Polytechnic of Leiria
School of Technology and Management
Department of Electrical Engineering
Bachelor's Degree in Electrical and Computer Engineering

BATTAIHEALTH
BATTERY CONDITION ESTIMATION IN AUTOMOTIVE AND RAILWAY APPLICATIONS USING AI

PEDRO ANDRÉ SILVA FERREIRA

Leiria, Junho de 2025

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Final report of the Project Curricular Unit of the Bachelor's Degree in Eletrotechnical and Computers Engineering, branch of Eletronics and Computers.

PEDRO ANDRÉ SILVA FERREIRA
N: 2222035

Work done under the guidance of Professor Luís Conde Bento (luis.conde@ipleiria.pt) and Professor Mónica Figueiredo (monica.figueiredo@ipleiria.pt).

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RESUMO

A estimativa precisa do Estado de Saúde (SoH), Estado de Carga (SoC) e Vida Útil Restante (RUL) das baterias é crucial para aplicações automóveis e ferroviárias, dado o papel essencial das baterias na eficiência energética e fiabilidade dos sistemas de transporte. A gestão eficaz destes parâmetros pode prevenir falhas inesperadas, otimizar os ciclos de carga e descarga, e prolongar a vida útil das baterias, contribuindo assim para uma redução significativa nos custos operacionais e ambientais. A Inteligência Artificial (IA) tem mostrado grande potencial na tarefa de estimar SoH, SoC e RUL das baterias. Algoritmos de machine learning e redes neuronais podem analisar grandes volumes de dados históricos e em tempo real, identificando padrões complexos que são difíceis de detectar com métodos tradicionais. A aplicação de IA permite uma previsão mais precisa e adaptativa das condições da bateria, melhorando a segurança e a eficiência operacional em veículos automóveis e ferroviários. Os datasets utilizados para a estimativa de SoH, SoC e RUL de baterias incluem uma variedade de dados recolhidos de ciclos de carga e descarga, condições de temperatura, tensões, correntes e outros parâmetros relevantes. Estes dados podem ser obtidos a partir de testes laboratoriais controlados, bem como de operações reais em campo. A qualidade e a abrangência dos datasets são essenciais para o treino eficaz dos modelos de IA, garantindo que eles possam generalizar bem para diferentes tipos de baterias e condições de operação. O desenvolvimento deste projeto envolve várias etapas-chave. Inicialmente, serão identificados os datasets e pré-processados os dados relevantes das baterias. Em seguida, serão desenvolvidos e treinados modelos de IA utilizando técnicas de machine learning supervisionado e não supervisionado. A validação dos modelos será realizada através de testes exaustivos com datasets distintos, assegurando a sua robustez e precisão. Finalmente, será implementado um sistema protótipo capaz de estimar em tempo real o SoH, SoC e RUL das baterias, com o objetivo de ser integrado em aplicações automóveis e ferroviárias, promovendo a inovação e a sustentabilidade nos sistemas de transporte.

ABSTRACT

Escrever o resumo em inglês.

INDEX

LIST OF FIGURES

LIST OF TABLES

LIST OF ACRONYMS

CNN Convolutional Neural Network

EFK Extended Kalman Filter

LSTM Long Short-Term Memory

SOC State of Charge

SOH State of Health

1

INTRODUCTION

2 BACKGROUND MATERIAL AND SUPPORTING TECHNOLOGIES

This chapter presents the foundational background material and supporting technologies that were used in the project. The first section covers the core theoretical concepts fundamental to battery health monitoring, including detailed explanations of key battery parameters such as State of Charge (SoC), State of Health (SoH), and Remaining Useful Life (RUL). Additionally, we cover the essential evaluation metrics used to assess model performance and provide an in-depth discussion of battery degradation mechanisms that directly impact health estimation accuracy. The chapter also addresses the technical challenges inherent in battery health monitoring, from the complexity of electrochemical processes to the practical difficulties of real-world implementation. The second section introduces the comprehensive suite of software tools and platforms that facilitated the research and development process, from hyperparameter optimization and experiment tracking to data visualization and version control. This comprehensive background establishes the technical foundation necessary for understanding the methodologies and results presented in subsequent chapters.

2.1 CORE CONCEPTS

This section covers the core theoretical concepts fundamental to battery health monitoring, including detailed explanations of key battery parameters, evaluation metrics, degradation mechanisms, and technical challenges. Battery technology serves as the foundation for energy storage systems across numerous applications, from portable electronics to electric vehicles and grid-scale storage. Modern batteries primarily fall into several categories, including lithium-ion, lead-acid, nickel-metal hydride, and flow batteries, each with distinct electrochemical properties, energy densities, and lifecycle characteristics. The health of these batteries is characterized by parameters such as state of charge

(SoC), state of health (SoH), capacity fade, internal resistance, and degradation rates, which collectively determine performance and longevity. Monitoring these parameters presents unique challenges due to the complex, nonlinear relationships between observable measurements and underlying battery conditions. Artificial intelligence and machine learning approaches offer powerful solutions to these challenges by enabling pattern recognition across multidimensional battery data. Supervised learning algorithms can predict remaining useful life, while unsupervised methods can detect anomalies indicative of impending failure. Deep learning architectures, particularly recurrent neural networks and transformers, have demonstrated exceptional capability in extracting temporal patterns from battery operational data, making them especially valuable for health prognostics in dynamic usage scenarios.

Time Series and Spectral Analysis of Battery Data

Time series analysis focuses on the temporal evolution of battery parameters such as voltage, current, and SoC, modeling and forecasting battery behavior, identifying trends, and detecting anomalies in the time domain. A comprehensive time series analysis framework decomposes battery data into three fundamental components that reveal distinct patterns in battery behavior and degradation processes.

Trend Component represents the long-term directional movement in battery parameters over extended periods, capturing the underlying degradation trajectory that reflects fundamental changes in battery chemistry and structure. In battery health monitoring, trend analysis reveals capacity fade patterns, where SoH exhibits a gradual declining trend over hundreds or thousands of charge-discharge cycles due to irreversible electrochemical processes such as SEI layer growth and active material loss. The trend component is particularly valuable for RUL prediction, as it provides insights into the rate of degradation and helps establish baseline expectations for battery performance decline under specific operational conditions.

Seasonal/Cyclic Component identifies recurring patterns that occur at regular intervals within battery operational data, reflecting periodic influences such as daily usage cycles, temperature variations, or charging schedules. In automotive applications, seasonal patterns may manifest as daily driving patterns that affect SoC fluctuations, while in stationary energy storage systems, seasonal components often correspond to diurnal energy demand cycles or seasonal temperature variations that influence battery efficiency and capacity. These cyclic patterns are essential for understanding how external factors systematically influence battery behavior and for developing models that can account for predictable variations in performance.

Irregular/Noise Component encompasses random fluctuations and unpredictable variations that cannot be attributed to trend or seasonal patterns, including measurement noise, sudden load changes, and stochastic environmental factors. In battery monitoring systems, irregular components may arise from sensor precision limitations, electromagnetic interference, sudden acceleration events in vehicles, or unexpected temperature spikes. While these components represent uncertainty in the data, proper characterization of noise patterns is crucial for developing robust estimation algorithms that can distinguish between genuine battery state changes and measurement artifacts.

Complementing this temporal approach, spectral analysis is a frequency-domain technique that characterizes the dynamic behavior of battery systems by decomposing time-series data into its frequency components, revealing periodic patterns, noise characteristics, or system resonances that may not be evident in the time domain. **Cascade spectrum analysis** can be integrated with traditional spectral methods to provide multi-resolution frequency domain decomposition, enabling the identification of both broad-band and narrow-band frequency characteristics across different temporal scales. This cascaded approach is particularly valuable for battery applications where degradation mechanisms operate at multiple frequency ranges, from high-frequency electrochemical impedance variations to low-frequency capacity fade trends, allowing for comprehensive characterization of battery dynamic behavior across the entire operational frequency spectrum. Together, these analytical frameworks provide comprehensive insights into battery degradation, thermal effects, and electrochemical processes across both temporal and frequency domains.

State of Charge (SoC)

The State of Charge represents the amount of energy remaining in a battery relative to its maximum capacity. It can be expressed as:

$$\text{SoC} = \frac{\text{Remaining Charge or Energy}}{\text{Maximum Charge or Energy Capacity}} \times 100\% \tag{1}$$

However, due to the chemical complexity of batteries and variations among individual cells, the SoC is always an approximate estimate. One factor contributing to the nonlinearity in its estimation is the formation of impurity layers in the pores of the electrodes. When these pores are blocked by impurities, electron movement is hindered, leading to irregular voltages and currents.

State of Health (SoH)

The State of Health reflects the battery's ability to store and deliver energy compared to its original specifications. It can be expressed as:

$$\text{SoH} = \frac{\text{Current Maximum Capacity}}{\text{Original Maximum Capacity}} \times 100\% \tag{2}$$

The nonlinearity in SoH estimation primarily arises from the progressive degradation of electrode materials. As impurities accumulate in the electrode pores, the available surface area for electrochemical reactions decreases, reducing the battery's effective capacity. This process is highly dependent on the number of charge/discharge cycles and operational conditions, making it difficult to model SoH linearly over time.

Remaining Useful Life (RUL)

The Remaining Useful Life quantifies the number of cycles remaining before the battery's performance degrades below a specified threshold. It can be expressed as:

$$\text{RUL} = \text{Total Expected Useful Life} - \text{Current Age} \tag{3}$$

Predicting RUL is particularly challenging due to the accumulation of impurities in the electrode pores. As the pores become obstructed, the degradation rate accelerates, leading to a sudden drop in battery performance. This nonlinear dynamic makes it difficult to accurately predict the exact point at which the battery will reach its end of useful life.

Mean Absolute Error (MAE)

The Mean Absolute Error measures the average magnitude of errors in a set of predictions, without considering their direction. It is calculated as:

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n} |y_i - \hat{y}_i| \tag{4}$$

where y_i is the actual value, $\hat{y}_i$ is the predicted value, and n is the number of observations. MAE is intuitive and robust to outliers, as it does not square the errors, but it does not penalize larger errors as heavily as other metrics. This makes it less sensitive to extreme deviations in predictions, which can be a limitation in contexts like battery performance where large errors may indicate critical failures.

Mean Squared Error (MSE)

The Mean Squared Error quantifies the average of the squared differences between predicted and actual values. It is expressed as:

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \tag{5}$$

MSE emphasizes larger errors due to the squaring of differences, making it sensitive to outliers. In battery modeling, this can be useful for detecting significant deviations in predictions of parameters like State of Charge or State of Health, but its sensitivity to outliers may amplify the impact of irregular data points caused by factors like electrode impurities or sensor noise.

Root Mean Squared Error (RMSE)

The Root Mean Squared Error is the square root of the MSE, providing an error metric in the same units as the original data. It is defined as:

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} (y_i - \hat{y}_i)^2} \tag{6}$$

RMSE balances the emphasis on larger errors from MSE while being more interpretable due to its unit consistency with the data. In battery applications, RMSE is often used to evaluate prediction accuracy for metrics like SoC or RUL, but its sensitivity to outliers can be a drawback when dealing with nonlinear degradation patterns caused by electrode pore blockages.

Mean Absolute Percentage Error (MAPE)

The Mean Absolute Percentage Error measures the average percentage error between predicted and actual values. It is calculated as:

$$\text{MAPE} = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i}\right| \times 100\% \tag{7}$$

MAPE is useful for comparing prediction accuracy across datasets with different scales, as it normalizes errors relative to the actual values. However, it can become problematic when actual values are close to zero, as in some battery SoC scenarios, leading to large percentage errors. Additionally, its reliance on relative errors may mask significant absolute deviations in critical battery performance metrics.

Neural Networks and Deep Learning Fundamentals

Neural Networks (NNs) are computational models inspired by the architecture and dynamics of networks of neurons in the brain, capable of performing various tasks such as classification, translation, prediction, and data generation. These networks possess the remarkable ability to learn from data through a process called training, where the network receives input-output pairs and adjusts its internal parameters, known as weights and activations, to minimize the loss function. The loss represents the difference between the network's predicted outputs and the true outputs, with various optimization algorithms such as gradient descent or stochastic gradient descent guiding the training process by iteratively updating the network's parameters to improve performance. Beyond their fundamental learning capabilities, neural networks demonstrate a crucial ability to generalize from training data to new, unseen data, achieved through the use of non-linear activation functions and regularization techniques that enable them to learn complex relationships between inputs and outputs.

Neural network methodologies can be broadly categorized into two main paradigms: **traditional machine learning methods** and **deep learning methods**. Traditional machine learning approaches, such as Support Vector Machines, Random Forests, and shallow neural networks, typically require manual feature engineering and domain expertise to extract relevant characteristics from raw data, demanding significant preprocessing effort and domain knowledge. In contrast, **deep learning methods** employ multi-layered neural networks that can automatically learn hierarchical feature representations directly from raw input data, eliminating the need for manual feature extraction and enabling end-to-end learning. Figure 1 illustrates this fundamental distinction between traditional neural networks and deep learning architectures, highlighting the increased complexity and hierarchical feature learning capabilities of deep learning systems.

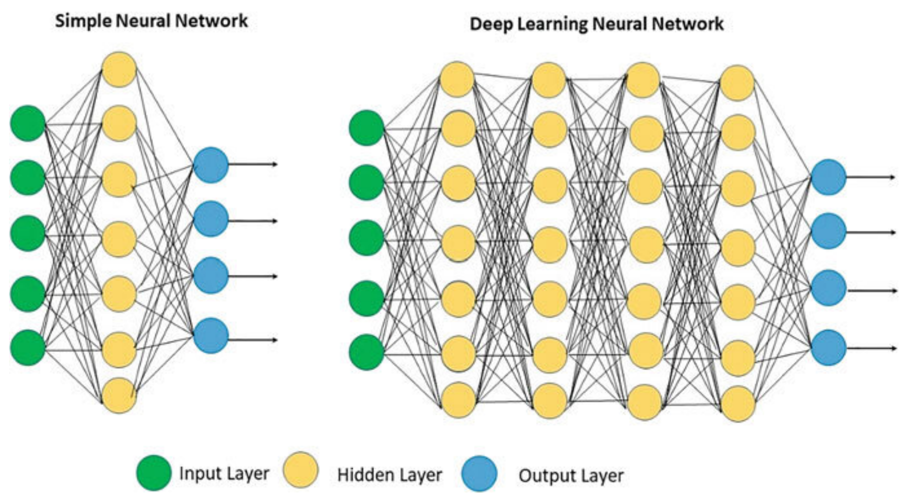

Figure 1: Comparison between traditional neural networks (left) and deep learning architectures (right), illustrating the difference in complexity and hierarchical feature learning capabilities.

Deep learning architectures consist of multiple hidden layers, each containing numerous artificial neurons (nodes) that process information through weighted connections. Each neuron receives inputs, applies a weighted sum followed by an activation function (such as ReLU, sigmoid, or tanh), and passes the result to subsequent layers. This layered structure enables the network to learn increasingly complex and abstract representations, with early layers capturing low-level features and deeper layers combining these into high-level patterns. The depth of these networks allows them to model intricate, non-linear relationships that are particularly valuable for complex temporal data such as battery degradation patterns.

For this project, the deep learning approach was specifically adopted due to its superior ability to capture complex temporal patterns inherent in battery degradation data and its capacity to handle the high-dimensional, sequential nature of battery health monitoring without requiring extensive domain-specific preprocessing or manual feature design. Deep learning excels in battery applications because it can automatically discover relevant features from raw sensor measurements (voltage, current, temperature) and learn the subtle, non-linear relationships between these measurements and battery health states. The hierarchical feature learning capability is particularly important for battery data, where degradation patterns manifest across multiple time scales and involve complex interactions between electrochemical processes. Furthermore, deep learning architectures such as recurrent neural networks (RNNs), Long Short-Term Memory (LSTM) networks, and Transformers are specifically designed to handle sequential data, making them ideal for modeling the temporal dependencies present in battery operational data and predicting future health states based on historical patterns.

Deep Learning Training Parameters and Optimization

Understanding key training parameters is crucial for developing effective battery state estimation models. **Epochs** represent complete passes through the training dataset, where 50–500 epochs are typical for battery data, carefully balancing the risk of underfitting with too few iterations against overfitting with excessive training on temporal sequences. **Batch Size** determines the number of samples processed simultaneously, where smaller batches (16–32) excel at capturing nonlinear patterns in battery behavior, while larger batches (128–256) provide more stable gradients but may struggle with the irregular nature of real-world battery data.

Patience in early stopping mechanisms defines how many epochs to wait without validation improvement before terminating training, with values of 5–20 epochs proving effective at preventing overfitting while allowing models sufficient time to generalize across different battery systems and operational conditions. **Learning Rate** controls the magnitude of parameter adjustments during training, requiring careful tuning for battery degradation patterns: rates too high (>0.01) risk missing subtle degradation signals, while rates too low (<0.0001) result in painfully slow convergence and potentially incomplete learning.

Optimizers play a critical role in training efficiency, with the Adam optimizer commonly chosen for its adaptive learning rate capabilities, while SGD with momentum provides more stable convergence but demands additional hyperparameter tuning specifically for battery applications. **Regularization** techniques, including L1/L2 regularization and dropout, become particularly important when working with limited battery datasets, especially when training data originates from only a few battery types or specific operational conditions.

Loss Functions must be carefully selected based on the specific task: MSE for regression problems like SoC and capacity prediction, MAE when robustness against outliers is paramount, cross-entropy for classification tasks such as fault detection, and custom loss functions that can elegantly incorporate domain-specific knowledge about battery behavior. Finally, **Validation** strategies require special consideration in battery applications, where time-based splitting ensures models are tested on genuinely future data, and cross-validation procedures must account for the inherent temporal dependencies present in battery degradation sequences.

Battery Degradation and Capacity Fade

Battery degradation refers to the gradual loss of a battery's ability to store and deliver energy, driven by chemical reactions, temperature fluctuations, charge/discharge cycles, and aging. This degradation manifests as capacity fade, resulting in reduced device runtime or diminished electric vehicle driving range. The key mechanisms contributing to this degradation include several interconnected processes. **Solid Electrolyte Interphase (SEI) Growth** occurs when a layer forms on the anode, consuming lithium ions and reducing capacity. This process is accelerated at high temperatures and currents, leading to an initial irreversible capacity loss of approximately 10% during formation cycles. **Lithium Plating** represents another critical mechanism where, at low temperatures or high charge rates, lithium deposits on the anode, forming "dead lithium" that contributes to irreversible capacity loss and increases safety risks. **Particle Fracture** results from mechanical stress during cycling, causing cracks in electrode materials that reduce active material availability and exacerbate capacity decline. **Positive Electrode (PE) Decomposition** involves structural changes in the cathode, such as spinel/rock salt phase formation, which degrade performance and contribute to active material loss. Finally, **Impedance Increase** manifests as rising interfacial resistance, predominantly at the positive electrode, which limits efficient charge transfer and indirectly reduces usable capacity. After 800 cycles, electrode resistance can increase tenfold, significantly impacting battery performance.

2.1.1 *Capacity Fade*

The [18] paper studies and explains very well the capacity fade refers to the progressive decline in a lithium-ion battery's ability to store energy, manifesting as reduced device runtime or diminished electric vehicle driving range. This phenomenon is driven by several key mechanisms:

Studies report capacity losses ranging from 12.4% to 32% after 500–800 cycles, corresponding to an average loss of 0.025–0.05% per cycle [18].

Internal Resistance Degradation in Lithium-Ion Batteries

As lithium-ion batteries age, their internal resistance increases, adversely affecting power delivery, charging efficiency, and thermal management. This degradation is particularly pronounced during calendar ageing, as detailed in the study by [13] on LFP/C-based batteries. The primary mechanisms contributing to this increase involve several interconnected processes. **Solid Electrolyte Interface (SEI) Growth** is characterized by the thickening of the SEI layer on the graphite anode over time, reducing Li^+ ion permeability. This growth follows a power law dependence (approximately $t^{0.8}$) and is accelerated at high temperatures and high state-of-charge (SOC) levels, leading to increased resistance and contact loss within the anode. **Lithium Plating** involves the deposition of metallic lithium on the anode, which clogs electrode pores, impeding ion transport and elevating resistance, particularly under high SOC conditions. **Cathode Structural Degradation** occurs at the LFP cathode, where binder decomposition, oxidation of conductive agents, and corrosion of current collectors reduce inter-particle conductivity, contributing to resistance increase, especially at elevated temperatures. Additionally, **Electrolyte Decomposition** produces decomposition products that form resistive surface layers on both electrodes, further increasing internal resistance, with effects amplified at high temperatures and SOC levels.

The study demonstrates that internal resistance increases nonlinearly with storage time, with exponential acceleration due to higher storage temperatures (e.g., 55°C) and SOC levels (e.g., 90%). For instance, after 20 years at 25°C and 50% SOC, resistance may rise by approximately 71%, doubling at 100% SOC. This increased resistance results in slower charging, diminished power output, and accelerated degradation due to enhanced heat generation, impacting battery performance and lifespan.

Battery Health Monitoring

Battery health monitoring is critical for ensuring reliability, safety, and longevity of battery systems. Monitoring involves assessing key parameters such as the state of charge and the state of health (SoH), which provide essential insights into battery performance and remaining operational capacity.

Technical Challenges

The technical challenges in monitoring battery health arise from the complex nature of battery systems and the difficulties in accurately estimating SOC and SOH.

Complexity of Battery Chemistry

Batteries, particularly lithium-ion batteries, have intricate internal chemistries that are difficult to model and monitor. Factors such as temperature, charge-discharge rates, and depth of discharge influence degradation, making accurate SOH estimation challenging. The nonlinear and complex degradation processes vary with usage conditions, environmental factors, and battery design, complicating predictive modeling.

Measurement Difficulties

Measuring individual battery parameters, such as internal resistance, temperature, and voltage, is technically challenging, especially in real-time applications. This requires precise sensors and sophisticated equipment, which may not be feasible in real-world scenarios. For instance, accurately measuring internal resistance or temperature in a moving vehicle is far more complex than in a controlled lab environment.

Modeling and Estimation

rever isto !!!

Developing accurate models for SOH estimation is complex. Electrochemical models, which simulate battery behavior based on physical and chemical principles, require extensive computational resources and detailed parameter inputs (e.g., electrolyte properties, reaction rates). Semi-empirical models often oversimplify electrochemical processes, reducing their effectiveness under extreme conditions. Equivalent circuit models (ECMs) may lack precision during high-rate charging/discharging or extreme temperatures due to their simplified nature.

Limitations of Data-Driven Methods

Data-driven approaches, such as machine learning techniques (e.g. Support Vector Regression, Gaussian Process Regression, Artificial Neural Networks), rely on large, high-quality datasets, which can be difficult to obtain. These methods also lack physical interpretability, making it difficult to understand their predictions. Additionally, issues like overfitting and high computational demands pose challenges for real-time applications.

Complexity of Hybrid Methods

Hybrid approaches, which combine model-based and data-driven methods, can improve accuracy but increase system complexity and computational costs. Interpreting errors in these systems remains a challenge, requiring further research to enhance transparency and efficiency.

Laboratory vs Real World Conditions

There is a significant discrepancy between laboratory-simulated conditions and actual operational environments. Laboratory settings often use sophisticated equipment that is not available in real-world applications, limiting the applicability of monitoring methods. For example, real-world conditions like varying temperatures or road vibrations are difficult to replicate in a lab, affecting SOH estimation accuracy.

Real-Time Monitoring

Achieving real-time, reliable SOH monitoring is crucial for safety-critical applications but is technically demanding. Battery management systems (BMS) must balance accuracy with computational efficiency to provide timely insights without overloading system resources.

Environmental Factors

Batteries are sensitive to environmental conditions such as temperature, humidity, and vibration. Monitoring systems must account for these factors, which can significantly impact battery health and performance. For example, high temperatures can accelerate battery degradation, while low temperatures may reduce capacity, complicating health estimation.

Cost of Monitoring Systems

Implementing sophisticated battery health monitoring systems can be expensive, both in terms of initial setup and ongoing maintenance. This includes the cost of sensors, data storage, and computational infrastructure, which can be prohibitive for smaller organizations or applications.

Data and Computational Costs

AI and data-driven methods require significant computational resources and high-quality data, which can be costly to acquire and process. The high demand for data and computing power presents challenges, particularly for real-time monitoring applications and edge devices.

2.2 SUPPORTING TECHNOLOGIES

This section describes the comprehensive suite of software tools and platforms that facilitated the research and development process, including analytical frameworks, optimization tools, and development environments.

Optuna

Optuna is an open-source hyperparameter optimization framework used to search for the best hyperparameters in machine learning models [1]. It employs efficient algorithms like Tree-structured Parzen Estimator (TPE) to systematically explore hyperparameter spaces, supporting parallel and distributed optimization. In this work, Optuna was utilized to automate the tuning process, enhancing model performance by identifying optimal hyperparameter configurations with reduced manual effort.

Weights and Biases (WandB)

Weights & Biases (WandB) is a machine learning platform designed for experiment tracking and visualization [15]. It enables real-time logging and monitoring of training metrics, hyperparameters, and model outputs. In this study, WandB was employed to keep track of training processes and visualize losses, providing interactive dashboards to analyze experiments, debug models, and ensure reproducible workflows across iterations.

PlotJuggler

PlotJuggler is an open-source time series visualization tool designed for fast, intuitive, and extensible data analysis [8]. It features a user-friendly drag-and-drop interface, enabling efficient visualization of large datasets, both offline and in real-time. In this work, PlotJuggler was highly effective for exploring and analyzing data within datasets, allowing for the visualization of time series, identification of patterns, and application of transformations like derivatives or moving averages through its Transform Editor. Its compatibility with formats such as CSV, ROS, and MQTT, along with plugin extensibility, made it a valuable tool for detailed data inspection and analysis.

Orange Data Mining

Orange Data Mining is an open-source data visualization and analysis platform designed for exploratory data analysis and machine learning workflows [4]. It provides a visual programming interface with drag-and-drop widgets that enable users to build data analysis pipelines without extensive coding. Orange offers comprehensive tools for data preprocessing, feature selection, correlation analysis, and outlier detection through interactive visualizations and statistical methods. In this work, Orange was instrumental for exploring correlations within battery datasets and identifying outliers that could potentially skew model performance. Its intuitive interface allowed for rapid prototyping of data cleaning pipelines, enabling efficient removal of anomalous data points while preserving the integrity of temporal relationships in battery time series data. The platform's correlation analysis capabilities were particularly valuable for understanding feature relationships and selecting relevant variables for subsequent machine learning models.

Git Version Control

Git is a distributed version control system designed to handle projects of all sizes with speed and efficiency [9]. It tracks changes in source code and files during software development, enabling multiple contributors to work on the same project simultaneously while maintaining a complete history of modifications. Git provides features such as branching, merging, and distributed workflows that facilitate collaborative development and experimentation. In this work, Git was employed to ensure robust version control throughout the research process, maintaining a comprehensive history of code changes, experimental iterations, and documentation updates. All project files, including machine learning models, data processing scripts, and analysis notebooks, were systematically committed and pushed to GitHub repositories. This approach guaranteed that all work was safely preserved, enabled rollback to previous versions when needed, and facilitated reproducible research by maintaining clear documentation of the project's evolution and experimental milestones.

PyTorch

PyTorch is an open-source machine learning framework developed by Facebook's AI Research lab, designed for deep learning applications with a focus on flexibility and ease of use [2]. It provides dynamic computational graphs, allowing for intuitive model development and debugging through its eager execution model. PyTorch features automatic differentiation capabilities through its autograd system, enabling efficient gradient computation for backpropagation in neural networks. The framework supports GPU acceleration through CUDA, making it suitable for training large-scale models efficiently.

PyTorch was specifically chosen over TensorFlow for this project due to several key advantages that align with the research requirements. **Research-oriented design** provides greater flexibility for implementing novel architectures and custom loss functions specific to battery degradation modeling, whereas TensorFlow's static graph approach can be more restrictive for experimental work. Additionally, **superior community support** in the academic research community and **extensive documentation** for cutting-edge architectures made PyTorch the preferred choice for this research-focused project.

In this work, PyTorch served as the primary framework for developing and training deep learning models for battery health monitoring applications. PyTorch seamlessly integrates with other tools in the machine learning pipeline, such as Optuna for hyperparameter optimization and WandB for experiment tracking, creating a cohesive development environment that supports reproducible research workflows.

Conda Environments

Conda is an open-source package management and environment management system that simplifies the installation, running, and updating of packages and their dependencies [6]. It creates isolated environments where different versions of Python, libraries, and dependencies can coexist without conflicts, making it particularly valuable for this projects.This approach ensured that version conflicts between packages were avoided, enabled seamless collaboration across different development machines, and guaranteed that the exact software environment could be recreated for reproducibility.

3

STATE OF THE ART

The accurate estimation of SoC, SoH, and RUL is critical for optimizing battery performance in automotive and railway applications. These metrics underpin the reliability and efficiency of battery management systems (BMS), providing essential indicators for battery health monitoring and predictive maintenance planning. Traditional methods, such as Coulomb Counting and Kalman Filters, often struggle with nonlinearities and dynamic operating conditions. Recent advancements in Artificial Intelligence (AI), particularly machine learning and deep learning, offer promising solutions by capturing complex patterns in battery data. This chapter reviews the state of the art in SoC, SoH, and RUL estimation, focusing on AI-based approaches.

Traditional Methods for SoC, SoH, and RUL Estimation Traditional methods for battery state estimation can be categorized into physics-based and statistical approaches, each with inherent limitations.

Physics-Based Methods Physics-based methods model the electrochemical and electrical behavior of batteries. Key approaches include:

- **Equivalent Circuit Models (ECMs)**: Represent batteries using electrical components (e.g., resistors, capacitors) to simulate voltage and current dynamics. ECMs are computationally efficient but lack precision under varying conditions.
- **Electrochemical Models**: Simulate internal chemical reactions, offering high accuracy but requiring significant computational resources and detailed parameter knowledge.

Statistical Methods Statistical techniques rely on empirical data to estimate battery states. Common methods include:

- **Coulomb Counting**: Integrates current over time to estimate SoC. This method is sensitive to measurement errors and initial SoC inaccuracies.

- **Kalman Filters**: Use recursive algorithms to refine state estimates by combining model predictions with noisy measurements. While effective for linear systems, they struggle with the nonlinear dynamics of batteries.

These methods often fail to capture subtle variations in battery behavior under dynamic operating conditions, necessitating advanced approaches.

AI-Based Methods for Battery State Estimation AI-based methods leverage machine learning and deep learning to model complex, nonlinear relationships in battery data. This section reviews key approaches, datasets, and their applications in the contex of the project.

Machine Learning Techniques Supervised machine learning algorithms, such as Support Vector Machines (SVMs) and Random Forests, have been applied to predict SoC and SoH using features like voltage, current, and temperature. For instance, [14] demonstrates SVMs achieving high accuracy in SoH estimation (98.26%) for lead-acid batteries under controlled conditions. However, these methods require extensive feature engineering and struggle with temporal dependencies.

Deep Learning Architectures Deep learning models excel at capturing temporal and spatial patterns in battery data. Key architectures include:

- **Convolutional Neural Networks (CNNs)**: Extract spatial features from battery data, such as voltage profiles. Combining CNNs with Long Short-Term Memory (LSTM) units, as implemented in the [5] paper, enhances forecasting accuracy by modeling temporal dependencies.
- **Recurrent Neural Networks (RNNs) and LSTMs**: Designed for sequential data, LSTMs are particularly effective for RUL prediction, as they capture long-term degradation trends. Studies using the NASA Battery Dataset [11] report LSTM-based models outperforming traditional methods in RUL estimation as implemented in the [10].
- **Transformer Models**: Emerging in battery state estimation, transformers leverage attention mechanisms to model complex dependencies, showing promise in handling variable-length sequences [17].

Datasets for AI-Based Estimation The quality and diversity of datasets are critical for training robust AI models. Notable datasets include:

- **NASA Battery Dataset** [11]: Provides voltage, current, temperature, and impedance data under various operating conditions, widely used for SoC and RUL estimation due to its diversity.
- **CALCE Battery Dataset** [3]:
- **MATR Battery Dataset** [7]:
- **HKUST Battery Dataset** [12]:

These datasets highlight the importance of incorporating real-world operating conditions and diagnostic measurements to improve model generalizability.

Hybrid Approaches Hybrid models combine physics-based and data-driven methods to enhance accuracy. For example, [] integrates ECMs with neural networks to refine SoC estimates, leveraging physical constraints to reduce training data requirements. Such approaches are particularly relevant for railway applications, where operational conditions vary widely.

Challenges and Research Gaps Despite advancements, several challenges persist in battery state estimation:

- **Data Requirements**: AI models, particularly deep learning, require large, diverse datasets, which are often limited or proprietary .
- **Operational Variability**: Battery performance varies due to temperature, load profiles, and aging, complicating model generalization .
- **Computational Complexity**: Real-time estimation in automotive and railway systems demands low-latency models, a challenge for complex deep learning architectures.
- **Lack of Standardized Datasets**: The absence of universal, open-source datasets for railway applications limits model benchmarking.

The *BattAIHealth* project addresses these gaps by developing AI models trained on both synthetic and real-world datasets, optimizing for robustness and real-time applicability in transportation systems.

Conclusion The state of the art in battery state estimation reveals a transition from traditional physics-based and statistical methods to AI-driven approaches. While machine learning and deep learning models, supported by datasets like the NASA Battery Dataset and Aging Dataset from EV, offer superior accuracy, challenges such as data scarcity and operational variability persist. This project builds on these advancements by developing robust AI models tailored for automotive and railway applications, aiming to enhance BMS reliability and efficiency.

4

DEVELOPMENT

4.1 INTRODUCTION

This chapter details the development phases of the battery health prediction system, encompassing the complete progression from initial MATLAB modeling to advanced deep learning implementation. The project evolved through distinct phases: (1) MATLAB-based modeling and simulation using traditional methods, (2) exploration of hybrid neural network approaches, (3) transition to pure data-driven models, and (4) implementation of state-of-the-art deep learning architectures for time series forecasting.

The development process was guided by the need to create accurate, robust, and scalable battery health prediction models capable of handling real-world applications. Each phase built upon lessons learned from previous approaches, ultimately leading to the implementation of TimesNet, a cutting-edge time series analysis architecture that demonstrates superior performance in battery degradation prediction tasks.

4.2 MATLAB MODELING AND SIMULATION

The initial development phase focused on implementing traditional battery modeling approaches in MATLAB to establish baseline performance and understand the fundamental characteristics of battery degradation patterns.

Kalman Filter Implementation

The Extended Kalman Filter (EFK) was implemented as the primary estimation algorithm for SOC and SOH prediction. The EFK approach was chosen for its proven effectiveness in handling the nonlinear dynamics of battery systems and its ability to provide uncertainty quantification.

Coulomb Counting Integration

Coulomb counting was integrated as a complementary method for SOC estimation, providing a reference baseline for comparison with the Kalman filter results. The implementation addressed several critical considerations to ensure accuracy and reliability. **Current integration accuracy and drift compensation** were prioritized to minimize cumulative errors that could significantly impact SOC estimates over extended periods. **Temperature effects on coulombic efficiency** were carefully analyzed, as thermal variations can substantially alter the charge-discharge efficiency and affect the accuracy of capacity calculations. **Aging effects on capacity estimation** were incorporated to account for the gradual degradation of battery capacity over operational lifetime, ensuring that SOC estimates remain accurate as the battery ages. Finally, **calibration procedures for initial SOC determination** were established to provide accurate baseline measurements, which are crucial for the cumulative nature of coulomb counting methods.

Batemo Model Integration

The Batemo battery model was incorporated to provide physics-based battery behavior simulation. This integration offered comprehensive capabilities for model development and validation. **Validation of estimation algorithms under controlled conditions** was enabled through the model's ability to simulate precise battery behaviors, allowing for systematic testing of algorithm performance across various operational scenarios. **Generation of synthetic data for algorithm testing** provided a valuable resource for training and evaluating neural networks when real-world data was limited or when specific degradation patterns needed to be studied. **Analysis of model sensitivity to various degradation mechanisms** was facilitated by the physics-based nature of the Batemo model, enabling detailed investigation of how different aging phenomena affect battery performance predictions. Additionally, **comparison between model-based and data-driven approaches** was made possible, allowing for comprehensive evaluation of different estimation methodologies and their respective strengths and limitations.

The MATLAB implementation served as a foundation for understanding battery dynamics and provided insights that informed subsequent neural network development phases.

4.3 NEURAL NETWORK DEVELOPMENT EVOLUTION

The neural network development process evolved through multiple iterations, each addressing specific limitations identified in previous approaches and incorporating lessons learned from the MATLAB modeling phase.

Initial CNN+LSTM Architecture

The first neural network implementation combined CNN with LSTM networks to leverage both spatial feature extraction and temporal sequence modeling capabilities.

Architecture Design

The CNN+LSTM architecture was structured to leverage the complementary strengths of both convolutional and recurrent neural networks. The design incorporated multiple specialized layers, each serving a distinct purpose in the feature extraction and temporal modeling pipeline. **CNN layers** were responsible for extracting local patterns and features from battery measurement sequences, identifying spatial relationships and important signal characteristics within the input data. **LSTM layers** focused on modeling long-term dependencies and temporal relationships, capturing the sequential nature of battery degradation and state evolution over time. Finally, **Dense layers** provided the final prediction mapping with appropriate activation functions, transforming the processed features into accurate SOC and SOH estimates.

Training Challenges and Limitations

Several significant challenges were encountered during the CNN+LSTM implementation that highlighted the complexity of applying deep learning to battery health monitoring. These obstacles required careful analysis and ultimately influenced the decision to pursue alternative approaches. **Gradient vanishing** emerged as a critical issue where long sequences caused training instability, preventing the network from effectively learning long-term dependencies essential for accurate battery state prediction. **Overfitting** presented another major concern, as the high model complexity led to poor generalization, with the network memorizing training patterns rather than learning transferable features applicable to new battery data. **Computational efficiency** posed practical limitations, with training time becoming prohibitively long for large datasets, making the approach unsuitable for real-world applications requiring timely model updates. Additionally,

Feature engineering proved challenging, as manual feature selection proved suboptimal, requiring extensive domain expertise and iterative refinement that limited the model's adaptability to different battery types and operating conditions.

Hybrid vs. Data-Driven Approach Evaluation

A systematic comparison was conducted between hybrid approaches (combining physics-based models with neural networks) and pure data-driven methods.

Hybrid Approach Implementation

The hybrid approach integrated multiple complementary techniques to leverage both physics-based understanding and data-driven learning capabilities. This comprehensive strategy incorporated several key components designed to enhance prediction accuracy and reliability. **Physics-based model outputs as additional input features** provided domain-specific insights that enriched the neural network's understanding of battery behavior, incorporating fundamental electrochemical principles into the learning process. **Kalman filter estimates as regularization terms** helped constrain the neural network training by incorporating well-established state estimation techniques, reducing the likelihood of unrealistic predictions and improving model stability. Furthermore, **domain knowledge constraints in loss function design** ensured that the learned models respected known physical limitations and relationships, preventing the network from learning patterns that violated fundamental battery physics principles.

Data-Driven Approach Focus

The pure data-driven approach emphasized maximum utilization of machine learning capabilities while minimizing reliance on explicit domain knowledge. This methodology focused on allowing the neural network to discover patterns and relationships directly from the data. **End-to-end learning from raw sensor data** enabled the model to process unfiltered battery measurements, potentially capturing subtle patterns that might be lost during manual preprocessing or feature engineering steps. **Automatic feature extraction and representation learning** allowed the network to identify the most relevant characteristics for battery health prediction without requiring extensive domain expertise or manual feature design. Additionally, **minimal domain-specific preprocessing requirements** reduced implementation complexity and improved the method's adaptability to different battery types and measurement configurations, making it more suitable for diverse real-world applications.

Comparative Analysis Results

The evaluation revealed that data-driven approaches demonstrated **superior generalization** across different battery chemistries, **reduced dependency** on accurate physics model parameters, **better scalability** to large datasets, and **more robust performance** under varying operating conditions.

This analysis motivated the transition to advanced pure data-driven architectures.

4.4 DATASET COLLECTION AND PREPROCESSING

The dataset development process was crucial for training robust and generalizable models, requiring careful consideration of data quality, diversity, and preprocessing strategies.

Primary Dataset Selection

The primary dataset utilized in this work is the CALCE (Center for Advanced Life Cycle Engineering) battery dataset, obtained from the University of Maryland's public repository. This dataset was selected for its:

- Comprehensive cycle life data spanning multiple battery chemistries
- High-quality measurements with consistent sampling rates
- Well-documented experimental conditions and procedures
- Established use in battery research community for benchmarking

Data Cleaning and Preprocessing

Several preprocessing steps were implemented to ensure data quality and model training stability:

Cycle Removal and Filtering

- **Initial cycle removal**: The first charge-discharge cycle was removed from each battery file to avoid initialization artifacts and inconsistent starting conditions

- **Incomplete cycle filtering**: Cycles with insufficient data points or incomplete charge/discharge sequences were excluded from the training set
- **Outlier detection**: Statistical methods were applied to identify and remove measurement outliers that could negatively impact model training

Battery-level partitioning was employed to prevent data leakage, ensuring that cycles from the same battery appeared in only one partition.

Input Data Formatting

The input data structure was designed to optimize model performance:

- **Sequence length**: Fixed-length sequences of 100 time steps were extracted from continuous battery operation data
- **Feature vector**: Each time step included voltage, current, temperature, and derived features such as power and energy
- **Target variables**: State of Health (SOH) values were calculated based on capacity fade measurements
- **Sliding window**: Overlapping sequences were generated to maximize training data utilization

Limitations of Previous Approaches

The evaluation of CNN+LSTM and hybrid approaches revealed several critical limitations:

- **Temporal modeling constraints**: Traditional LSTM architectures struggled with very long sequences typical in battery degradation analysis
- **Multi-scale pattern recognition**: Difficulty in capturing both short-term fluctuations and long-term degradation trends simultaneously
- **Computational efficiency**: High computational requirements limited the scalability to large datasets
- **Generalization issues**: Poor performance when applied to battery chemistries or operating conditions not seen during training

Requirements for Advanced Architecture

The identified requirements for an improved architecture included:

- **Multi-periodicity detection**: Ability to automatically identify and exploit multiple periodic patterns in battery data
- **Long-range dependency modeling**: Effective capture of dependencies across extended time horizons
- **Parameter efficiency**: Reduced model complexity while maintaining or improving performance
- **Versatility**: Capability to handle various time series analysis tasks beyond just forecasting

These requirements led to the selection and implementation of TimesNet, a cutting-edge architecture specifically designed for general time series analysis.

4.5 UTILIZED MODEL (TIMESNET)

TimesNet is a state-of-the-art neural network architecture specifically designed for general time series analysis tasks [16]. This model addresses the fundamental challenge of temporal variation modeling by transforming the complex problem from 1D time series analysis into 2D space analysis. The key innovation of TimesNet lies in its ability to discover multi-periodicity patterns in time series data and decompose intricate temporal variations into intraperiod and interperiod variations.

The architecture works by converting 1D time series into a set of 2D tensors based on multiple identified periods. This transformation embeds intraperiod variations into the columns and interperiod variations into the rows of the 2D tensors, making temporal patterns more accessible for analysis through 2D convolution operations. The core component, TimesBlock, can adaptively discover multi-periodicity and extract complex temporal variations using parameter-efficient inception blocks.

TimesNet demonstrates superior performance across five mainstream time series analysis tasks: short-term and long-term forecasting, imputation, classification, and anomaly detection. This versatility makes it particularly suitable for battery health prediction tasks, where complex temporal dependencies and multi-scale patterns are crucial for accurate state-of-health estimation. The model's ability to handle various sequence lengths and its robust architecture for capturing temporal dynamics align well with the requirements of battery degradation modeling, where both short-term fluctuations and long-term trends must be considered simultaneously.

Architecture Adaptation for Battery Health Prediction

The TimesNet architecture was adapted for battery health prediction with several key modifications:

- **Input preprocessing**: Battery measurement sequences (voltage, current, temperature) were formatted to exploit the multi-periodicity detection capabilities
- **Output configuration**: Modified for regression tasks to predict continuous SOH values rather than classification outputs
- **Loss function**: Implemented Mean Squared Error (MSE) with additional regularization terms to prevent overfitting
- **Feature engineering**: Minimal manual feature engineering to leverage the model's automatic pattern discovery capabilities

4.6 MODEL OPTIMIZATION

For model optimization, the Optuna tool was utilized, which enables hyperparameter optimization for machine learning models, integrated with Weights & Biases (WandB), which allows for result visualization and model comparison.

Dataset Preparation for Optimization

For this test, the dataset was reduced to only 1/10 of the data, equally distributed from the original dataset, with the objective of reducing the time required for finding the best hyperparameters, since this process took approximately one week even with this reduction.

Optimization Process

For the hyperparameter search, 50 trials were performed, with 50 epochs each, using an early stopping patience of 5 epochs to avoid overfitting and accelerate the optimization process.

Optimized Parameters

The parameters that were optimized through Optuna include:

- **e_layers**: Number of encoder layers (1–3) — controls the depth of the encoder stack
- **d_layers**: Number of decoder layers (1–3) — controls the depth of the decoder stack
- **factor**: Expansion factor for the FFN (1–5) — controls the complexity of frequency components in TimesNet
- **freq**: Frequency for time features encoding ("s", "t", "h") — seconds, minutes, hours
- **d_model**: Model dimension (fixed at 16)
- **top_k**: Top-k dominant frequencies in TimesNet (1–5) — controls how many frequency components to consider

Parameter Importance Analysis

Through this optimization, it was possible to detect the importance of the hyperparameters. We observed that the importance factor of the **e_layers** parameter (number of encoder layers) is the parameter that most influences the result when changed, demonstrating that the depth of the encoder architecture is critical for model performance.

Best Trial Results

The most successful trial was trial 15, which presented the following results:

- **MSE Value**: 0.0015545075293630362
- **Optimal Parameters**:
  - e_layers: 2
  - factor: 4
  - d_model: 16

  - top_k: 9
  - n_heads: 16
- **Duration**: 7770232 ms (approximately 2 hours and 10 minutes)

The results show that using 2 encoder layers works better than deeper networks, likely avoiding overfitting on the battery dataset. The high expansion factor of 4 allows the model to capture more complex patterns, while setting top_k to 9 means the model considers more frequency components than the default range, which helps capture the various periodic behaviors in battery degradation cycles.

5 CONCLUSIONS

A apresentação das conclusões tem como objetivo realizar uma síntese, acompanhada de um conjunto de observações acerca do que foi escrito anteriormente.

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