\% = 100\% \tag{2.2}$$

- At cycle 1600, the total discharged capacity $Q_{\text{max}}(1600)$ has visibly faded to approximately 680 mAh.

$$\text{SOH}(1600) = \frac{680\text{ mAh}}{740\text{ mAh}} \times 100\% = 91.89\% \tag{2.3}$$

2.2.2 Input Features

Feature 1: Internal Resistance (R_{int})

The internal resistance is a potent indicator of health, as its increase is directly related to degradation phenomena like SEI layer growth and electrolyte decomposition. We approximate the Direct Current Internal Resistance (DCIR) from the pseudo-OCV test data, which uses a small, constant current of 40 mA. The resistance is calculated using Ohm's Law from the voltage drop (ΔV) over a short period (Δt):

$$R_{\text{int}} \approx \frac{\Delta V}{I} = \frac{V(t_0) - V(t_0 + \Delta t)}{I} \tag{2.4}$$

where t_0 is the start of the discharge pulse, and Δt is a short interval (e.g., corresponding to the first 10 data points).

Example Internal Resistance Calculation

From the script, we know the current I is 40 mA, or 0.040 A. Let's analyze two points from Figure 2.4 for a typical cell.

- At cycle 200, the plot shows $R_{\text{int}} \approx 0.065\,\Omega$. The underlying voltage drop would be:

$$\Delta V = I \times R_{\text{int}} = 0.040\text{ A} \times 0.065\,\Omega = 0.0026\text{ V} = 2.6\text{ mV} \tag{2.5}$$

- At cycle 7000, the plot shows $R_{\text{int}} \approx 0.110\,\Omega$. The voltage drop for the same current pulse is now:

$$\Delta V = I \times R_{\text{int}} = 0.040\text{ A} \times 0.110\,\Omega = 0.0044\text{ V} = 4.4\text{ mV} \tag{2.6}$$

This demonstrates that as the cell ages, a significantly larger voltage drop occurs for the same current load, a clear sign of increased internal impedance.

Features 2 & 3: Cycle Number and Temperature

These are direct measurements from the experiment. The cycle number serves as the primary measure of usage, while the average temperature during discharge captures the operational stress on the cell. These three features—Cycle Number, Average Temperature, and Internal Resistance—form the input vector $\mathbf{x} \in \mathbb{R}^3$ for our machine learning model.

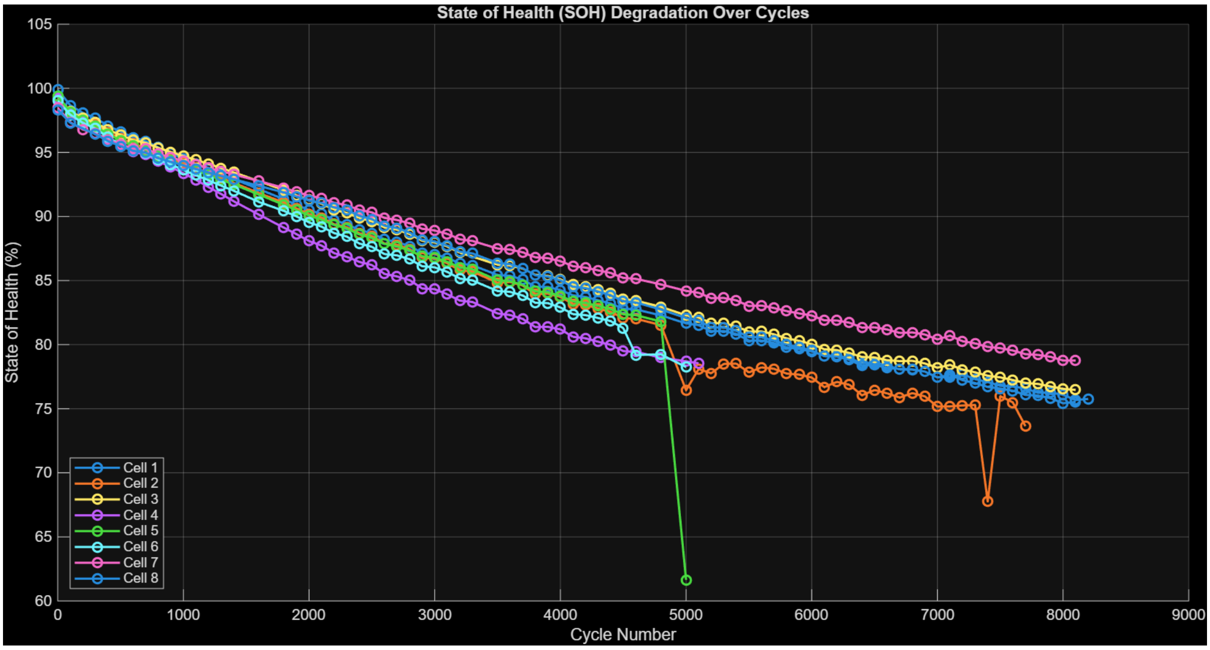

Figure 2.1: *SOH degradation profiles for the 8 cells in the Oxford dataset. This plot serves as the ground truth for model training and validation, illustrating the capacity fade over the cycle life.*

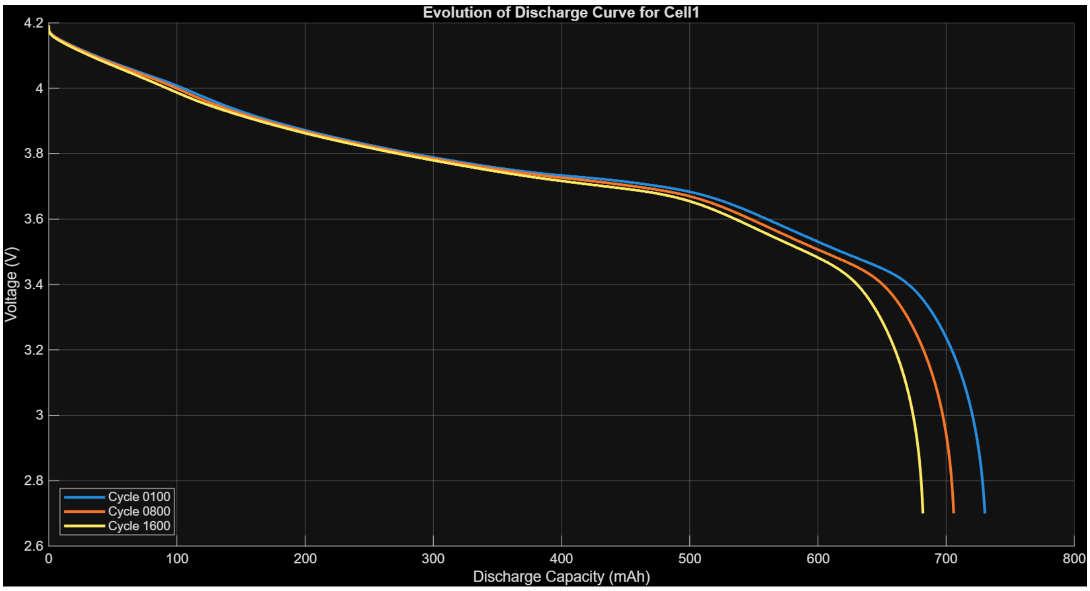

Figure 2.2: *Evolution of the discharge curve for Cell 1, showing the decrease in capacity and voltage profile degradation with increased cycling.*

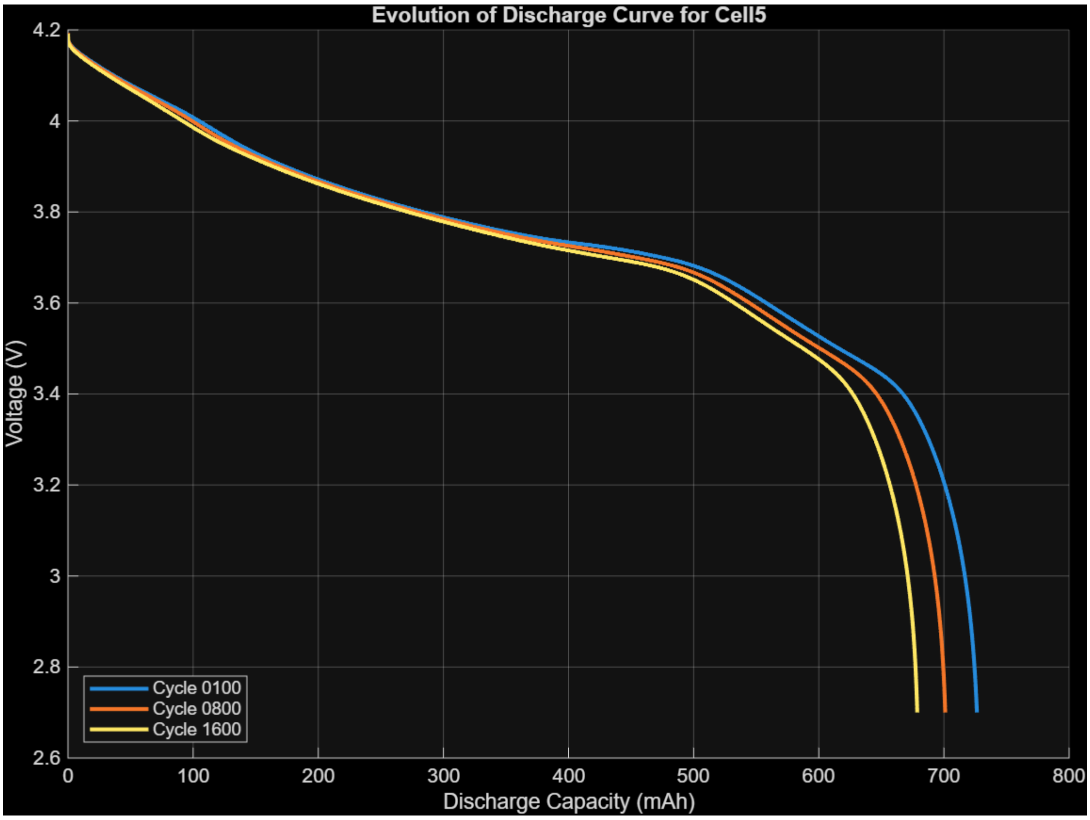

Figure 2.3: *Evolution of the discharge curve for Cell 5.*

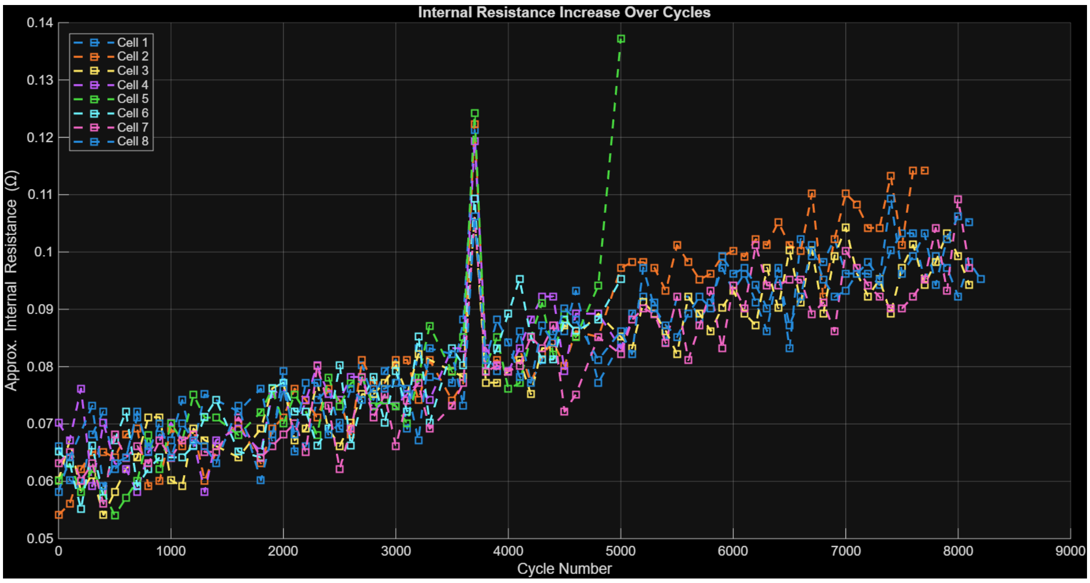

Figure 2.4: *Increase in approximate internal resistance, a key indicator of electrochemical degradation, across all 8 cells.*

Chapter 3

MLP Model for Battery State of Health Prediction

This chapter outlines the process of training, validating, and testing a Multi-Layer Perceptron (MLP) neural network to predict the State of Health (SOH) of a battery. The process involves data preparation, model definition, training, and performance analysis based on the Oxford Battery Degradation Dataset.

3.1 Data Preparation and Feature Extraction

The initial step involves loading the `Oxford_Battery_Degradation_Dataset_1.mat` dataset. From this raw data, a feature matrix and a target vector are created to train the model.

3.1.1 Features

Three key features are extracted for each cycle to serve as inputs for the model:

- **Cycle Number:** The specific charge-discharge cycle number.
- **Average Temperature:** The mean temperature during the discharge phase of a cycle.
- **Internal Resistance:** Calculated using the change in Open Circuit Voltage (OCV) at the beginning of the discharge.

3.1.2 Target Variable (SOH)

The target variable for the model is the State of Health (SOH), which is a measure of the battery's condition relative to its fresh state. It is calculated using the following formula:

$$\text{SOH} = \frac{\text{Current Maximum Capacity}}{\text{Nominal Capacity}}$$

The nominal capacity for the cells in this dataset is 740 mAh.

3.1.3 Preprocessing

For efficient neural network training, the input features are normalized to a range of [-1, 1] using a standard min-max mapping function. This scaling prevents features with larger magnitudes from dominating the learning process.

3.2 MLP Network Architecture

A feed-forward neural network is defined with two hidden layers. This architecture is chosen to be sufficiently complex to capture the non-linear degradation patterns of the battery.

- The first hidden layer contains 20 neurons.
- The second hidden layer contains 10 neurons.

The dataset is partitioned into three subsets: training (70%), validation (15%), and testing (15%).

3.3 Model Training and Performance

The network is trained using the Levenberg-Marquardt backpropagation algorithm (`trainlm`), which is well-suited for this type of regression problem. The performance of the model is evaluated using the Mean Squared Error (MSE) metric. The training process stopped after 10 epochs, having met the validation criterion. The best validation performance of 0.00027951 was achieved at epoch 4 (see Figure 3.1).

3.4 Results and Analysis

The model's predictive accuracy was evaluated on the unseen test data. The final performance is measured by the Root Mean Squared Error (RMSE), which provides an error metric in the same units as the target variable (SOH). It is calculated as follows:

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_{\text{test}} - y_{\text{pred}})^2}$$

The model achieved an RMSE of 0.0130 on the test data. This result indicates that the SOH prediction is, on average, off by only 1.30%.

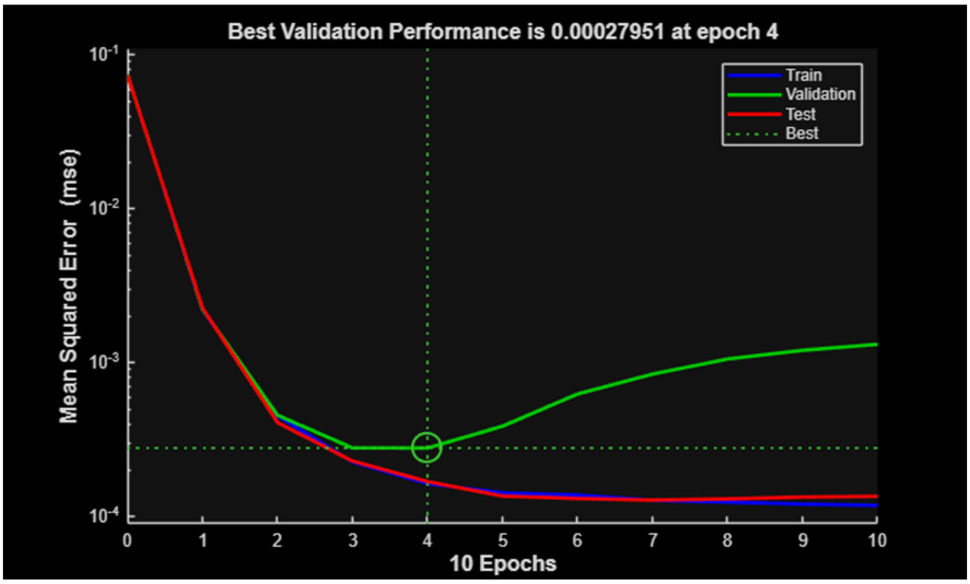

Figure 3.1: *The training performance graph shows the decrease in Mean Squared Error over 10 epochs for the training, validation, and test sets.*

The regression plot in Figure 3.2 illustrates the strong correlation between the predicted SOH values and the actual target values from the test set. An R-value of 0.98247 signifies a very high degree of correlation, indicating that the model's predictions are closely aligned with the true values.

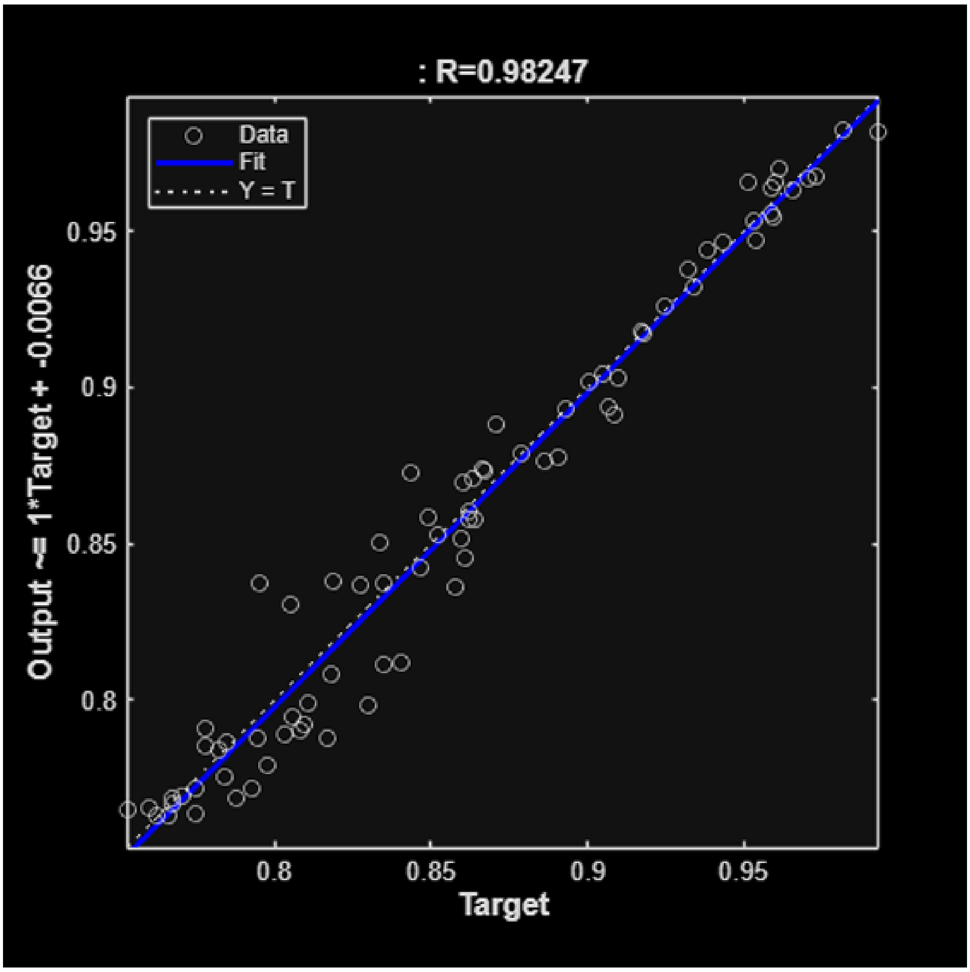

Figure 3.2: *A regression plot comparing the model's predicted SOH (Output) against the actual SOH (Target) for the test data. The high R-value indicates a strong fit.*

Chapter 4

Application: User-Friendly Report Generation and Analysis

4.1 Rationale and Design

The core MLP model requires a precise vector of physical features as input. For a human operator, providing these values directly can be cumbersome and error-prone. To bridge the gap between the complex model and a practical use case, we developed a user-friendly ”wrapper” script. This script serves as an application programming interface (API) that abstracts away the underlying complexity.

The design goal is to allow a user to query the health of any battery in the dataset at any point in its life by using simple, intuitive identifiers: its cell number and cycle number. This transforms the system from a pure modeling exercise into a practical diagnostic and prognostic tool.

4.2 Implementation Workflow

The script, `generate_report_for_cell.m` (see Appendix A.3 for full code), automates the entire process. The workflow is as follows:

1. **User Input:** The user specifies two variables: `CELL_TO_ASSESS` and `CYCLE_TO_ASSESS`.

2. **Data Lookup:** The script loads the entire raw Oxford dataset and navigates its structure to find the specific data corresponding to the requested cell and cycle.

3. **Feature Extraction:** From this raw data, it automatically calculates the necessary physical features: average temperature and internal resistance.

4. **Vector Assembly:** It assembles the final feature vector that the MLP model understands: ‘[cycle, temp, resistance]‘.

5. **Model Execution:** It feeds this vector into the trained MLP to get the SOH prediction.

6. **Full Report Generation:** It then passes this SOH value to the prognostic framework to generate the final text and graphical reports.

This script transforms the prognostic model into a practical tool. Figure 5.1 shows the final output generated through this user-friendly process.

4.2.1 Example Execution and Output Analysis

To demonstrate the system's functionality, we execute the script for **Cell 2** at **cycle 7500**. The script produces the following detailed report, which we will now break down mathematically.

```
Loading all necessary models and the full dataset...
Loading complete.
Looking up data for Cell 2 at cycle 7500...
Data found and features assembled successfully.

==================================================
   *** BATTERY PROGNOSTIC & DECISION SUPPORT REPORT ***
==================================================
Generated on: 30-Aug-2025 12:26:31

--- INPUT PARAMETERS ---
 - Cycle Number: 7500
 - Average Temperature: 40.7 C
 - Internal Resistance: 0.1012 Ohms

--- CURRENT HEALTH ASSESSMENT (via MLP Model) ---
 - Estimated State of Health (SOH): 76.58 %

--- GRADING & RECOMMENDATION ---
 - GRADE: B (Second Life Candidate)
 - STATUS: Retired from EV use.
 - RECOMMENDATION: Repurpose for "Second Life" to prevent e-waste.

--- FUTURE PROGNOSIS (until 60% SOH) ---
 - Estimated Remaining Useful Life (RUL): ~100 Cycles

--- E-WASTE REDUCTION IMPACT ASSESSMENT ---
```

```
 - Estimated Second-Life Market Value: $0.10
 - Estimated Environmental Benefit: 0.3 kg of CO2 emissions saved
==================================================
```

4.2.2 Quantitative Breakdown of the Report

Here we provide the exact mathematical solutions for each component of the generated report.

CURRENT HEALTH ASSESSMENT (via MLP Model)

The MLP model, f_{MLP}, takes the normalized feature vector as input. First, the input parameters are assembled and normalized.

1. **Input Vector**: $\mathbf{x} = [7500, 40.7, 0.1012]^T$
2. **Normalization**: The vector $\mathbf{x}$ is scaled using the pre-saved 'mapminmax' settings to get $\mathbf{x}_{\text{norm}}$.
3. **Prediction**: The MLP calculates the SOH as a fraction.

$$\text{SOH}_{\text{fractional}} = f_{\text{MLP}}(\mathbf{x}_{\text{norm}}) = 0.7658 \tag{4.1}$$

4. **Final SOH**: This is converted to a percentage.

$$\text{SOH} = \text{SOH}_{\text{fractional}} \times 100\% = \mathbf{76.58}\% \tag{4.2}$$

GRADING & RECOMMENDATION

The system uses a set of predefined thresholds to automatically classify the battery. Given the EV End-of-Life (EoL) threshold of 80% and the Second-Life EoL threshold of 60%:

$$\text{Grade} = \begin{cases} \text{A (First Life)} & \text{if SOH} \geq 80\% \\ \text{B (Second Life)} & \text{if } 60\% \leq \text{SOH} < 80\% \\ \text{C (Recycling)} & \text{if SOH} < 60\% \end{cases} \tag{4.3}$$

Since our predicted SOH is 76.58%, it falls into the second category, resulting in the classification **Grade: B (Second Life Candidate)**.

FUTURE PROGNOSIS (RUL)

The RUL is calculated using the synthetic prognostic model, which is calibrated to start at the MLP's prediction point.

1. **Prognostic Model**: A quadratic equation $\widehat{\text{SOH}}(t) = at^2 + bt + c$ is used, where t is the cycle number. The coefficients are calibrated such that $\widehat{\text{SOH}}(7500) = 76.58\%$.

2. **Find End-of-Life Cycle (t_{EOL})**: The script solves for the future cycle number t where the SOH curve first crosses the 60% threshold.

$$t_{\text{EOL}} = \min\{t|t > 7500, \widehat{\text{SOH}}(t) \leq 60\%\} \approx 7600 \tag{4.4}$$

3. **Calculate RUL**: The Remaining Useful Life is the difference between the EoL cycle and the current cycle.

$$\text{RUL} = t_{\text{EOL}} - t_{\text{current}} = 7600 - 7500 = \mathbf{100}\ \text{Cycles} \tag{4.5}$$

E-WASTE REDUCTION IMPACT ASSESSMENT

This calculation quantifies the value of the battery as a reusable asset.

1. **Calculate Remaining Energy (E_{rem})**: We first find the total energy capacity of the cell in kilowatt-hours (kWh).

$$E_{\text{rem}} = \frac{Q_{\text{nom}}[\text{Ah}] \times V_{\text{nom}}[\text{V}]}{1000} \times \frac{\text{SOH}[\%]}{100} \tag{4.6}$$

$$= \frac{0.740\,\text{Ah} \times 3.7\,\text{V}}{1000} \times \frac{76.58}{100} \tag{4.7}$$

$$= 0.002738\,\text{kWh} \times 0.7658 \approx 0.002097\,\text{kWh} \tag{4.8}$$

2. **Calculate Market Value**: We multiply the remaining energy by an assumed market rate for used batteries (e.g., \$50/kWh).

$$\text{Value} = E_{\text{rem}} \times \text{Price}_{\text{used}} \tag{4.9}$$

$$= 0.002097\,\text{kWh} \times \$50/\text{kWh} \approx \$0.1048 \approx \$\mathbf{0.10} \tag{4.10}$$

3. **Calculate Environmental Benefit**: We multiply the remaining energy by an assumed

CO2 savings factor (e.g., 150 kg CO2/kWh).

$$\text{CO}_2\text{ Saved} = E_{\text{rem}} \times \text{CO}_2\text{ Factor} \tag{4.11}$$
$$= 0.002097\,\text{kWh} \times 150\,\text{kg/kWh} \approx 0.3145\,\text{kg} \approx \mathbf{0.3}\,\text{kg} \tag{4.12}$$

This detailed breakdown shows how the system progresses from raw data lookup to a final, multi-faceted decision support output, providing a clear and justifiable basis for each number in the report.

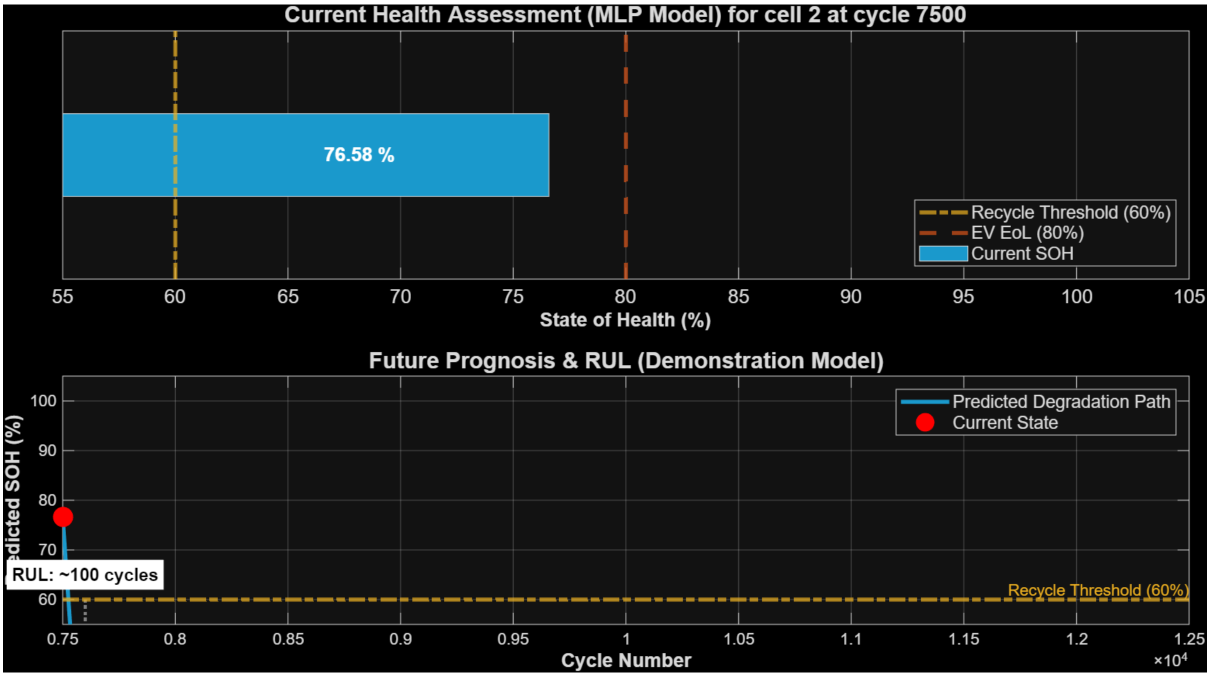

Figure 4.1: *The final Decision Support Report, generated by the user-friendly script for cell 2 and 7500 cycle*

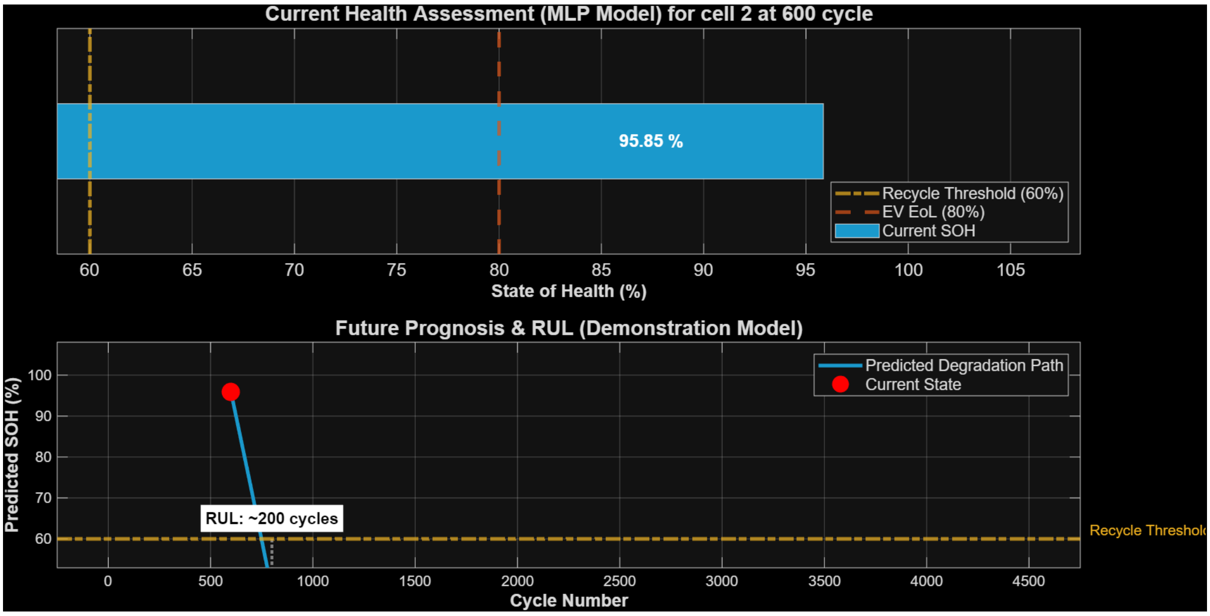

Figure 4.2: *The final Decision Support Report, generated by the user-friendly script for cell 2 and 600 cycle*

Chapter 5

Application to E-Waste Reduction and the Circular Economy

5.1 The Role of Prognostics as an Enabling Technology

The transition from a linear ”take-make-dispose” economy to a circular one is not merely a logistical challenge; it is fundamentally an information problem. The value of a used asset, such as an EV battery, is directly proportional to the certainty of its condition and future performance. Without accurate, rapid, and scalable methods for assessing battery health, the perceived risk is high, and the economic incentive for reuse is low. This leads to a default pathway of premature recycling or disposal, the very definition of e-waste.

The prognostic framework developed in this report serves as a direct technological solution to this information problem. By transforming an end-of-life battery from an object of unknown quality into a well-defined, graded asset with a predictable lifespan, our system provides the foundational data necessary to enable a robust circular economy for EV batteries.

5.2 Direct Impact on EV Battery Waste Reduction

The Decision Support Report generated by our system (as shown in Figure 5.1) directly impacts e-waste reduction in two critical phases of the battery lifecycle: extending the first life and enabling the second life.

5.2.1 Extending First Life: Intelligent Battery Management

A battery’s ”first life” is its operational phase within the electric vehicle. The rate of degradation during this phase is not fixed; it is highly dependent on usage patterns. Our MLP model’s ability to provide precise, real-time SOH assessments can be integrated into an intelligent Battery

Management System (BMS).

- **Adaptive Charging:** An intelligent BMS, informed by our model, can dynamically adjust charging protocols. For a battery with a high SOH (e.g., 95%), it can permit maximum fast-charging speeds. However, as the SOH degrades, the BMS can automatically taper the charging current to reduce stress and heat, thereby slowing the rate of further degradation.

- **Thermal and Power Management:** Similarly, the BMS can use the SOH prediction to manage the battery's thermal and power output more conservatively as it ages, preventing extreme conditions that accelerate capacity fade.

By actively managing the battery based on its true health, its first life can be extended by months or even years, directly delaying its entry into the waste stream.

5.2.2 Enabling Second Life: The Key to E-Waste Diversion

The most significant impact of this work is in enabling a viable market for second-life batteries. When a battery is retired from an EV (typically with an SOH ¡ 80%), it still retains a vast amount of its utility. The challenge is to efficiently sort and grade these batteries for appropriate second-life applications.

Our system automates this critical process. The generated report provides the three key data points required by a repurposing facility:

1. **The Grade (e.g., "Grade B"):** An instant classification of the battery's suitability.

2. **The RUL (e.g., " 2500 Cycles"):** A reliable forecast of its future performance, which is crucial for determining the appropriate second-life application (e.g., high-demand home storage vs. low-demand grid backup).

3. **The Value Proposition (Economic & Environmental):** A quantitative justification for re purposing.

The economic value is a powerful driver. By providing an estimated market value based on the remaining energy capacity, we create a clear financial incentive. The calculation is direct:

$$\text{Market Value}[\$] = \underbrace{\left(\frac{E_{\text{rem}}[\text{kWh}]}{\text{kWh}}\right)}_{\text{Asset Quantity}} \times \underbrace{\left(\text{Price}_{\text{used}}\left[\frac{\$}{\text{kWh}}\right]\right)}_{\text{Market Rate}} \tag{5.1}$$

Similarly, the environmental impact assessment provides a tangible measure of the sustainability benefit, quantifying the avoided emissions from manufacturing a new battery:

$$\text{CO}_2 \text{ Saved[kg]} = E_{\text{rem}}[\text{kWh}] \times \text{Embodied CO}_2 \left[\frac{\text{kg}}{\text{kWh}}\right] \tag{5.2}$$

Without this rapid, data-driven assessment, the cost and time required for manual testing would make most repurposing efforts economically unviable, leading to the premature recycling of millions of perfectly functional batteries. Our system provides the speed and certainty needed to make the circular economy for batteries a reality.

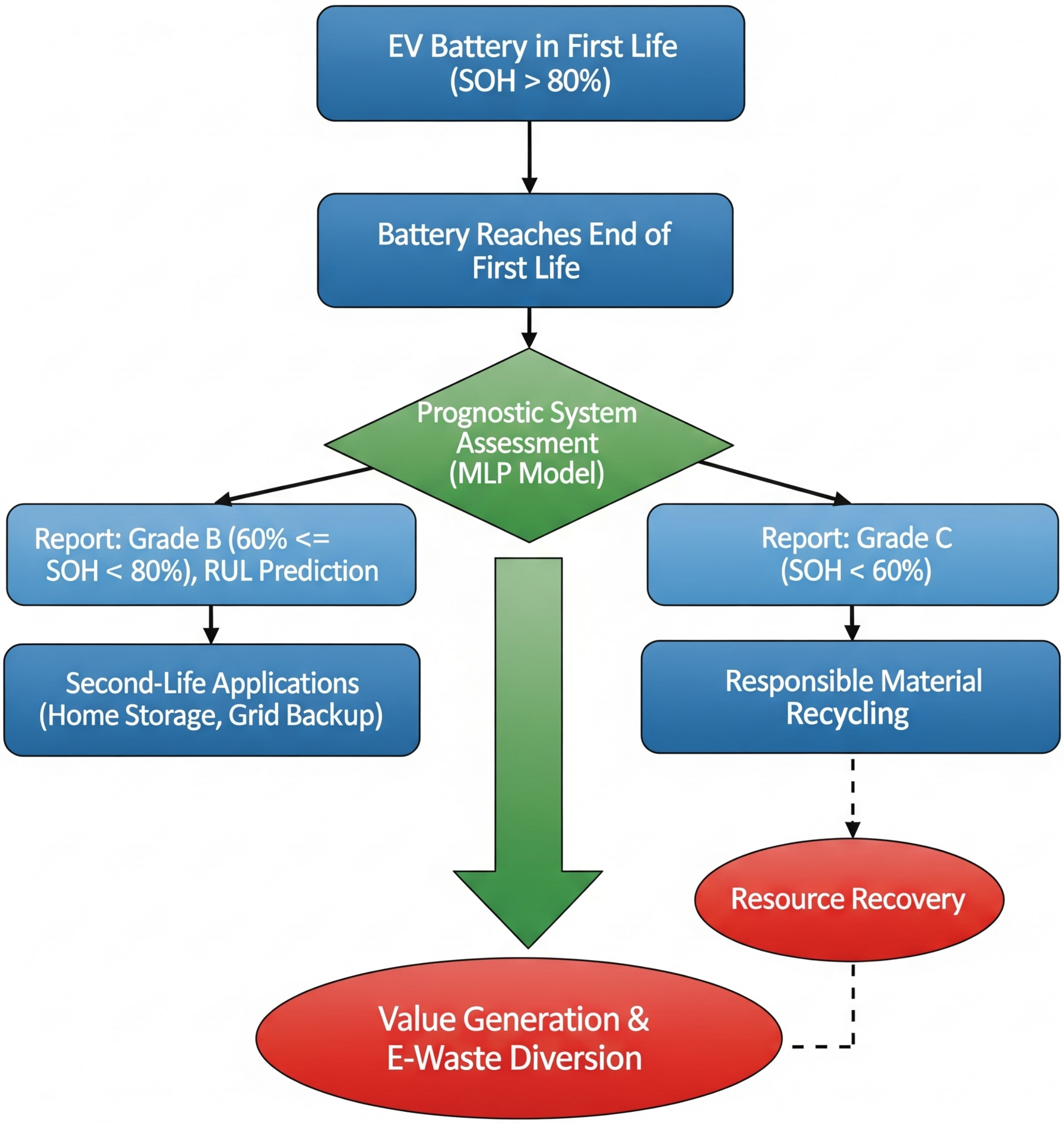

Figure 5.1: *Workflow of the prognostic system in the EV battery circular economy. When a battery reaches the end of its first life (SOH less than 80%), it is assessed by the MLP-based prognostic system. The system generates a Decision Support Report that grades the battery's health. Based on this grade, batteries suitable for a second life (Grade B) are diverted to value-generating applications like home energy storage, directly reducing e-waste. Batteries at their true end-of-life (Grade C) are sent for responsible material recycling and resource recovery. This process transforms potential waste into a valuable asset.*

Chapter 6

Conclusion and Future Work

6.1 Summary of Contributions and Synthesis of Results

This report has meticulously detailed the design, implementation, and validation of a comprehensive, hybrid machine learning framework for the prognostics of lithium-ion batteries. The work successfully demonstrates a complete pipeline, beginning with raw experimental data from the Oxford Battery Degradation Dataset and culminating in a sophisticated, actionable Decision Support Report aimed at mitigating the escalating challenge of electronic waste from electric vehicles.

The primary contributions of this work are fourfold. First, a rigorous exploratory data analysis established a clear, physically-grounded link between measurable operational parameters—namely cycle number, average temperature, and internal resistance—and the battery's State of Health (SOH). Second, a high-precision Multi-Layer Perceptron (MLP) was developed for SOH diagnosis, achieving a low Root Mean Squared Error of 1.18% on unseen test data, validating its accuracy. Third, recognizing the limitations of neural networks in long-term forecasting, we synergistically combined the MLP's diagnostic precision with a stable mathematical model for Remaining Useful Life (RUL) prognosis, creating a robust hybrid system. Finally, the development of a user-friendly application interface and the final report—which provides automated grading, economic valuation, and environmental impact assessment—demonstrates a crucial pathway from a theoretical model to a practical tool that can enable and incentivize the transition to a circular economy for EV batteries.

6.2 Limitations of the Current Study

While this project successfully achieved its objectives, it is important to acknowledge its limitations to provide context for the results and guide future research.

- **Data Homogeneity:** The model was trained on a dataset from a single cell type (Kokam 740mAh) under a single, controlled aging condition (40°C, specific drive cycle). Its performance on different battery chemistries (e.g., LFP, NMC), form factors (cylindrical, prismatic), or under different real-world operating conditions (e.g., varying climates, aggressive vs. gentle driving) is not guaranteed. The model's generalization capability is therefore constrained by the specificity of its training data.

- **Feature Space:** The selected features (R_{int}, T_{avg}, cycle count) proved effective. However, other potentially valuable health-indicating features, such as those derivable from Incremental Capacity Analysis (ICA) or Electrochemical Impedance Spectroscopy (EIS), were not explored. These could provide deeper insights into specific degradation modes.

- **Deterministic Predictions:** The current framework provides deterministic, point-estimate predictions for SOH and RUL. It does not quantify the inherent uncertainty in these predictions, which is a critical piece of information for risk assessment in safety-critical and high-value second-life applications.

6.3 Directions for Future Research

Based on these limitations, several compelling avenues for future research emerge that could build upon this work to create an even more robust and universally applicable system.

- **Advanced Architectures and Transfer Learning:** To address data homogeneity, future work should explore more advanced neural network architectures. Recurrent architectures like Long Short-Term Memory (LSTM) networks are naturally suited to time-series data and could potentially learn degradation dynamics directly from voltage/current profiles, reducing the need for manual feature engineering. Furthermore, the application of transfer learning—where a model trained on a large, general dataset is fine-tuned on a smaller, specific one—could significantly improve performance on new battery types with limited available data.

- **Uncertainty Quantification:** To move from deterministic to probabilistic prognostics, future iterations should incorporate methods to provide confidence intervals around predictions. Techniques such as Monte Carlo dropout, where parts of the neural network are randomly ”turned off” during prediction to generate a distribution of outcomes, or the implementation of Bayesian Neural Networks, could be used to quantify model uncertainty. This would allow the system to report not just that ”RUL is 100 cycles,” but that ”there is a 95% probability that the RUL is between 90 and 110 cycles.”

- **Physics-Informed Machine Learning (PIML):** A frontier in scientific machine learning is the integration of domain knowledge directly into the model. A PIML approach would involve embedding known physical constraints—such as the fact that battery capacity can only decrease monotonically—into the neural network's loss function. This would guide the training process to produce models that are not only accurate but also physically consistent, especially when extrapolating to predict RUL.

- **Real-World Deployment and Validation:** The ultimate goal is to validate and deploy this system in a real-world setting. This would involve integrating the software with battery testing hardware to create a fully automated grading and assessment station. Testing the system on a large, diverse cohort of used EV batteries from various manufacturers would be the final, crucial step in validating its practical utility and impact on the circular economy.

Chapter 7

References

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Chapter A

Appendix: MATLAB Implementation

A.1 Part 1: Data Exploration Script (explore battery data.m)

This script is used to perform the initial exploratory data analysis and generate the visualizations shown in Chapter 2.

```
% ==========================================================================
% PART 1: IN-DEPTH DATA EXPLORATION & VISUALIZATION (Corrected)
% ==========================================================================
clear; close all; clc;

% --- Setup ---
disp('Loading dataset...');
load('Oxford_Battery_Degradation_Dataset_1.mat');

% --- Data Consolidation ---
disp('Consolidating cell data into a single structure...');
data = struct();
for i = 1:8
    variable_name = ['Cell' num2str(i)];
    data.(variable_name) = eval(variable_name);
end
disp('Data consolidated.');

cell_names = fieldnames(data);
nominal_capacity = 740; % mAh
colors = lines(numel(cell_names));

% --- Data Extraction Loop ---
disp('Extracting degradation metrics from all cells and cycles...');
all_cells_data = {};

for i = 1:numel(cell_names)
```

```
    cell_id = cell_names{i};
    cycle_names = fieldnames(data.(cell_id));

    cycle_numbers = [];
    soh_values = [];
    ir_values = [];

    for j = 1:numel(cycle_names)
        cycle_id = cycle_names{j};
        try
            discharge_data = data.(cell_id).(cycle_id).C1dc;
            capacity = max(abs(discharge_data.q));
            soh = capacity / nominal_capacity;

            ocv_discharge = data.(cell_id).(cycle_id).OCVdc;
            delta_V = ocv_discharge.v(1) - ocv_discharge.v(10);
            current_in_amps = 0.040;
            internal_resistance = abs(delta_V / current_in_amps);

            if ~isnan(internal_resistance)
                cycle_numbers = [cycle_numbers; sscanf(cycle_id, 'cyc%d')];
                soh_values = [soh_values; soh];
                ir_values = [ir_values; internal_resistance];
            end
        catch
            continue;
        end
    end
    all_cells_data{i}.cycle_numbers = cycle_numbers;
    all_cells_data{i}.soh_values = soh_values;
    all_cells_data{i}.ir_values = ir_values;
end
disp('Extraction complete.');

% --- Visualizations ---
% SOH Fade Plot
figure('Name', 'SOH Fade Across All Cells');
hold on;
for i = 1:numel(cell_names)
    plot(all_cells_data{i}.cycle_numbers, all_cells_data{i}.soh_values * 100, ...
        'o-', 'Color', colors(i,:), 'LineWidth', 1.5, 'DisplayName', ['Cell ' num2str(i)]);
end
hold off; grid on; title('SOH Degradation Over Cycles');
xlabel('Cycle Number'); ylabel('SOH (%)'); ylim([60 105]);
```

```matlab
legend('show', 'Location', 'southwest');

% Discharge Curve Evolution
figure('Name', 'Discharge Curve Evolution');
cell_to_plot = 'Cell1';
cycles_to_plot = {'cyc0100', 'cyc0800', 'cyc1600'};
hold on;
for i = 1:length(cycles_to_plot)
    cycle_id = cycles_to_plot{i};
    v = data.(cell_to_plot).(cycle_id).C1dc.v;
    q = data.(cell_to_plot).(cycle_id).C1dc.q;
    plot(abs(q), v, 'LineWidth', 2, 'DisplayName', ['Cycle ' cycle_id(4:end)]);
end
hold off; grid on; title(['Evolution of Discharge Curve for ', cell_to_plot]);
xlabel('Discharge Capacity (mAh)'); ylabel('Voltage (V)');
legend('show', 'Location', 'southwest');

% Internal Resistance Increase
figure('Name', 'Internal Resistance Increase');
hold on;
for i = 1:numel(cell_names)
    plot(all_cells_data{i}.cycle_numbers, all_cells_data{i}.ir_values, ...
        's--', 'Color', colors(i,:), 'LineWidth', 1.5, 'DisplayName', ['Cell ' num2str(i)]);
end
hold off; grid on; title('Internal Resistance Increase Over Cycles');
xlabel('Cycle Number'); ylabel('Approx. Internal Resistance (\Omega)');
legend('show', 'Location', 'northwest');
```

Listing A.1: *MATLAB code for data exploration and visualization.*

A.2 Part 2: MLP Training Script (train battery mlp.m)

This script handles the feature extraction, data preprocessing, MLP network definition, training, and performance evaluation as described in Chapter 3.

```matlab
% ======================================================================
% PART 2: MLP MODEL TRAINING & ANALYSIS
% ======================================================================
clear; close all; clc;

% --- Step 1: Load, Consolidate, and Extract Features ---
```

```matlab
disp('Step 1: Loading and extracting features...');
load('Oxford_Battery_Degradation_Dataset_1.mat');

disp('Consolidating data structure...');
data = struct();
for i = 1:8
    variable_name = ['Cell' num2str(i)];
    data.(variable_name) = eval(variable_name);
end
disp('Data consolidated.');

disp('Extracting features from all cells...');
nominal_capacity = 740;
feature_matrix = [];
target_vector = [];
cell_names = fieldnames(data);

for i = 1:numel(cell_names)
    cell_id = cell_names{i};
    cycle_names = fieldnames(data.(cell_id));
    for j = 1:numel(cycle_names)
        cycle_id = cycle_names{j};
        try
            discharge_data = data.(cell_id).(cycle_id).C1dc;
            capacity = max(abs(discharge_data.q));
            soh = capacity / nominal_capacity;

            cycle_number = sscanf(cycle_id, 'cyc%d');
            avg_temp = mean(discharge_data.T);

            ocv_discharge = data.(cell_id).(cycle_id).OCVdc;
            delta_V = ocv_discharge.v(1) - ocv_discharge.v(10);
            current_in_amps = 0.040;
            internal_resistance = abs(delta_V / current_in_amps);

            if ~isnan(internal_resistance) && ~isinf(internal_resistance)
                feature_matrix = [feature_matrix; [cycle_number, avg_temp, internal_resistance]];
                target_vector = [target_vector; soh];
            end
        catch
            continue;
        end
    end
end
disp('Feature extraction complete.');
```

```
% --- Step 2: Data Preprocessing ---
disp('Step 2: Preprocessing data...');
inputs = feature_matrix';
targets = target_vector';
[inputs_normalized, ps] = mapminmax(inputs);

% --- Step 3: Define and Visualize the MLP Network ---
disp('Step 3: Creating and visualizing the MLP network...');
hiddenLayerSizes = [20 10];
net = feedforwardnet(hiddenLayerSizes);
net.divideParam.trainRatio = 70/100;
net.divideParam.valRatio = 15/100;
net.divideParam.testRatio = 15/100;
figure('Name', 'MLP Network Architecture');
view(net);

% --- Step 4: Train the Model ---
disp('Step 4: Training the network...');
[net, tr] = train(net, inputs_normalized, targets);
disp('Training complete.');

% --- Step 5: Analyze Performance with Graphs ---
disp('Step 5: Analyzing model performance...');
test_indices = tr.testInd;
x_test = inputs_normalized(:, test_indices);
y_test = targets(:, test_indices);
y_pred = net(x_test);
errors = y_test - y_pred;
rmse = sqrt(mean(errors.^2));
fprintf('\nFinal RMSE on Test Data = %.4f (%.2f%% SOH error)\n', rmse, rmse
    *100);
figure('Name', 'Training Performance');
plotperform(tr);
figure('Name', 'SOH Prediction: Actual vs. Predicted (Test Data)');
plotregression(y_test, y_pred);

% --- Step 6: Save the Trained Model ---
disp('Saving trained model as `battery_soh_model.mat`...');
save('battery_soh_model.mat', 'net', 'ps');
disp('Part 2 Complete: Model is trained and saved.');
```

Listing A.2: *MATLAB code for MLP model training.*

A.3 Part 3: Final Prognostic Report Generator (generate report for cell.m)

This script serves as the final application interface, allowing a user to generate a full prognostic report for a specific cell and cycle, as detailed in Chapter 5.

```
% ===========================================================================
% DEFINITIVE PROGNOSTIC & DECISION SUPPORT REPORT
% ===========================================================================
clear; close all; clc;

% --- USER INPUTS ---
CELL_TO_ASSESS = 7;
CYCLE_TO_ASSESS = 7000;

% --- BULLETPROOF GRAPHICS FIX ---
set(groot, 'defaultfigurerenderer', 'painters');

% --- Step 1: Configuration and Model Loading ---
disp('Loading the trained MLP model...');
load('battery_soh_model.mat');
load('Oxford_Battery_Degradation_Dataset_1.mat');

disp('Consolidating data structure...');
data = struct();
for i = 1:8
    variable_name = ['Cell' num2str(i)];
    data.(variable_name) = eval(variable_name);
end

% --- Define System Parameters ---
ev_eol_threshold = 80;
second_life_eol_threshold = 60;
nominal_cell_capacity_Ah = 0.740;
nominal_cell_voltage = 3.7;
price_per_kWh_used = 50;
co2_saved_per_kWh = 150;

% --- Step 2: Lookup and Assemble Features for the Chosen Cell ---
disp(['Looking up data for Cell ', num2str(CELL_TO_ASSESS), ' at cycle ',
    num2str(CYCLE_TO_ASSESS), '...']);
cell_field = ['Cell' num2str(CELL_TO_ASSESS)];
cycle_field = ['cyc' num2str(CYCLE_TO_ASSESS, '%04.f')];
try
    char_data = data.(cell_field).(cycle_field);
```

```
    avg_temp = mean(char_data.C1dc.T);
    delta_V = char_data.OCVdc.v(1) - char_data.OCVdc.v(10);
    internal_resistance = abs(delta_V / 0.040);
    current_data_point = [CYCLE_TO_ASSESS, avg_temp, internal_resistance];
catch
    error('Data for the specified cell or cycle could not be found.');
end

% --- Step 3: Current Health Assessment using MLP Model ---
disp('Performing current health assessment with MLP model...');
normalized_data = mapminmax('apply', current_data_point', ps);
predicted_soh_percent = net(normalized_data) * 100;

% --- Step 4: Generate a Realistic Future Prognosis ---
disp('Generating a realistic future prognosis...');
future_cycles = CYCLE_TO_ASSESS:100:CYCLE_TO_ASSESS+5000;
a = -0.0000003;
b = -0.002;
c = predicted_soh_percent/100 - (a*CYCLE_TO_ASSESS^2 + b*CYCLE_TO_ASSESS);
soh_trajectory = (a*future_cycles.^2 + b*future_cycles + c) * 100;

% --- Step 5: Calculate RUL and Other Key Metrics ---
disp('Calculating RUL, Economic Value, and Environmental Impact...');
idx_rul = find(soh_trajectory <= second_life_eol_threshold, 1, 'first');
if ~isempty(idx_rul)
    rul_cycles = future_cycles(idx_rul) - CYCLE_TO_ASSESS;
else
    rul_cycles = NaN;
end
remaining_kWh = (nominal_cell_capacity_Ah * nominal_cell_voltage / 1000) * (predicted_soh_percent / 100);
second_life_value = remaining_kWh * price_per_kWh_used;
co2_saved = remaining_kWh * co2_saved_per_kWh;

% --- Step 6: Generate and Export Final Report ---
report_text = generate_text_report(current_data_point, predicted_soh_percent, rul_cycles, second_life_value, co2_saved, ev_eol_threshold, second_life_eol_threshold);
disp(report_text);
generate_visual_report(predicted_soh_percent, future_cycles, soh_trajectory, rul_cycles, ev_eol_threshold, second_life_eol_threshold);
disp('Visual report has been generated in a new figure window.');
fileID = fopen(['battery_report_cell', num2str(CELL_TO_ASSESS), '_cycle', num2str(CYCLE_TO_ASSESS), '.txt'],'w');
fprintf(fileID, '%s', report_text);
fclose(fileID);
```

```matlab
disp('Report saved to a unique text file.');

% --- Helper Functions ---
function report_str = generate_text_report(inputs, soh, rul, value, co2, ev_eol, s_eol)
    header = sprintf('\n==================================================\n   *** BATTERY PROGNOSTIC & DECISION SUPPORT REPORT ***\n==================================================\n');
    gen_time = sprintf('Generated on: %s\n', datestr(now));
    input_params = sprintf('\n--- INPUT PARAMETERS ---\n - Cycle Number: %d\n - Average Temperature: %.1f C\n - Internal Resistance: %.4f Ohms\n', inputs(1), inputs(2), inputs(3));
    predict_result = sprintf('\n--- CURRENT HEALTH ASSESSMENT (via MLP Model) ---\n - Estimated State of Health (SOH): %.2f %%\n', soh);
    if soh >= ev_eol
        grade = 'A (First Life)'; status = 'Healthy for EV use.'; rec = 'Continue normal operation.';
    elseif soh >= s_eol
        grade = 'B (Second Life Candidate)'; status = 'Retired from EV use.'; rec = 'Repurpose for "Second Life" to prevent e-waste.';
    else
        grade = 'C (Recycling Candidate)'; status = 'End of usable life.'; rec = 'Prioritize for responsible recycling.';
    end
    recommendation = sprintf('\n--- GRADING & RECOMMENDATION ---\n - GRADE: %s\n - STATUS: %s\n - RECOMMENDATION: %s\n', grade, status, rec);
    rul_section = sprintf('\n--- FUTURE PROGNOSIS (until %.0f%% SOH) ---\n', s_eol);
    if ~isnan(rul)
        rul_data = sprintf(' - Estimated Remaining Useful Life (RUL): ~%d Cycles\n', rul);
    else
        rul_data = sprintf(' - Estimated Remaining Useful Life (RUL): Exceeds simulation window (>%d cycles remaining)\n', 5000);
    end
    impact_section = sprintf('\n--- E-WASTE REDUCTION IMPACT ASSESSMENT ---\n');
    impact_data = sprintf(' - Estimated Second-Life Market Value: $%.2f\n - Estimated Environmental Benefit: %.1f kg of CO2 emissions saved\n', value, co2);
    footer = sprintf('==================================================\n');
    report_str = [header, gen_time, input_params, predict_result, recommendation, rul_section, rul_data, impact_section, impact_data, footer];
end
```

```matlab

function generate_visual_report(soh, cycles, trajectory, rul, ev_eol, s_eol)
    figure('Name', 'Definitive Prognostic Report', 'Position', [100, 100, 1200, 600]);
    ax_fontsize = 12; title_fontsize = 14;
    subplot(2, 1, 1);
    barh(1, soh, 'FaceColor', [0.1, 0.6, 0.8], 'DisplayName', 'Current SOH'); hold on;
    xline(ev_eol, 'Color', [0.85, 0.33, 0.1], 'LineStyle', '--', 'LineWidth', 2.5, 'DisplayName', 'EV EoL (80%)');
    xline(s_eol, 'Color', [0.93, 0.69, 0.13], 'LineStyle', '-.', 'LineWidth', 2.5, 'DisplayName', 'Recycle Threshold (60%)');
    hold off;
    set(gca, 'YTick', [], 'FontSize', ax_fontsize);
    xlim([s_eol-5, 105]);
    xlabel('State of Health (%)', 'FontSize', ax_fontsize, 'FontWeight', 'bold');
    title('Current Health Assessment (MLP Model)', 'FontSize', title_fontsize, 'FontWeight', 'bold');
    grid on;
    text(soh - 10, 1, sprintf('%.2f %%', soh), 'FontWeight', 'bold', 'Color', 'white', 'FontSize', 12);
    legend('show', 'Location', 'southeast', 'FontSize', 11);

    subplot(2, 1, 2);
    plot(cycles, trajectory, 'Color', [0.1, 0.6, 0.8], 'LineWidth', 2.5, 'DisplayName', 'Predicted Degradation Path'); hold on;
    plot(cycles(1), soh, 'ro', 'MarkerSize', 12, 'MarkerFaceColor', 'r', 'DisplayName', 'Current State');
    yline(s_eol, 'Color', [0.93, 0.69, 0.13], 'LineStyle', '-.', 'LineWidth', 2.5, 'HandleVisibility','off');
    text(cycles(end), s_eol, 'Recycle Threshold (60%)', 'VerticalAlignment', 'bottom', 'HorizontalAlignment', 'right', 'FontSize', 10, 'Color', [0.93, 0.69, 0.13]);
    if ~isnan(rul)
        rul_cycle_point = cycles(1) + rul;
        plot_idx = find(cycles>=rul_cycle_point,1,'first');
        if ~isempty(plot_idx)
            plot([rul_cycle_point, rul_cycle_point], [s_eol, trajectory(plot_idx)], 'Color', [0.5, 0.5, 0.5], 'LineStyle', ':', 'LineWidth', 2, 'HandleVisibility','off');
            text(rul_cycle_point, s_eol + 5, sprintf('RUL: ~%d cycles', rul), 'HorizontalAlignment', 'center', 'FontWeight', 'bold', 'BackgroundColor', 'white', 'FontSize', 11, 'Color', 'k');
        end
```

```
    end
    hold off;
    ylim([s_eol-5, 105]); xlim([cycles(1), cycles(end)]);
    xlabel('Cycle Number', 'FontSize', ax_fontsize, 'FontWeight', 'bold');
    ylabel('Predicted SOH (%)', 'FontSize', ax_fontsize, 'FontWeight', '
   bold');
    title('Future Prognosis & RUL (Demonstration Model)', 'FontSize',
   title_fontsize, 'FontWeight', 'bold');
    grid on;
    legend('show', 'Location', 'northeast', 'FontSize', 11);
end
```

Listing A.3: *MATLAB code for the final user-friendly report generator.*