Digital Twin Battery Storage in Energy Storage System

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A thesis submitted to Cardiff University

for the degree of Doctor of Philosophy

December 2024

Acknowledgements

First and foremost, I would like to express my heartfelt gratitude to my family for their unwavering support and encouragement throughout my academic journey. Their belief in my potential has been a source of strength and motivation during times of joy and difficulty. Their support, not only financially but also emotionally, has provided me with the stability and confidence to keep pushing forward. I am particularly indebted to my parents, who have always supported me. I also extend my sincerest thanks to my girlfriend, who has stood by me through thick and thin. Her understanding, care, and companionship have been invaluable, and her unwavering belief in me has provided immense emotional strength during challenging times.

Next, I would like to express my sincere appreciation to my supervisors: Prof Ying Liu, Prof Jianzhong Wu, Dr Wenlong Ming, and Dr Yue Zhou. Their mentorship and guidance have been critical in helping me navigate my academic pursuits and overcome various obstacles. I am truly grateful for their selfless dedication to my education and research. Their insights, feedback, and expertise have not only enhanced my knowledge and skills but have also inspired me to approach my work with greater passion and diligence. I am immensely grateful for their generous support and belief in my potential.

I would also like to extend my appreciation to my colleagues, lab mates, and friends who have accompanied me throughout this journey. Their camaraderie and shared experiences have made my academic life more vibrant and enjoyable. I am especially grateful for the friendships I have formed during this period; these relationships have provided me with much-needed balance and emotional support outside of my studies.

As I conclude this chapter of my academic journey, I am filled with immense gratitude for all the people who have contributed to my growth and success. I sincerely hope to continue making meaningful contributions in my field and to honour the trust and support that so many have shown me throughout these years.

Abstract

Battery Energy Storage Systems (BESS) play a key role in supporting the transition to renewable energy by providing stability to energy grids. However, the increasing complexity of managing BESS presents significant challenges regarding real-time monitoring, accurate state estimation, and predictive maintenance. Estimating key battery states, such as State of Charge (SOC), State of Health (SOH), and Remaining Useful Life (RUL), is important for enabling the operational efficiency and longevity of these systems. Traditional methods often struggle to account for the complex and dynamic behaviour of battery systems, leading to inefficiencies in decision-making and system performance. This thesis proposes a Digital Twin (DT)-driven approach to enhance decision support for BESS, focusing on improving the accuracy of battery state estimations and optimising system operations through the integration of real-time data with advanced analytical models.

The thesis begins by outlining the development of a DT framework tailored specifically for BESS. The proposed framework creates a digital model of the physical system, enabling continuous synchronisation of real-time data between the physical and digital environments. This integration allows for real-time updates of battery states, providing operators with a comprehensive view of system performance. The framework includes detailed data acquisition and preprocessing procedures, which are essential for keeping the accuracy of the DT model. Additionally, advanced deep learning algorithms are applied to enhance the framework's capacity for decision support. This approach provides a robust foundation for improving operational decision-making by offering insights into potential outcomes based on various operational scenarios.

Secondly, this thesis presents a detailed examination of battery state estimation methods, with a focus on advanced deep learning techniques. Temporal Convolutional Networks (TCN) and Long Short-Term Memory (LSTM) networks are used to estimate SOC and SOH, and predict RUL. These models are capable of processing both historical and real-time data, allowing them to adapt to dynamic changes in the operational environment. Compared to traditional methods, the TCN-LSTM model demonstrates improved accuracy in estimating battery states, which is critical for proactive maintenance and efficient resource allocation. The results of the experimental analysis validate the effectiveness of these models, highlighting their ability to provide reliable predictions that support the management of BESS.

Thirdly, the thesis addresses the importance of situational awareness in managing BESS operations. Situational awareness is essential for managing multiple operational objectives, including load balancing, energy dispatch, and system reliability. A multi-faceted optimisation strategy is proposed, leveraging real-time data from the DT to address these objectives simultaneously. This approach can provide operators with a detailed understanding of system conditions and the ability to simulate various operational scenarios. The optimisation approach improves system efficiency under varying conditions, allowing for more informed decisions that reduce the risk of unexpected system failures.

Finally, the thesis introduces a DT-supported decision support system designed to optimise BESS maintenance and operational efficiency. The proposed method extends DT to support operational decision-making by incorporating real-time health monitoring, fault detection, and predictive maintenance strategies. The decision support system presented leverages predicted RUL. These predicted RUL to inform a maintenance scheduling and spare parts ordering policy, aimed at minimising system downtime and reducing operational costs. Additionally, large language models (LLMs), are introduced to enhance the system's capability for intelligent fault diagnosis and maintenance recommendations through the analysis of unstructured data, such as maintenance logs and technical documentation.

This thesis presents a comprehensive DT-driven approach for enhancing the management and operation of BESS. The proposed framework integrates data with advanced deep learning models, providing more accurate estimations of battery states and supporting more effective decision-making. The findings of this research contribute to the broader field of energy management by demonstrating the potential of DT to improve the reliability and efficiency of BESS operations. As renewable energy continues to play an increasingly important role in global energy systems, the adoption of DT will be critical in supporting the long-term sustainability and performance of energy storage infrastructures.

Research Achievements

Journal papers:

1. K. Zhao, Y. Liu, W. Ming, Y. Zhou and J. Wu. Digital twin-supported battery state estimation based on TCN-LSTM neural networks and transfer learning[J]. CSEE Journal of Power and Energy Systems, 2024, DOI:10.17775/CSEEJPES.2024.00900. **(Impact factor: 6.9) (Published)**

2. K. Zhao, Y. Liu, W. Ming, Y. Zhou and J. Wu. A Hierarchical and Self-Evolving Digital Twin (HSE-DT) method for multi-faceted battery situation awareness realisation[J]. Machines, 2025, 13(3): 175. https://doi.org/10.3390/machines13030175 **(Impact factor: 2.2) (Published)**

3. K. Zhao, Y. Liu, W. Ming, Y. Zhou and J. Wu. DT-Supported Operational Decision Support in BESS by RUL-Based Optimisation and LLM-Driven Fault Analysis. **(intended for Digiatl Engineering)**

Conference papers:

1. **K. Zhao**, Y. Liu, W. Ming, Y. Zhou and J. Wu. Digital twin-driven estimation of the state of charge for Li-ion battery[C], 2022 IEEE 7th International Energy Conference (ENERGYCON). IEEE, 2022: 1-6. **(Published)**

2. **K. Zhao**, Y. Liu, W. Ming, Y. Zhou and J. Wu. Digital Twin-supported BESS Operational Decision Support of RUL-Based Maintenance. 2025 IEEE 31st International Conference on Engineering. **(Under review)**

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$SOC(t)$: SOC values at instances t

$SOC(t_0)$: SOC values at the commencement time t_0,

Q_a: Fraction of the nominal capacity Q_n

Q_n: The peak charge a battery can retain

$C_s(t)$: The mean surface lithium-ion concentration at instance t

$C_{s,min}$and $C_{s,max}$: Surface lithium-ion concentrations at battery states of full charge

C_a and C_r: Capacity values

R_r and R_a: Nominal and present internal resistances.

t_{EOL}: The cycle count upon the battery's EOL

SOC_{ei} and SOC_{ti} The ith estimated SOC and true SOC

η: The Coulombic efficiency of the battery

I: Current

E: The battery capacity in Amp Hour

R_0: The internal resistance

R_1: The polarisation resistance

C_1: The polarisation capacitance

U_1 and U_L: The terminal voltage of the polarisation capacitance and the battery cell

ω1 and ω2: The process noise

β: The measurement noise

U_{oc}: The open circuit voltage is dependent on SOC.

$l(k)$: The actual capacity

$\hat{l}(k)$: The estimated capacity

z_i: The values of the x-variable in a sample

Z: The mean of the values of the x-variable

q_i: The values of the y-variable in a sample

$\bar{q}$: The mean of the values of the y-variable

A_i: The inherent availability

A_a: The achieved availability and

A_0: The operational availability

T: The mean maintenance time interval

q: Average repair or preventive maintenance time, including corrective or preventive maintenance intervals

RUL_k: The RUL of the equipment at time k

L: The spare parts lead time

$E(C_i(L_p, q))$: The expected cost

$E(L_i(L_p, q))$: The expected length

C_{eo}: The cost of placing an emergency order

C_0: The cost of placing a normal order

C_s: The shortage cost per unit of time and t is

C_h: The holding cost per unit of time

A and B: The trainable matrices,

W_0: The pre-trained weight matrix,

ΔW: The parameter update during fine-tuning

x: The word embedding vector input

h: The output.

c: The number of characters in the candidate translation sentence

r: The number of characters in the reference translation sentence.

List of Abbreviation

Li-ion: Lithium-ion

DT: Digital Twin

SOC: State of Charge

SOH: State of Health

RUL: Remaining Useful Life

BESS: Battery Energy Storage System

BMS: Battery Management Systems

V2G: Vehicle-to-grid

PCS: Power Conversion System

DC: Direct Current

AC: Alternating Current

AI: Artificial Intelligence

ML: Machine Learning

IoT: Internet of Things

LSTM: Long Short-Term Memory

TCN: Temporal Convolutional Network

CNN: Convolutional Neural Network

PGD: Proper Generalised Decomposition

HI: Health Indicator

RNN: Recurrent Neural Networks

PdM: Predictive Maintenance

ADC: Analogue-to-digital Converter

EIS: Electrochemical Impedance Spectroscopy

EKF: Extended Kalman Filter

UKF: Unscented Kalman Filter

SVM: Support Vector Machines

ECM: Equivalent Circuit Model

PV: Photovoltaic

EOL: End-of-Life

ReLU: Rectified Linear Unit

NASA: National Aeronautics and Space Administration's

V: Voltage

I: Current

T: Temperature

MAE: Mean Absolute Error

RMSE: Root Mean Square Error

MSE: Mean Squared Error

PCC: Pearson correlation coefficient

LLMs: Large Language Models

NLP: Natural Language Processing

Q&A: Question-Answer

LoRA: Low-Rank Adaptation

MTBM: Mean Time Between Maintenance

MCMT: Mean Corrective Maintenance Time

MLDT: Mean Logistic Delay Time

SLES: Smart Local Energy Systems

Chapter 1 Introduction

1.1 Background

With the global shift toward renewable energy sources such as solar and wind, Battery Energy Storage Systems (BESS) have become essential in addressing the intermittent nature of renewable generation (Mahela and Shaik, 2016). BESS enables surplus energy storage during periods of low demand and its release when demand exceeds supply. This energy-buffering capability stabilises supply and enhances the integration of renewable energy into modern grids (Hu et al., 2018a). However, as BESS demand increases, the challenges of effective system management have become more evident.

One of the challenges faced by BESS management lies in accurately estimating critical parameters such as State of Charge (SOC), State of Health (SOH), and Remaining Useful Life (RUL). SOC refers to the quantity of charge accessible in a battery compared to the total charge possible. All measurements are important for forming practical maintenance schemes. These factors are essential for improving system effectiveness and avoiding breakdowns as well as cutting back on upkeep costs (Drath and Horch, 2014).

Standard techniques for assessing battery metrics are often constrained by static models that do not adequately portray the changing behaviour of batteries across diverse operating environments. Battery systems are intricate and affected by factors like temperature and current; thus, accurate forecasts need sophisticated algorithms to handle the nonlinearities in performance. Standard practices such as ampere-hour integration and look-up tables can be misled by faulty sensor data causing inefficient battery management and increased financial burden (Tuegel et al., 2011).

The combined effects led to the growth of the Digital Twin (DT) as a valuable resource for enhancing BESS handling (Reniers and Howey, 2023). A combined approach to modelling data from the physical asset in real-time allows DT to adjust itself effectively for accurate assessment and future projection (Dong et al., 2014). Through DT in BESS environments, operators can observe battery behaviour and determine SOC and SOH for effective charge and discharge decisions (Mahela and Shaik, 2016). By merging sensor data and historical performance with environmental contexts DT offers a detailed perspective on battery performance issues and advancements (Li et al., 2020). In place of standard maintenance schedules based on time intervals, DT supplies predictive maintenance options. Maintenance needs are anticipated by the system for operators to lessen unforeseen failures and cut down on downtime while increasing battery lifespan. This capability proves to be essential for large-scale BESS deployments because unanticipated maintenance may result in costly and chaotic situations (Killer et al., 2020). Additionally, DT helps operators model different operational situations with efficient energy storage and discharge methods which increases system effectiveness and lowers expenses (You et al., 2022).

While DT offers benefits challenges arise during its implementation in BESS. Complexities in merging DT systems with the already established grid infrastructure create the foremost issue. As renewable energy sources grow in number, they add complexity to the relationship between demand and storage. DT must manage these interactions immediately while requiring smooth connexions with other grid management tools and platforms. For smaller operators integration can prove to be costly and complicated (Dileep, 2020). The amount and accuracy of data required by DT present a major issue (Fuller et al., 2020). To function properly a DT requires dependable data from its physical asset. Lacking or incorrect data could generate flawed forecasts and poor decisions possibly leading to system breakdowns or inefficiencies (Koziel et al., 2021).

To overcome these obstacles researchers have crafted sophisticated strategies for merging data. The application of cloud-based systems has been investigated to boost the scalability and flexibility of DT (Alam and El Saddik, 2017). New developments in Machine Learning and Artificial Intelligence have enhanced the accuracy of estimating SOC and SOH and enabled DT to adapt to variable operating scenarios (Singh et al., 2021a).

The creation of hierarchical DT frameworks for combining data from multiple origins at diverse granularities is an active area of research (Wang et al., 2023). By adopting this strategy, we gain a deeper understanding of the battery system which increases the reliability of estimations and supports better management of BESS. The adoption of deep learning methods like convolutional neural networks (CNN) and long short-term memory (LSTM) networks has enhanced the precision of SOC and SOH estimations. By identifying detailed patterns of battery data these algorithms improve the precision and trustworthiness of battery state estimations (Yang et al., 2021b). Utilising transfer learning strategies enables DT systems to react to new data faster and boost their response to variations in battery performance. Adjustments in the market present multiple chances to improve the functionality of BESS using DT. Operators receive guidance on charging or discharging the battery to enhance profit or lower expenses by utilising simulations of various market scenarios provided by DT systems (Mirsaeidi et al., 2022). This function is especially important in unregulated energy sectors where prices shift according to both supply and demand. By using DT technology, the connections between BESS and variable renewable energy forms like solar and wind can be improved (Agostinelli et al., 2021).

Even if the potential gains from DT technology for BESS are visible significant hurdles persist before it can be embraced. Alongside the previously mentioned technical issues are economic and regulatory challenges (Verbruggen et al., 2010). The steep financial requirements for establishing and managing DT systems might hinder smaller operators, especially in places with minimal capital or government incentives. The regulations that oversee DT applications in energy sectors continue to change and clearer standards are necessary to guarantee the safe and proper functioning of these systems (Yu et al., 2022).

DT represents a major improvement in the control of BESS. With their ability to deliver insights immediately and promote predictive maintenance DTs present a strong tool to tackle the challenges linked to renewable energy expansion. The effective use of DT systems involves addressing multiple technical and economic obstacles. Research developing in this area will probably lead to an enhanced importance of DT for energy storage and grid operations (Bhatti et al., 2021).

DT technology brings attractive advantages to BESS; however considerable hurdles remain for acceptance on a larger scale. Along with the technological barriers listed above are multiple economic and regulatory issues that will influence the situation. The total price of launching and maintaining DT systems might be too steep for smaller operators in places that lack capital or government incentives for deployment. Regulatory rules for using DT in energy markets have not been finalised; clearer guidelines and standards must be established to enable the safety and efficiency of these systems (Onile et al., 2021).

DT technology marks a major progress in managing BESS. These tools deliver timely battery analytics and facilitate predictive upkeep while solving problems linked to the rise of renewable energy systems. To apply DT systems successfully one must address multiple challenges relating to technology and economics. Ongoing studies should enhance the importance of DT technology in shaping energy storage and grid management (Boicea, 2014, Meliani et al., 2021).

1.2 Motivations

The global demand for renewable energy has led to the rapid development of BESS to **mitigate** the variability of solar and wind energy. The systems contribute significantly to grid stability by capturing excess energy during low-demand times and then supplying it when demand spikes. As renewable energy sources become more prominent managing BESS presents considerable difficulties. Although improvements in battery technology have increased energy storage efficiency and capacity, current battery management strategies are still unable to cope with the complex operating behaviour of batteries. (Li and Wang, 2019).

Traditional monitoring approaches are the primary basis for existing battery management tools in determining important battery characteristics such as SOC and SOH (Lipu et al., 2022). These values are important for judging the efficiency and lifespan of the battery alongside its safety concerns. Traditional techniques rely on fixed models and set maintenance plans and fail to capture the changing behaviour of battery systems. Insufficient real-time data integration and predictive functions result in inefficiencies during energy storage management and raise operational expenditures as well as the chance of unforeseen failures (Krishna et al., 2022). These constraints emphasise the urgency for enhanced methodologies that increase the fidelity of battery state evaluations and allow for anticipatory maintenance practises.

DT stands out as a potential answer to the issues encountered in managing BESS. The DT functions as an immediate virtual model of a physical system that consistently incorporates data from sensors alongside historical statistics and environmental conditions. With the simulation of the physical system's behaviour, DT improves monitoring and decision processes in BESS. With the help of DT technology operators gain full visibility of battery operations that facilitates the optimisation of charge and discharge schedules and forecasts failure risks while increasing battery lifespan (Wu et al., 2020).

Though DT technology offers benefits potential hurdles continue in implementing it for BESS. Combining DT systems with existing grid systems poses significant difficulties (Jafari et al., 2023). Managing energy generation and storage is becoming complex and needs data to move smoothly between physical and digital systems. For smaller operators integrating DT with the existing grid poses technical challenges and high costs (Xu et al., 2016). Reliable prediction depends on the essential need to allow the quality and correctness of the data integral to DT. Lacking or incorrect data can result in bad decisions that might cause less efficient system operation or even breakdowns (Koziel et al., 2021). Overcoming the financial and technical obstacles of DT implementation in BESS is an essential research topic.

Battery management systems struggle with the absence of predictive maintenance methods. Old practices of maintenance typically depend on established schedules that overlook the battery's true condition causing either extra interventions or unanticipated breakdowns (Koziel et al., 2021). By analysing real-time data predictive maintenance determines when maintenance is essential thereby decreasing downtime and lowering operational costs. By tracking the battery's state and running simulations across different scenarios DT supports predictive maintenance (Chen et al., 2023). By employing predictive strategies ahead of failures operators boost system reliability while decreasing their maintenance costs.

Improving battery monitoring and upkeep is just one benefit of DT; it can also allow the BESS to operate more efficiently in reaction to market changes. As renewable energy enters the grid more prominently energy markets experience greater volatility as prices shift with supply and demand. With DT technology available operators can handle these variations by modelling diverse market situations and discovering the optimal methods for storing and distributing energy. A quick response to market changes creates a notable advantage in deregulated energy markets.

Adopting DT technology for BESS carries various obstacles. A major technical issue lies in the necessity for accurate data. A DT performs efficiently if it obtains reliable and timely data from the physical system. Missing or incorrect data may cause wrong forecasts and poor choices. As BESS systems become more interconnected they create risks related to cybersecurity that necessitate securing the data's integrity and guaranteeing safe communication between the physical and digital realms (Ünal et al., 2023, Kharlamova et al., 2022).

New techniques for boosting data quality and harmonisation in DT systems are being examined by researchers. Applying ML algorithms acts as a technique to improve the prediction skills of DTs. Through the training of ML models with extensive datasets researchers can boost the accuracy of predicting SOC and SOH. The connection of cloud platforms to DT systems may boost scalability and alleviate the local devices' computational strain. DTs hosted on the cloud enable immediate data analysis and processing for operators to gain precise and prompt information about battery performance (Semeraro et al., 2023b).

Building hierarchical DT systems represents an additional field of current research. Such systems support the unification of analytics from multiple resources offering a more in-depth perspective of system dynamics. For BESS applications this strategy is vital as monitoring both individual cells and the entire system is key to improving performance. Combining sensor information with historical data and external inputs allows hierarchical DTs to generate a reliable and extensive analysis of battery efficiency (Semeraro et al., 2023b).

With the ongoing rise of renewable energy use comes an increasing demand for advanced energy storage options. BESS will significantly contribute to maintaining the dependability and consistency of the grid; however, for effective management of these systems new tools and technologies are essential. By supplying instantaneous information about battery performance and supporting predictive maintenance methods DT technology becomes a beneficial tool in addressing BESS management difficulties. To fully utilise DT technology for BESS we must navigate numerous challenges including technical and financial issues. Current explorations in this domain will play a vital role in forming scalable and affordable approaches that address the demands of a rapidly changing and decentralised energy framework (Bao et al., 2024).

This study aims to develop a robust, data-driven DT framework for BESS management to enhance operational efficiency, extend battery lifespan, and reduce costs. Through the integration of machine learning algorithms and hierarchical DT architectures, the research seeks to improve real-time accuracy in SOC and SOH estimations, while enabling predictive maintenance strategies to minimize downtime. Additionally, the framework will incorporate dynamic updating models to optimise model responsiveness. By resolving technical challenges related to state monitoring and estimation, the proposed DT aims to provide scalable and cost-effective tools for operators, ultimately advancing system reliability, accelerating renewable energy integration, and supporting global decarbonization efforts in an increasingly decentralized energy landscape.

1.3 Research Questions and Objectives

Following the background and motivations, under the context of renewable energy integration and BESS management, this research aims to investigate a Digital Twin-driven approach for improving battery state estimation, situational awareness, and operational decision support. The following research questions have been formulated to achieve this goal:

1. *With the development of emerging technologies such as DT and real-time data analytics, the management of BESS has shifted towards a data-driven and real-time operational environment. In this context, what is an appropriate Digital Twin-driven framework for optimising the management and performance of BESS?*

2. *Battery state estimation is important for the efficient operation of BESS, and a data-driven approach has been widely adopted. However, existing research on*

state estimation often lacks a comprehensive explanation of how key variables are determined for predicting battery state metrics such as SOC and SOH. Therefore, how can battery state estimation be achieved in a predictive manner with proper justification of the variables affecting SOC, SOH, and RUL?

3. *Battery optimisation is critical for enhancing the performance and lifespan of BESS, and data-driven approaches are commonly used. However, existing optimisation research often focuses on isolated parameters without fully explaining or justifying the selection of variables influencing battery performance. Therefore, how can battery optimisation be achieved in a predictive manner, with proper justification of the factors affecting energy storage, discharge efficiency, and long-term operational reliability?*

4. *With the advancement of DT technology and machine learning techniques, DT can be applied for operational decision-making with the unique advantage of real-time data integration and predictive analytics. Therefore, how can DT be utilised for computational modelling and decision support in BESS, particularly for predictive maintenance and operational decision-making, considering operational and technical constraints?*

With the identification of the research questions, the research objectives following these research questions are listed below:

1. *To propose a framework for DT-driven management of BESS that can integrate real-time data, historical performance, and environmental factors to optimise battery performance and reliability.*

2. *To apply the proposed DT-support framework for battery state estimation tasks that improve the accuracy of SOC, SOH, and RUL predictions and integrate real-time data for updating.*

3. *To propose a DT-driven optimisation method for BESS. The method will integrate real-time sensor data, historical data, and environmental factors to enhance battery situational awareness.*

4. *To study a DT-driven approach for operational decision support in BESS for predictive maintenance and providing maintenance strategies.*

The details of this research will be reported in Chapters 3, 4, 5 and 6.

1.4 Thesis Outline

In **Chapter 1**, a broader context and background are provided as to the motivation and significance of this research.

Chapter 2 presents a detailed review of the existing literature related to Battery Digital Twin (BDT) technology and BESS. The chapter is divided into four sections: (1) an overview of the BDT, including its definition, evolution, and current research trends; (2) a review of the key components, benefits, and challenges of BESS; (3) the research and applications of DT in energy system; and (4) a summary of the literature, linking the key findings to the research questions of this study. This review provides an understanding of the current research landscape and highlights areas that will be addressed through the research questions in the following chapters.

In **Chapter 3**, a framework is introduced for the DT-driven management of BESS. This framework is designed to support real-time monitoring, predictive maintenance, and operational optimisation. The framework consists of several components, each focusing on different aspects of BESS management and digital representation. These components include data description, data pre-processing and integration, analytical methods for optimisation, and model collaboration.

Chapter 4 presents a method for battery state estimation and RUL prediction. Utilising an equivalent circuit model as its foundational basis, a DT model has been developed, integrating factors such as voltage, current, and ambient temperature. Recognising the complexities of battery state estimation, we introduced the temporal convolutional networks (TCN)-LSTM approach. This advanced algorithm is specifically designed to reduce dependence on initial values, especially with limited training data as input. To support this, we incorporated the battery digital twin framework and used transfer learning techniques to enable continuous model refinement while working through rolling learning.

Chapter 5 aims to introduce the hierarchical and self-evolving digital twin (HSE-DT) method, designed to enhance battery situational awareness. Utilising a structured DT model, the method integrates critical parameters such as voltage, current, and temperature, alongside advanced estimation techniques. Recognising the complexities of battery situational awareness, The HSE-DT method employs the Transformer-CNN model to accurately identify spatial and temporal characteristics of battery conditions.

In **Chapter 6**, the integration of advanced data-driven approaches (e.g., spare parts ordering strategy combining RUL prediction and availability, and LLM-based fault diagnosis and decision support) into DT to enhance maintenance decision support for BESS is explored. The results of the experiment indicate that integrating the spare parts ordering strategy based on RUL and availability with LLM insights can greatly enhance maintenance planning and fault detection. This chapter focuses on the special qualities of these models and proposes that unifying them under a DT framework might generate a more thorough and versatile strategy for overseeing BESS and boosting system dependability while cutting maintenance expenses.

Chapter 7 concludes the thesis, and a summary of its achievements is presented. There is a discussion of the limitations and future work. As a final note, the main contributions to the body of knowledge resulting from this research are summarised.

1.5 Research Contributions

This thesis makes several contributions to the wider body of knowledge.

1. A DT framework for BESS management is presented that prioritises real-time monitoring and optimisation. This approach delivers a clear strategy to collect data from multiple sources and enhance the accuracy of battery state estimations. The framework enhances the efficiency of BESS operations through real-time data-driven decision support.

2. A method for battery state estimation is introduced, including SOC, SOH and RUL. By integrating machine learning techniques and real-time data, the proposed methodology offers a more reliable approach to estimating these critical battery parameters. This can lead to better decision-making and improved battery performance in real-world applications.

3. A multi-faceted optimisation method is proposed for situational awareness in BESS. The optimisation model contributes to improving the adaptability and reliability of BESS under changing operational conditions.

4. A decision support system is introduced within the DT framework, focusing on predictive maintenance and providing a question-answer maintenance strategy. This system enables operators to predict potential failures and plan maintenance activities, reducing downtime of BESS. This contribution addresses a gap in current battery management practices by providing a more proactive approach to maintenance and operational decision support.

Chapter 2 Literature Review

2.1 Introduction

As outlined previously, this chapter reviews the related works and relevant research in three main areas: battery energy storage systems, battery digital twins, and the research and applications of digital twins in energy systems. Section 2.2 explores BESS by reviewing its key components, the associated benefits and challenges, and emerging innovations in this field. The discussion on battery digital twins is divided into three aspects: the definition and evolution of the technology, its advantages and limitations, and the current trends shaping future research. These topics are covered in Section 2.3. Section 2.4 reviews the broader applications of digital twin technology in energy systems, particularly its role in renewable energy integration, system optimisation, and potential implications for energy transitions. Finally, Section 2.5 summarises the chapter concerning the research questions posed in this study.

2.2 Battery Energy Storage System

In the contemporary energy landscape, BESS has appeared as a critical asset for managing renewable energy integration and providing grid stability (Kortmann et al., 2021). The global shift towards decarbonisation and the development of sustainable energy infrastructures underscore the significance of BESS (Dunn et al., 2011). These systems store excess energy generated from intermittent renewable sources, such as solar and wind, for later use, thereby enabling a reliable power supply (Castelletto and

Boretti, 2022). This capability mitigates fluctuations in energy availability, particularly during periods of low generation or high demand, enhancing the efficiency and resilience of modern energy systems (Nazar and Anwer, 2020). Consequently, BESS have become indispensable in both grid-level applications and decentralised energy networks, such as electric vehicles (EVs) (Mendi et al., 2021).

Despite significant technological advancements, particularly in lithium-ion (Li-ion) batteries, several critical issues hinder the optimal performance and widespread adoption of BESS. These include battery degradation, energy density limitations, and the economic feasibility of long-term operations (Nechaieva, 2019). Furthermore, the complexity of integrating BESS into diverse energy systems introduces additional challenges in maintaining operational safety and efficiency (Beltramin, 2018). To address these issues and unlock the full potential of BESS, continuous research and innovation are needed.

This section reviews the literature on BESS, focusing on its core components, the benefits it offers, the challenges it faces, and the emerging innovations that aim to address these challenges. This review lays the groundwork for understanding the subsequent discussion on DT and its applications in battery management, which will be explored in greater depth in the following sections.

2.2.1 Overview of Battery Energy Storage Systems

BESS are fundamental to modern energy infrastructures, balancing energy supply and demand, facilitating the integration of renewable energy sources, and enhancing the stability of power grids (Dunn et al., 2011). As reliance on renewable energy, particularly variable sources such as solar and wind, increases, the need for advanced energy storage solutions capable of mitigating fluctuations in energy production and consumption becomes more urgent (Zuo et al., 2021). BESS offer the flexibility to store surplus energy generated during periods of low demand and release it during peak demand, thus preventing power outages and providing grid stability (Al Essa, 2020).

The success of BESS is largely attributed to the widespread adoption of Li-ion batteries, which dominate the market due to their high energy density, long cycle life, and relatively low maintenance requirements (Nazar and Anwer, 2020). However, these batteries are not without limitations. Safety risks related to thermal runaway, constraints on raw material availability, and environmental concerns associated with lithium and cobalt extraction and processing pose significant barriers to broader adoption (Fauzan et al., 2016). Addressing these issues is critical to meet the growing demand for sustainable and resilient energy solutions (Fang et al., 2020).

One promising research direction involves exploring alternative battery chemistries, such as sodium-ion and solid-state batteries, to overcome the limitations of Li-ion technologies (Xu et al., 2020). Sodium-ion batteries, for instance, offer a more sustainable and cost-effective option for large-scale energy storage, as sodium is more abundant and less expensive compared to lithium (Namekar and Pathak, 2020). Similarly, solid-state batteries, which replace the liquid electrolyte in Li-ion batteries with a solid electrolyte, improve safety by reducing the risk of thermal runaway (Wang et al., 2021b). These innovations hold the potential to significantly enhance the performance, safety, and scalability of BESS for both grid-level and transportation applications (Wang et al., 2022).

In addition to advancements in battery chemistry, significant progress has been made in optimising BESS operation through the integration of Battery Management Systems (BMS) and DT technology. BMS play a critical role in providing the safe and efficient functioning of battery systems by monitoring and estimating parameters such as SOC, SOH, voltage, and temperature (Anandavel et al., 2021). Real-time data provided by BMS enable operators to adjust system operations to prevent adverse conditions and extend battery lifespan.

Digital Twin technology further enhances BESS optimisation by creating a virtual model of the physical battery system that mirrors its real-time operation (Mihai et al., 2022). This virtual representation allows for precise monitoring, predictive maintenance, and performance optimisation. By integrating data from embedded sensors, the DT can simulate various operating scenarios, predict potential failures, and provide actionable insights to enhance system performance and longevity (Mihai et al., 2022). In EVs, DTs are used to monitor battery health, predict the RUL, and optimise charging and discharging cycles, thus extending battery life (Mihai et al., 2022).

The deployment of BESS has extended beyond grid-level applications to diverse sectors, particularly transportation. Within power grids, BESS provide essential services such as frequency regulation, voltage support, and peak shaving. Fast adaptation to shifts in grid frequency and voltage allows BESS to support grid stability and secure the dependable supply of electricity. (Fellah et al., 2021). Peak shaving, specifically, involves discharging stored energy during periods of high demand to reduce the grid load, thereby minimising the need to activate costly and less efficient peaker plants (Uddin et al., 2018).

In the transportation sector, BESS serve as a foundational technology for vehicle electrification. EVs rely on advanced battery technologies for propulsion, and as demand for EVs continues to grow, the need for efficient, durable, and safe battery systems becomes even more critical (Xu et al., 2020). Vehicle-to-grid (V2G) technology exemplifies an innovative use case for BESS in transportation, wherein EVs can supply excess energy stored in their batteries back into the grid during peak demand periods (Anandavel et al., 2021). This bidirectional energy flow enhances grid flexibility and provides opportunities for optimising energy utilisation across both transportation and energy sectors.

2.2.2 Components and Architectures of BESS

BESS is composed of several integral components, each playing a critical role in ensuring system efficiency, safety, and operational reliability (Pham et al., 2020). These components are systematically integrated within a sophisticated architecture that enables BESS to perform a wide range of applications, such as grid stabilisation, renewable energy integration, and EV propulsion (Schimpe et al., 2018). A comprehensive understanding of these components and their interactions is essential for optimising BESS performance and enhancing their long-term sustainability (Vartanian, 2010).

The core of any BESS is the battery cells, which serve as the primary storage units for electrical energy. The predominant technology in BESS is Li-ion batteries, known for their high energy density, long cycle life, and overall efficiency (Diao et al., 2016). These battery cells are typically assembled into modules, which are then organised into larger battery packs. This modular configuration facilitates scalability, allowing BESS to accommodate varying energy storage requirements, from small-scale residential systems to large-scale utility applications (Ma et al., 2023). The modular structure also simplifies maintenance and replacement of individual components, thereby minimising system downtime (Soni and Fernandez, 2023).

The BMS is a pivotal component that supports battery cells by monitoring and regulating their operating conditions (Ausswamaykin and Plangklang, 2014). By tracking critical parameters such as SOC, SOH, voltage, temperature, and current, the BMS helps prevent issues such as overcharging, overheating, or deep discharge, all of which can significantly impair battery performance and lifespan (Lipu et al., 2021). Moreover, the BMS not only safeguards the battery cells but also provides actionable data for optimising system efficiency and enabling predictive maintenance, helping operators anticipate potential failures before they occur (Inderwildi et al., 2020).

Another essential component in BESS architecture is the Power Conversion System (PCS), which manages energy conversion between the direct current (DC) stored in the batteries and the alternating current (AC) used by most electrical grids and devices (Soong and Lehn, 2014). The PCS includes inverters to convert DC to AC for grid applications, as well as converters that govern the charging and discharging processes (Zhao et al., 2014). This conversion capability is important in grid-connected systems, ensuring that energy storage can be efficiently utilised by the grid and various electrical loads while minimising energy losses during the conversion process (Lo Franco et al., 2021).

Effective thermal management is a critical aspect of BESS design, as it maintains optimal operating temperatures for battery cells, which is vital for both performance and safety (Liu et al., 2017). Li-ion batteries, in particular, are highly sensitive to extreme temperatures, and their efficiency can be significantly compromised when exposed to conditions that are either overheating or overcooling (Qian et al., 2016). A well-engineered thermal management system may employ air cooling, liquid cooling, or phase-change materials to regulate temperature and prevent overheating (Wang et al., 2020a). In some advanced BESS configurations, thermal management is integrated with DT, allowing real-time simulations that can predict and pre-empt potential overheating or other temperature-related issues (Patil et al., 2021).

The integration of DT technology into BESS architecture represents a significant advancement in system management and optimisation (Padmawansa et al., 2023). Digital twins create a virtual replica of the physical system, enabling operators to monitor performance, conduct simulations, and predict future behaviour based on real-time data. Continuously updated using sensor inputs from the physical BESS, the digital twin provides an accurate, up-to-date representation of the system's status. This technology facilitates more precise control, improved maintenance strategies, and enhanced operational efficiency, particularly in large-scale applications where even minor improvements can yield substantial cost savings and performance gains.

2.2.3 Challenges and Opportunities of BESS

Despite the rapid advancement and growing adoption of BESS, numerous technical, economic, and environmental challenges persist, impeding their full-scale deployment and optimisation (Krishna et al., 2022). These barriers not only limit the efficiency and longevity of current BESS installations but also raise concerns about the sustainability and long-term feasibility of using such systems for extensive grid and transportation applications (Krishna et al., 2022). Consequently, addressing these challenges is imperative for realising the full potential of BESS and enabling a more sustainable and resilient energy future (Sun et al., 2023).

One of the foremost barriers to the widespread adoption of BESS is the high upfront capital cost associated with battery technologies, particularly Li-ion batteries (Sparacino et al., 2012). Although significant reductions in manufacturing costs and improvements in material sourcing have been achieved in recent years, the initial investment required for installing large-scale BESS remains a formidable barrier, particularly in regions where renewable energy project financing is constrained (Hossain et al., 2020). The overall cost of BESS deployment encompasses not only the batteries themselves but also the expenses related to power conversion systems, BMS, and thermal management solutions (Mitali et al., 2022). To overcome these economic challenges, ongoing research is focused on developing cost-effective battery chemistries, enhancing manufacturing efficiency, and achieving economies of scale in production (Akram et al., 2020).

In addition to high costs, battery degradation and limited lifespan present significant technical challenges for BESS (Liu et al., 2021a). Repeated charging and discharging cycles, fluctuations in operating temperature, and external environmental factors contribute to the gradual degradation of battery cells, leading to a decline in overall energy storage capacity and system efficiency over time (Pan et al., 2019). Degradation mechanisms such as capacity fading, increased internal resistance, and electrode deterioration not only reduce the operational lifespan of batteries but also necessitate frequent maintenance and replacement, thereby increasing the long-term operational costs of BESS. These issues are particularly problematic for lithium-ion batteries, which are highly sensitive to temperature variations and prone to safety risks such as thermal runaway under extreme operating conditions.

Efforts to address battery degradation have spurred research into alternative battery chemistries, such as sodium-ion and solid-state batteries, which offer potential improvements in lifespan, safety, and environmental sustainability (Hasan et al., 2021). Sodium-ion batteries, for example, use sodium—a more abundant and less expensive material compared to lithium—as the primary charge carrier, making them a cost-effective option for large-scale energy storage applications (Zhao et al., 2023). However, sodium-ion batteries currently face challenges related to lower energy density and shorter cycle life compared to their lithium-ion counterparts, which limits their competitiveness in high-energy applications (Hirsh et al., 2020). Meanwhile, solid-state batteries, which utilise solid electrolytes instead of liquid ones, drop the risk of leakage and significantly reduce the likelihood of thermal runaway (Velumani and Bansal, 2022). Despite these advantages, solid-state batteries are still in the experimental stage, and their commercial viability remains constrained by issues related to material stability and manufacturability at scale (Yang et al., 2021a).

Another significant technical challenge in the deployment of BESS is to offer the operational safety and reliability of these systems, especially when integrated with diverse energy infrastructures (Nazaralizadeh et al., 2024). Safety concerns stem from the complex chemical reactions within batteries, which can lead to issues such as overheating, short-circuiting, and in extreme cases, fires or explosions (Chen et al., 2021c). These safety risks are further exacerbated by the increased energy densities of advanced battery technologies, making effective safety management a critical priority. BMS play a critical role in mitigating these risks by continuously monitoring key parameters such as voltage, temperature, and SOC and implementing protective measures to prevent hazardous conditions (Wu et al., 2019, Chen et al., 2021b). However, the complexity of integrating BMS with multiple energy systems and enabling real-time responsiveness remains a considerable challenge.

DT technology has emerged as a promising solution to enhance the safety, efficiency, and reliability of BESS (Waseem et al., 2023). By creating a virtual representation of the physical battery system, DT technology enables real-time monitoring, predictive maintenance, and optimisation of battery performance. The integration of DT with BESS allows operators to simulate various operating scenarios, predict potential failures, and implement pre-emptive measures to prevent safety incidents. Moreover, DT technology facilitates a deeper understanding of complex degradation mechanisms, enabling more accurate predictions of RUL and enhancing decision-making processes related to maintenance and replacement schedules (Bhatti et al., 2021). Despite these advantages, the implementation of DT in large-scale BESS is still in its nascent stages, and further research is needed to develop standardised frameworks and protocols for DT integration.

Environmental sustainability represents another major challenge for BESS, primarily due to the extraction and processing of materials like lithium, cobalt, and nickel, which are associated with significant environmental and social impacts (Dehghani-Sanij et al., 2019). The mining of these materials not only results in habitat destruction, soil degradation, and water contamination but also raises ethical concerns regarding labour practices, particularly in regions with limited regulatory oversight (Hannan et al., 2021). For instance, cobalt mining in the Democratic Republic of the Congo has been widely criticised for its reliance on child labour and hazardous working conditions. The improper disposal of spent batteries poses additional environmental risks, as hazardous chemicals can leach into soil and groundwater, leading to long-term ecological damage (Chowdhury et al., 2020).

Despite these challenges, BESS present numerous opportunities for supporting the global transition to sustainable energy systems (Branco et al., 2018). One of the most promising areas of opportunity lies in the integration of BESS with renewable energy sources, such as solar and wind, to enhance grid flexibility and stability (Worku, 2022). By providing critical services such as frequency regulation, voltage support, and peak shaving, BESS can help balance supply and demand in real-time, thereby reducing the reliance on fossil-fuel-based peaker plants and minimising greenhouse gas emissions (Worku, 2022). Moreover, the deployment of BESS in microgrid and off-grid applications can provide reliable energy access in remote and underserved regions, contributing to energy equity and resilience.

The adoption of V2G technology offers another significant opportunity for BESS in the transportation sector (Lund and Kempton, 2008). V2G technology enables bidirectional energy flow between EVs and the grid, allowing EVs to supply excess energy stored in their batteries back to the grid during peak demand periods. This bidirectional energy flow not only enhances grid stability but also provides additional revenue streams for EV owners, incentivising the adoption of EVs and supporting the decarbonisation of the transportation sector (Upputuri and Subudhi, 2023). However, the implementation of V2G technology requires the development of compatible charging infrastructure and regulatory frameworks, as well as advancements in communication and control systems to manage energy flows effectively (Sovacool et al., 2018).

Artificial Intelligence (AI) and machine learning (ML) technologies are poised to play a transformative role in the optimisation of BESS operation and management (Yao et al., 2023, Gao and Lu, 2021). AI-driven algorithms can analyse vast amounts of operational data to identify patterns and anomalies, enabling real-time optimisation of charging and discharging cycles, predictive maintenance, and fault detection (Guo et al., 2021b). The integration of AI with BMS and DT systems can further enhance the performance and safety of BESS by enabling autonomous decision-making and adaptive control. As AI and ML technologies continue to mature, their application in BESS is expected to reduce operational costs, improve system efficiency, and extend battery lifespan (Chen et al., 2012).

In conclusion, while BESS faces various technical, economic, and environmental challenges, the opportunities for growth and optimisation remain vast. By overcoming issues related to high costs, battery degradation, and environmental sustainability, and capitalising on advancements in digitalisation, AI, and energy management, BESS can continue to play a pivotal role in the global transition towards sustainable energy systems (Andal and Jayapal, 2022). Continued research and innovation in battery chemistries, recycling technologies, and system integration will be critical for unlocking the full potential of BESS and achieving a more resilient and sustainable energy future. As the energy storage landscape evolves, BESS is poised to become a cornerstone technology in modern energy infrastructures, driving the decarbonisation of power grids and transportation systems worldwide.

2.3 Digital Twin of BESS

The integration of DT technology into BESS represents a significant advancement in the management and optimisation of energy storage solutions (Kharlamova et al., 2022). A digital twin is a dynamic, virtual model of a physical system that replicates real-time operations by continuously syncing with sensor data from the physical counterpart (Ibrahim et al., 2023). In the context of BESS, this technology enables enhanced monitoring, predictive maintenance, and performance optimisation by simulating various operating conditions and predicting potential failures (Song et al., 2024). As BESS becomes more complex and widespread in applications like grid stabilisation, renewable energy integration, and electric vehicles, the use of Digital Twins provides operators with a powerful tool for improving system efficiency, safety, and lifespan. This section will explore the core concepts of DT, its development, key techniques and the opportunities it presents when integrated with BESS, providing a detailed overview of the role it plays in modern energy management systems.

2.3.1 Definition and Evolution of Digital Twin

The concept of the DT has evolved significantly since its inception, becoming an integral part of numerous industrial and technological sectors, including energy storage systems (Tao et al., 2018). At its core, a digital twin is a virtual representation of a physical system that replicates the system's behaviour, processes, and characteristics in real-time by utilising data from various sources. This digital entity allows for enhanced monitoring, predictive maintenance, and optimisation of the physical system, making it a vital tool in the modern energy landscape (Hu et al., 2021).

The term "digital twin" was first introduced by NASA in 2012 to describe a high-fidelity digital model that could simulate the behaviour of aerospace systems during missions (Glaessgen and Stargel, 2012). It was envisioned as a tool to predict system behaviour, assess performance, and optimise operations in space environments. The idea quickly gained traction across various sectors, including manufacturing, where Michael Grieves further developed the concept by introducing a framework that described the digital twin as a digital counterpart to a physical product or system (Grieves and Vickers, 2017). This concept formed the foundation for further technological advancements, eventually being adopted in fields such as aerospace, automotive, and, more recently, energy systems.

A key feature of the digital twin is its bidirectional nature, wherein data flows between the physical system and its virtual counterpart in real-time (Yaqoob et al., 2020). This connection creates a dynamic feedback loop, allowing the digital twin to provide accurate assessments of the physical system's state and performance, predict potential failures, and optimise operations based on real-time data. This real-time synchronisation is made possible through the integration of Internet of Things (IoT) technologies and advanced data processing algorithms.

In the context of BESS, digital twin technology has become invaluable due to its ability to enhance the efficiency and reliability of energy storage systems. BESS face a variety of challenges, including battery degradation, safety risks, and efficiency losses, particularly with lithium-ion batteries (Lo Franco et al., 2021). Digital twins offer solutions by providing detailed, real-time insights into the SOC, SOH and RUL of batteries, enabling more effective battery management and optimisation (Li et al., 2020).

The evolution of digital twin technology in energy systems can be attributed to advancements in data analytics, machine learning, and cloud computing (Mihai et al., 2022). As data collection methods have improved and become more sophisticated, digital twins have evolved from simple static models to highly dynamic systems that continuously update themselves with real-time data from sensors embedded in the physical systems. This shift has made digital twins indispensable for optimising complex systems, such as BESS, where continuous monitoring and predictive capabilities can significantly enhance system performance and longevity (Ibrahim et al., 2023).

Another significant aspect of digital twin evolution is its application in smart grids (Jafari et al., 2023). In modern energy infrastructures, the ability to predict and respond to fluctuations in energy supply and demand is critical, particularly as more renewable energy sources, such as wind and solar, are integrated into the grid. Digital twins enable smart grids to become more adaptive and responsive by providing operators with real-time insights into energy flows and potential bottlenecks. This capability is essential for optimising the use of BESS, as it helps balance the intermittent nature of renewable energy sources by allowing operators to store excess energy during periods of low demand and release it when demand peaks (Sifat et al., 2023).

As digital twin technology continues to evolve, its applications are expanding beyond traditional industrial uses to encompass new and emerging fields, such as EVs and renewable energy integration. In the EV sector, digital twins are being used to monitor battery health, optimise charging cycles, and predict the performance of battery systems over time (Bhatti et al., 2021). This capability is critical for ensuring the safety and longevity of EV batteries, which are subject to repeated charging and discharging cycles.

In summary, the digital twin has evolved from a theoretical concept to a highly practical tool that is transforming how complex systems are managed and optimised. Its ability to provide real-time, data-driven insights into physical systems makes it an indispensable asset in fields such as energy storage, where efficiency, reliability, and safety are paramount. As advancements in data processing, machine learning, and IoT continue to accelerate, the role of digital twins in optimising BESS and other energy systems will only become more critical.

2.3.2 Key Techniques in Battery Digital Twin Development

The development of battery digital twins involves the integration of various techniques, enabling accurate modelling, real-time monitoring, and predictive maintenance for BESS (Li et al., 2024). These techniques help create digital twins that provide reliable simulations, informed decision-making, and system-wide optimisation. For BESS, digital twin technology is evolving through the use of machine learning models, real-time data processing, and advanced modelling strategies to improve system performance.

A key technique in digital twin development is real-time data acquisition and integration. Sensors embedded in the physical battery system continuously collect data on parameters such as voltage, temperature, and current. This data feeds directly into the digital twin, allowing the virtual model to stay aligned with the real-time conditions of the battery. IoT technology plays a role in maintaining the flow of data between the physical and virtual environments. The regular acquisition of data allows the digital twin to stay informed and delivers a fluid depiction of how the battery is functioning. (Uhlemann et al., 2017).

Advanced modelling and simulation techniques are another critical element in battery digital twin development. These models replicate the electrochemical processes within battery cells, helping to predict how the system will behave under different conditions. Various approaches, such as electrochemical models and thermal models, are employed to represent the battery's physical behaviour and identify the factors that impact performance and lifespan (Singh et al., 2021b). By simulating a range of scenarios, such as extreme conditions or degradation over time, the digital twin helps assess potential risks and system vulnerabilities, contributing to long-term operational planning (Alcaraz and Lopez, 2022).

ML algorithms enhance the predictive capabilities of digital twins by analysing both historical and real-time data to forecast future battery performance and identify potential issues (Rathore et al., 2021). LSTM networks, for instance, are effective in handling time-series data, making them suitable for predicting battery health and RUL (He et al., 2021). Similarly, TCN and CNN are used to detect patterns in battery data, offering valuable insights into the system's operational trends (Hong et al., 2021). These models can process complex datasets generated by BESS, providing more reliable predictions about the system's future behaviour.

Cloud computing plays a significant role in digital twin technology by enabling large-scale data processing and analysis (Hong et al., 2021). Cloud-based platforms offer the necessary computational resources for handling the vast amounts of data generated by BESS. Furthermore, edge computing complements cloud infrastructure by enabling real-time processing closer to the physical system. Time-sensitive tasks, such as monitoring critical operational changes, can be executed locally, while more complex simulations and analyses are conducted in the cloud (Wu et al., 2021). This balance between cloud and edge computing improves the responsiveness of the digital twin.

Predictive maintenance is another important technique used in digital twin technology (Chen et al., 2023). By analysing operational data, the digital twin can predict when certain components of the battery may fail or degrade, allowing for maintenance to be scheduled in advance. This predictive capability helps reduce unexpected system downtime and lowers maintenance costs (Peng et al., 2019). Through continuous monitoring and forecasting, digital twins enable more informed decisions about when and how to perform maintenance, thereby extending the battery’s operational life.

Thermal management is also a vital consideration for battery systems, particularly in lithium-ion batteries, where temperature fluctuations can affect performance (Wang et al., 2021b). In digital twins, real-time temperature data is combined with thermal models to predict changes in battery temperature during operation (Reniers and Howey, 2023). By simulating thermal conditions, the digital twin assists in maintaining the battery's optimal temperature range, which is essential for safe and efficient operation. Effective thermal management contributes to prolonging battery life and preventing safety issues related to overheating (Zhang et al., 2022).

Cybersecurity is another aspect that has gained attention with the increasing digitalisation of energy systems (Shitole et al., 2021). Digital twins are vulnerable to cyber threats, particularly when cloud computing and IoT are involved. Protecting the data integrity of digital twins is necessary to ensure that the physical systems they represent are not compromised. Techniques such as encryption, real-time system monitoring, and anomaly detection help maintain the security of the digital twin infrastructure, safeguarding against disruptions and unauthorised access.

In summary, the development of battery digital twins depends on the integration of several techniques, including real-time data acquisition, advanced modelling, machine learning, cloud computing, predictive maintenance, thermal management, and cybersecurity. These techniques contribute to improving the efficiency, safety, and reliability of BESS, supporting better decision-making and operational optimisation. As digital twin technology continues to evolve, the incorporation of more advanced models and techniques will further refine the functionality of battery digital twins, promoting progress in energy storage technologies.

2.3.3 Trends and Future Directions in Digital Twin for Energy Systems

The integration of DT into energy systems has accelerated in recent years, with increasing interest in its potential to enhance the performance, safety, and efficiency of energy storage systems. While much progress has been made, ongoing research continues to explore emerging trends and address challenges that will shape the future development of digital twins in this domain. These trends include the growing role of ML, advancements in real-time data analytics, the increasing importance of cybersecurity, and the expansion of digital twin applications beyond traditional energy storage systems.

One of the most significant trends in digital twin research is the use of AI and machine learning to enhance the predictive capabilities of digital twins. The integration of ML models has enabled more accurate forecasting of battery performance, degradation, and faults in energy storage systems-driven models allowing digital twins to process and analyse vast datasets, identifying patterns in system behaviour and predicting future outcomes with greater accuracy (Kaleem et al., 2023). By leveraging machine learning, digital twins can improve the efficiency of energy systems by optimising operational parameters and anticipating maintenance needs (Agostinelli et al., 2021).

Another key trend is the increasing focus on real-time data analytics and the development of robust data management (Wang et al., 2021b). Digital twins depend on continuous data streams from physical systems, while advancements in data analytics enable more efficient processing and interpretation of this information. Real-time monitoring and control of energy storage systems are essential to maintaining stability, optimising energy use, and ensuring reliable performance under varying demand conditions. The development of advanced data architectures, such as cloud-based and edge computing platforms, enables the real-time operation of digital twins. These architectures facilitate large-scale data processing and support localised decision-making, which is critical for responsive energy management systems.

Cybersecurity is becoming increasingly vital in digital twin research as energy systems become more interconnected and reliant on digital infrastructure (Wang et al., 2023). The growing adoption of IoT technologies in energy systems makes it imperative to secure the data integrity on which digital twins rely. Cyberattacks present significant risks to energy infrastructure, potentially compromising system performance or leading to catastrophic failures. Research on secure architectures, encryption methods, and fault-tolerant systems is critical to protecting energy storage systems from external threats. Future advancements in cybersecurity protocols for digital twins are likely to become a primary focus, particularly for critical infrastructures like power grids

(Shitole et al., 2021).

Extending digital twin applications beyond conventional BESS is another critical future direction. While digital twins are well-established for lithium-ion battery management, there is growing interest in applying them to other energy storage systems, such as fuel cells, pumped hydro, thermal energy storage, and supercapacitors (Kharlamova et al., 2022, Li et al., 2020). Such diverse applications create new opportunities for research and innovation in digital twins. For instance, digital twins can monitor and manage heat transfer processes in thermal energy storage systems, while fuel cell systems could benefit from advanced fault diagnosis and lifetime prediction. Expanding digital twins to include these systems can provide more comprehensive solutions for energy storage and management.

Lifecycle integration has emerged as a core focus in digital twin research, underscoring the deployment of these technologies across the entire lifecycle of energy systems—from design and production to operation and maintenance (Merkle et al., 2019). This holistic approach facilitates system optimisation, cost-efficiency, and enhanced operational performance across the entire system's lifecycle (Naseri et al., 2023). Moreover, lifecycle integration enables predictive maintenance through real-time monitoring and comprehensive data analysis during the operational phase. Consequently, future research is anticipated to prioritise the refinement of DT models to ensure seamless integration across each phase of energy system development, thereby enhancing overall system efficiency and reducing operational risks.

Finally, the formulation of standardised digital twin frameworks and protocols is pivotal for advancing research in this domain. The lack of universally accepted standards for digital twin deployment, coupled with inconsistencies in system design, data management, and communication protocols, poses considerable challenges for large-scale implementation. As digital twin technology advances, the establishment of standardised frameworks ensuring interoperability and scalability across a diverse array of energy storage systems will emerge as a top research priority. Such frameworks will facilitate the seamless integration of digital twins into diverse energy infrastructures, thereby promoting widespread adoption and optimising overall system performance.

In conclusion, the future of digital twin research for energy systems is driven by advancements in AI, real-time data analytics, cybersecurity, and the expansion of applications across various energy storage technologies. As digital twin technologies continue to evolve, their potential to optimise energy storage and management systems will become increasingly important, particularly in supporting the transition to more resilient and sustainable energy grids. By addressing current challenges and exploring new applications, digital twin research will play a pivotal role in shaping the energy systems of the future.

2.4 Research and Applications of Battery Digital Twin

The development of BDT technology has seen considerable progress, driven by its ability to transform the management of energy storage systems through advanced monitoring, predictive maintenance, and optimisation. A digital twin replicates the physical battery system in a virtual environment, providing real-time insights into its performance. This section investigates the current research and various applications of BDT, focusing on its role in improving grid stability, integrating renewable energy, and managing EV batteries. By exploring both theoretical advancements and practical implementations, this section sheds light on how BDT is evolving within the energy sector.

2.4.1 Battery Digital Twin

Digital twin technology harnesses sophisticated physical models, intelligent sensor readings, and comprehensive operation and maintenance data history, amalgamating multidisciplinary insights for a simulation process that spans various physical quantities, temporal scales, and probability scenarios. Such twins provide an authentic representation of energy storage systems within a virtual domain, capable of real-time updates and dynamic evolution, thereby mirroring the full lifecycle of the pertinent energy system (Zhou et al., 2019).

While research into batteries has deepened and advanced over the years, numerous challenges persist. State estimation for Li-ion batteries serves as a foundational element for both battery management systems and battery equilibrium management, critical in averting overcharge or over-discharge situations. Nevertheless, crafting accurate models for lithium-ion batteries remains an intricate task, given the pronounced non-linearity and tight interrelation of internal battery dynamics (Rae and Bradley, 2012). DT technologies have demonstrated notable efficacy in the aerospace domain, particularly in SOC estimation, RUL predictions, and optimal controls (Wu et al., 2020), suggesting their potential applicability to battery state management issues.

The integration of DT with BMS commenced recently, further enhanced by the incorporation of cloud computing and IoT frameworks (Botta et al., 2016). Present-day investigations into battery digital twins primarily address three core challenges inherent to contemporary BMS: the complexities in data integration from diverse BMS providers, the constrained computing power of embedded systems, and the restricted data storage capabilities. A synthesis of battery management systems utilising digital twin technologies, alongside their functionalities and methodologies, is outlined in Table 1.1.

To address the data-sharing challenges in battery management, Li (Li et al., 2020) integrated DT technology, consolidating all battery-related data into a cloud-based platform to enhance the BMS structure. This integration is critical as the volume of battery data surges, resulting in exponential increases in computational and storage demands for BMS. To navigate these complexities, machine learning approaches, particularly data scarcity models, are utilised to predict and refine system states, offering new insights into battery ageing processes. A notable example is the study,

Table 1.1 Battery digital twin in literature

Years	The functionality of applying DT	Related methods and algorithms
2018 (Baumann et al., 2018)	Monitoring cell voltage and temperature for decision-making	Cloud-connected BMS; electric-thermal model and empirical ageing model
2019 (Peng et al., 2019)	Assessment of spacecraft lithium-ion battery pack degradation based on low-cost modules and software	ECM with SVM and filter algorithms; LabVIEW for visualisation
2019 (Ramachandran et al., 2019)	Estimation of SOC	ECM and EFK algorithm
2020 (Qu et al., 2020)	Estimation of the battery discharge capacity	Health indicator and LSTM algorithm
2020 (Li et al., 2020)	Estimation of SOC and SOH	AEHF-based SOC estimation algorithm and PSO-based SOH estimation algorithm
2021 (Sancarlos et al., 2021)	Estimation of cell voltage, anode/cathode bulk SOC and surface SOC	Sparse-Proper Generalised Decomposition (s-PGD) and dynamic mode decomposition technique
2021 (Merkle et al., 2021)	Estimation of SOC, capacity and internal resistance	ECM model parameter fitting, curve fitting and SOC-OCV curve
2021 (Tang et al., 2021)	Estimation of SOC and monitoring and visualisation of real-time voltage and current	ECM and joint HIF-PF online estimation of SOC
2022 (Qin et al., 2023)	SOH Estimation	Gaussian Regression, LSTM, Dropout in LSTM, Cycling synchronisation, MPC
2023 (Reniers and Howey, 2023)	Thermal Management, Electrical Coupling, Degradation Analysis	'Always on' method, PI controller, SEI growth model

(Qu et al., 2020), which combines a Health Indicator (HI) with the LSTM network for precise estimation of battery discharge capacities.

However, the digital twins' real-time and self-evolving capabilities warrant further improvement. The following sections delve into the use of digital twins for SOC estimation. Research (Sancarlos et al., 2021) introduces a 'Hybrid Twin', a pioneering DT model for lithium-ion batteries in the automotive sector. These methods significantly boost the real-time performance and flexibility of BMS. Similarly, a study (Merkle et al., 2021) establishes a digital battery twin and data pipeline for electric vehicle batteries, leveraging a cloud-based system for health and performance analysis, underscoring digital twins' role in enhancing battery system management in vehicles. Tang (Tang et al., 2021) proposes a digital twin-supported framework to surmount BMS constraints, using a joint HIF-PF online algorithm for precise SOC estimation and efficient real-time monitoring. This approach exemplifies the transformative impact of digital twin technology in BMS. Paper (Qin et al., 2023) details a digital twin framework for real-time SOH assessment of lithium-ion batteries under variable conditions, utilising a unique method that incorporates energy discrepancy-aware cycling synchronisation and time-attention modelling, facilitating accurate SOH predictions without complete discharge cycles. Lastly, another study (Reniers and Howey, 2023) models a large-scale, grid-connected lithium-ion battery system through a digital twin methodology, focusing on the influence of system design and ancillary controls on degradation and efficiency, thereby highlighting digital twins' effectiveness in optimising battery system performance.

Deep learning, a specialised branch of machine learning, has gained prominence across various scientific disciplines, primarily due to its exceptional capability to model complex non-linear relationships. Utilising architectures like neural networks, and deep learning algorithms autonomously extract feature representations from raw data, eliminating the necessity for manual feature engineering. This unique strength has elevated deep learning to a pivotal role in numerous applications, ranging from computer vision to natural language processing.

Within the context of Li-ion battery research, deep learning's integration has marked a significant paradigm shift. The inherent complex dynamics and non-linear behaviours of Li-ion batteries pose challenges that often surpass the capabilities of traditional modelling techniques. However, deep learning, adept at unravelling these complex patterns, provides a solution to these intricacies.

LSTM, a specialised form of Recurrent Neural Networks (RNN), are particularly lauded for their proficiency in processing sequential data. A testament presented the Auto-CNN-LSTM model. By merging convolutional neural networks with LSTM, this model offers enhanced predictions for the remaining useful life of lithium-ion batteries, marking a milestone in battery prognostics (Ren et al., 2020). Reinforcing this, a study highlighted the superiority of LSTM-based models over traditional neural networks in predicting the RUL of such batteries (Long et al., 2019).

TCN, characterised by its sequence-focused convolutional design, have also made significant strides in Li-ion battery research. For instance, Bi et al. undertook a comparative analysis of LSTM and TCN for estimating the SOH of lithium-ion batteries. Their research accentuated the advantages of TCN in recognising long-term data patterns, indicating a promising avenue for subsequent studies (Bi et al., 2022). Further emphasising the adaptability of TCN, Liu delved into the combination of TCN with transfer learning, revealing breakthroughs in SOC estimation for lithium-ion batteries (Liu et al., 2021b).

To conclude, the adoption of deep learning architectures, especially LSTM and TCN, has undeniably advanced the domain of Li-ion battery research. Their advanced methodologies in analysing sequential data forecast a bright future for the development of battery management systems, prognostics, and health monitoring.

2.4.2 Battery Situational Awareness

Digital twin applied physical models, intelligent sensors, comprehensive operation and maintenance data history, amalgamating multidisciplinary insights for a simulation process that spans various physical quantities, temporal scales, and probability scenarios. Such DT provides an authentic representation of energy storage systems within a virtual domain, capable of real-time updates and dynamic evolution, thereby mirroring the full lifecycle of the pertinent energy system (Zhou et al., 2019).

Battery situation awareness (BSA) is important for the effective management of battery systems, encompassing the monitoring of key parameters, accurate state estimation, and predictive maintenance (PdM). This section reviews existing methodologies and recent advancements in BSA, focusing on battery monitoring and state estimation.

Battery monitoring is a foundational aspect of BSA, providing essential data to understand and manage battery performance. Effective monitoring involves the continuous measurement of critical parameters such as current, voltage, and temperature. These parameters are important for assessing the operational state and health of battery systems, especially in high-demand applications like electric vehicles and renewable energy storage.

The complexity and non-linearity of battery systems necessitate advanced monitoring techniques to enable safety, reliability, and optimal performance. Traditional BMS rely on embedded sensors to capture these metrics in real-time, providing important data for evaluating battery health and performance.

Precise monitoring of current, voltage, and temperature is important for efficient battery management, as each parameter significantly influences battery performance, safety, and lifespan. Current monitoring is essential for determining charge and discharge rates, which directly impact the calculation of the SOC and the prediction of battery behaviour under varying load conditions. Traditional methods, such as the use of shunt resistors and Hall-effect sensors, provide highly accurate real-time current data (Plett, 2004). However, recent advances in sensor technology and data acquisition systems have further improved measurement precision and reliability (Khaneghah et al., 2023). Similarly, voltage monitoring plays a pivotal role in SOC estimation and anomaly detection, including the prevention of overcharging and deep discharging. Advanced voltage monitoring systems, which employ differential voltage techniques and high-precision analogue-to-digital converters (ADCs), are capable of detecting minute voltage variations, providing valuable insights into battery dynamics and aiding in the identification of cell imbalances within battery packs (Ci et al., 2020). This capability is critical for implementing effective balancing strategies that enhance battery longevity and performance. Temperature monitoring, another key factor, directly impacts battery efficiency and safety. Modern battery management systems employ multiple temperature sensors distributed throughout the battery pack, utilising methods such as infrared thermography and fibre optic sensing for high-resolution temperature mapping (Lin et al., 2021). This comprehensive thermal management strategy allows the battery to operate within optimal temperature ranges, thereby extending its lifespan and enabling overall safety.

Recent advancements in battery monitoring have introduced techniques like Electrochemical Impedance Spectroscopy (EIS) and fibre optic sensing. EIS measures the impedance of the battery across a range of frequencies, providing detailed insights into the electrochemical processes and the health status of the battery. This technique helps in identifying internal degradation mechanisms that are not detectable through traditional monitoring methods. Fibre optic sensors offer high sensitivity and immunity to electromagnetic interference, making them ideal for monitoring in harsh environments (He et al., 2013). These advanced techniques complement traditional monitoring methods by providing additional layers of diagnostic information, enhancing the overall accuracy and robustness of battery monitoring systems. By continuously monitoring these parameters, battery management systems can detect early signs of degradation, optimise charging and discharging cycles, and enable the overall safety and reliability of the battery system. The integration of advanced monitoring techniques enhances the accuracy and robustness of data, providing a solid foundation for further state estimation and predictive maintenance.

Battery state estimation is another important component of BSA, providing key insights into the battery's current status and predicting future performance. Accurate estimation of battery state such as SOC and SOH is essential for enabling the reliability, efficiency, and safety of battery systems. The inherent complexity and non-linearity of battery systems pose significant challenges for state estimation. Advanced methodologies and models are necessary to achieve accurate and reliable estimations, which are vital for effective battery management.

SOC estimation represents the available capacity of the battery relative to its total capacity. It is a fundamental metric for managing battery operations and informing decisions on charging and discharging cycles. Various methods for SOC estimation have been developed, each with its advantages and limitations: a) Coulomb Counting: This method tracks the charge entering and leaving the battery. It is straightforward and widely used but susceptible to cumulative errors over time due to current measurement inaccuracies and initial SOC estimation errors (Plett, 2004). b) Voltage-Based Methods: These methods correlate the battery voltage with its SOC. While simple and easy to implement, they can be inaccurate due to the non-linear relationship between voltage and SOC, especially under varying load conditions (He et al., 2013) c) Model-Based Approaches: Techniques such as Kalman filters and neural networks utilise mathematical models to estimate SOC with higher accuracy. Kalman filters, including the Extended Kalman Filter (EKF) and Unscented Kalman Filter (UKF), are popular due to their ability to handle non-linear systems and incorporate measurement noise. Neural networks offer the potential to learn complex patterns in the data, further enhancing SOC estimation accuracy. Recent advancements have seen the integration of machine learning algorithms to further refine SOC estimation. These approaches leverage large datasets and advanced computational techniques to improve accuracy and robustness across various operating conditions.

SOH estimation provides insights into the overall condition and degradation of the battery. It typically involves evaluating parameters such as capacity fade, internal resistance increase, and self-discharge rates. Accurate SOH estimation is important for predicting battery lifespan and scheduling maintenance. Advanced techniques for SOH estimation include a) EIS: EIS measures the impedance of the battery across a range of frequencies, providing detailed insights into the electrochemical processes and health status of the battery. This technique can identify internal degradation mechanisms not detectable through traditional monitoring methods (Hu et al., 2012). b) Data-driven approaches: These models analyse historical performance data to predict future health trends. Techniques such as support vector machines (SVM), random forests, and deep learning models have been employed to enhance the accuracy and reliability of SOH estimations. These models can capture complex relationships between different health indicators and the overall battery condition (Fan et al., 2019).

2.4.3 Battery Digital Twin for Decision Support

DT technology in battery systems is critical for supporting decision-making processes, especially in energy management, maintenance scheduling, and optimising energy storage operations (Jafari and Byun, 2022). By establishing a real-time, data-driven virtual replica of a physical battery, the DT simulates various scenarios, predicts outcomes, and supports key operational decisions. Combining real-time monitoring with predictive capabilities allows optimal energy system performance, reduces operational costs, and mitigates potential risks.

A key function of DTs in decision support is optimising battery management (Wang et al., 2022). DT enables operators to simulate various charging and discharging patterns, identify inefficiencies, and optimise energy flows to match grid or end-user requirements. For instance, by leveraging historical and real-time data, the DT can predict peak demand periods and adjust charging cycles to ensure energy availability when needed, thereby preventing grid overload and lowering electricity costs (Tang et al., 2022).

For predictive maintenance, DT provides significant decision support by forecasting the optimal timing and location for maintenance activities (Krishna et al., 2022). Batteries degrade over time, and without timely intervention, their efficiency decreases, resulting in higher operational costs and potential system failures. DT can monitor the key parameters in real-time, enabling operators to predict when maintenance or replacement is necessary. This capability decreases the likelihood of unexpected breakdowns and prolongs battery lifespan. Predicting maintenance needs based on real-time data enables operators to avoid reactive maintenance strategies, which are typically more costly and disruptive.

DT also facilitates fault diagnostics, enabling rapid decision-making when issues arise (Xu et al., 2019). By continuously analysing battery system data, the DT identifies abnormalities, such as unexpected temperature fluctuations, voltage irregularities, or sudden capacity drops, which may signal faults or potential failures. The DT can simulate the impact of these faults on system performance and suggest corrective actions. This is particularly valuable for ensuring the safe operation of lithium-ion batteries, where undetected issues could cause hazardous situations like thermal runaway. Through real-time diagnostics, DTs enhance the overall safety and reliability of energy storage systems.

2.5 Summary

This chapter provides a comprehensive review of the literature on BESS and their integration with DT technology, focusing on three main areas: fundamental components and architectures of BESS, the evolution and applications of DT in battery systems, and emerging research trends and practical implementations of DT in energy systems.

The review emphasises the role of BESS in modern energy infrastructures, particularly in supporting renewable energy integration and ensuring grid stability. Despite significant technological advancements, challenges including battery degradation, limited energy density, and high operational costs still hinder the widespread adoption of BESS. To address these limitations, research focuses on alternative battery chemistries, such as sodium-ion and solid-state batteries, while also enhancing BMS through advanced operational strategies. However, existing frameworks for BESS management lack a cohesive integration of multi-source data such as sensor inputs and environmental factors with adaptive decision-making capabilities to address dynamic operational uncertainties.

The examination of digital twin technology highlights its evolution from a theoretical framework to a robust tool for real-time monitoring, predictive maintenance, and operational optimisation. When integrated with BESS, DT technology offers advanced capabilities for SOC, SOH estimation and RUL prediction, thereby enabling more precise and effective battery management. Integrating DT with BMS enhances the system's predictive and analytical capabilities, which are essential for mitigating safety risks and optimising battery performance throughout its operational life. Yet, prior studies hard to unify physics-based models with machine learning algorithms in hierarchical DT architectures to improve state estimation accuracy.

The chapter also explores practical applications and current research in battery digital twin technology, demonstrating its potential to optimise the performance, safety, and sustainability of energy storage systems. Advanced modelling techniques, machine learning algorithms, and real-time data analytics significantly enhance the predictive and diagnostic capabilities of digital twins. These methodologies enable more accurate predictions of battery degradation and maintenance needs, minimising operational disruptions and extending BESS lifespan. Nonetheless, current DT implementations neglect the integration of multi-faceted situational awareness such as real-time technical performance, economic constraints, and environmental impacts into unified operational strategies.

The chapter concludes by summarising the key findings and identifying research gaps that need to be addressed to fully leverage the benefits of digital twin technology in BESS. Future research should focus on developing standardised frameworks for DT integration, refining real-time analytic algorithms, and expanding DT applications to emerging battery chemistries and diverse energy storage systems. Critically, existing literature does not bridge the gap between RUL predictions and actionable operational optimisation strategies, leaving a disconnect between degradation analytics and decision support. Addressing these challenges will position DT technology as an essential tool for optimising BESS efficiency, reliability, and safety, ultimately contributing to broader energy sustainability and decarbonisation goals.

Chapter 3 A Framework for Digital Twin-Driven of Battery Storage

3.1 Introduction

Battery storage systems are becoming increasingly critical in modern energy infrastructures, especially with the rise of renewable energy sources (Nazaralizadeh et al., 2024). Emerging technologies such as digital twins, artificial intelligence, and the IoT have accelerated advancements in battery management and optimisation. DT technology, which involves creating a virtual replica of physical systems, is being integrated into battery storage solutions to enhance performance and predictive maintenance. However, traditional methods for battery state estimation and management have been applied in a limited number of studies, as reviewed in Chapter 2. Currently, there is a lack of comprehensive frameworks that address the complexities of battery systems under dynamic conditions. The industry must explore a framework that utilises DT technology to improve battery situation awareness and extend battery life. In this chapter, a framework is designed for digital twin-driven battery storage based on multi-source data and advanced machine learning techniques. The data and methodologies relevant to the proposed framework are introduced in Section 3.2.

3.2 DT-Driven Framework of Battery Energy Storage Systems

According to the literature review in Chapter 2, besides traditional battery state estimation methods, it is acknowledged that integrating multi-source data and domain knowledge is of great significance in enhancing the accuracy and reliability of BESS. Existing studies mainly focus on modelling based on either physical battery models or data-driven approaches, while the combination of these methods, along with the utilisation of multi-source data, is not fully exploited. With the development of the IoT and advanced machine learning techniques, it is now possible to collect and process comprehensive data concerning battery performance and state estimation. Hence, it is of great importance to introduce a framework that leverages multi-source data and integrates both model-driven and data-driven techniques for improved battery state estimation and management.

Meanwhile, DT technology exhibits remarkable potential in providing dynamic and accurate representations of physical battery systems, enabling real-time monitoring and predictive maintenance (Chen et al., 2023). By integrating advanced machine learning models, such as TCN, LSTM, CNN, and Transformer models, the DT framework offers a more comprehensive solution than traditional methods. While other techniques may struggle to adapt to the nonlinearities and temporal dependencies inherent in battery data, the proposed framework effectively handles these complexities. Furthermore, the inclusion of rolling transfer learning and self-evolution mechanisms allows the DT to adapt and evolve as new data and conditions emerge, allowing continuous accuracy and relevance.

In this context, exploring how to combine different techniques is essential for the development of an effective framework. The proposed framework is illustrated in Figure 3.1. It includes the following stages: multi-source data acquisition on the physical end, data preprocessing and integration on the cloud end, DT model development on the digital end, advanced state estimation using machine learning algorithms on the output end, and decision support for operators. The framework is designed concerning concepts in DT technology and advanced machine learning, which are detailed in the Appendix. Firstly, comprehensive data from various sources, including real-time sensor data and historical records, are collected alongside domain knowledge from empirical studies and existing literature. Secondly, data preprocessing is conducted to filter noise and normalise the data for consistency. Thirdly, the DT model is constructed, serving as a dynamic representation of the physical BESS. Then, by employing advanced machine learning techniques, the model enhances SOC and SOH estimations. Lastly, the results from the machine learning models are used for decision support regarding predictive maintenance, optimisation strategies, and extending the lifespan of the battery system.

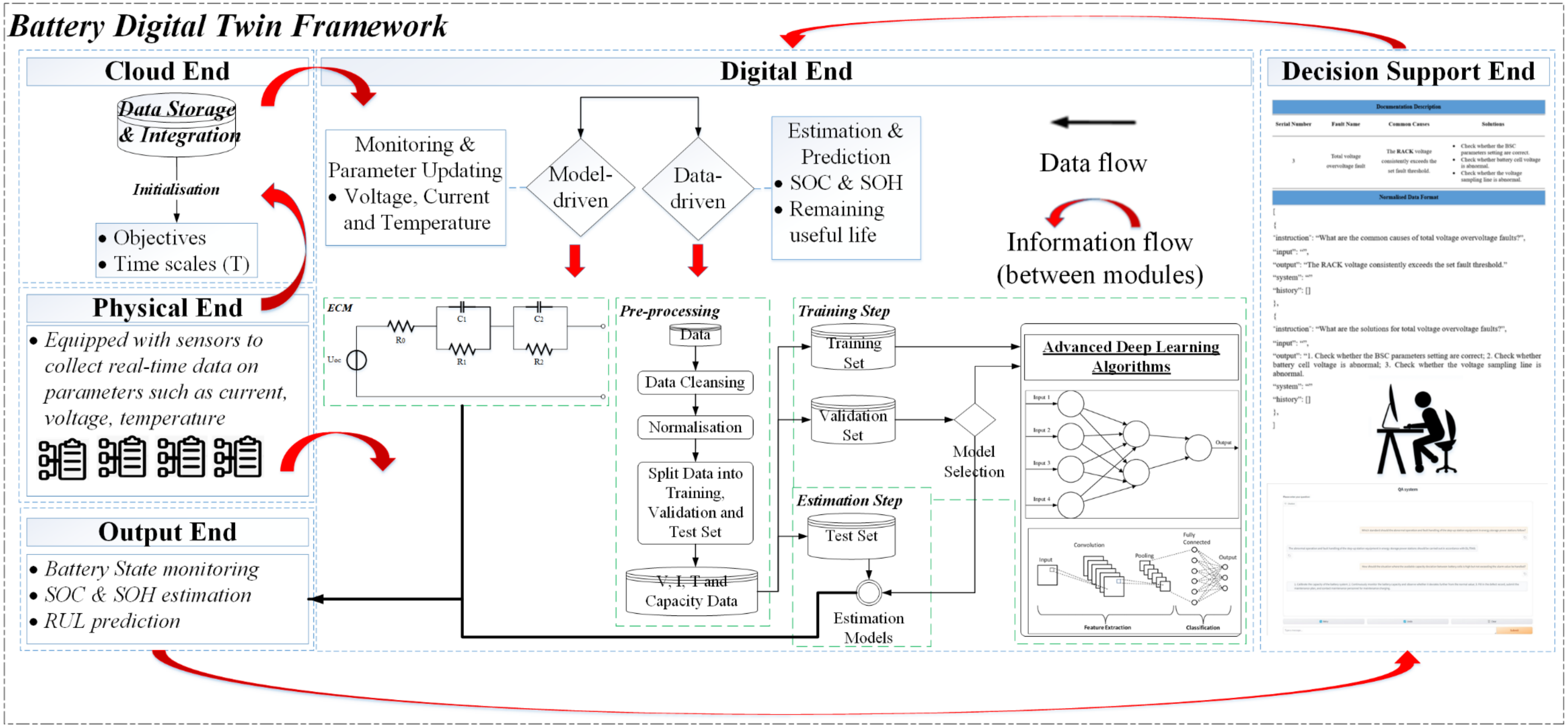


Figure 3.1 The proposed overall digital twin framework for battery.

Physical End: This end comprises the actual battery system equipped with sensors that collect real-time data on parameters such as current, voltage and temperature. These sensors provide the foundational data required for accurate state estimation.

Cloud End: Data collected from the physical layer is transmitted to this end, where it is integrated and pre-processed. This involves filtering noise, normalising data, and enabling consistency across different data sources.

Digital End: This end hosts the DT models that replicate the physical battery's behaviour. It includes electrochemical models, thermal models, and ageing models that work together to provide a comprehensive representation of the battery's state. The models are continuously updated with real-time data to maintain accuracy. Advanced algorithms, such as CNN and Transformer models, are employed on the digital end to estimate SOC and SOH. These models analyse historical and real-time data, leveraging machine learning techniques to predict future states and detect anomalies.

Output End: This end delivers critical outputs such as cell status monitoring, SOC estimation, and reliability recommendations, which assist technicians in making informed decisions.

Decision Support end: The topmost end provides insights and recommendations based on the estimations and predictions. This layer includes user interfaces that allow stakeholders to interact with the digital twin, visualise data, and make informed decisions regarding battery management.

The Digital End hosts comprehensive DT models—including electrochemical, thermal, and ageing models—utilising advanced algorithms (such as CNN and Transformer) to replicate the physical battery's behaviour, estimate critical parameters (SOC, SOH), predict future states, and detect anomalies. Conversely, the Cloud End primarily functions as a data integration and pre-processing hub, managing data filtering, noise reduction, and normalisation to ensure consistent, high-quality inputs to the DT models.

The Digital End operates locally, offering real-time state estimation and immediate response capabilities directly at the battery system, while the Cloud End performs more computationally intensive predictive tasks, such as long-term degradation modeling and fleet-level optimisation.

3.2.1 Multi-source Data Acquisition

The processes preceding battery performance degradation are considered potentially significant. For instance, data related to charging and discharging cycles, as well as environmental conditions, should be collected throughout all operational stages of BESS. It is important to note that when collecting battery data—typically recorded in a multivariate time-series format—the temporal relevance and quality of the data must be carefully considered. Since battery performance can fluctuate due to various factors, continuous monitoring provides valuable information about the system's behaviour over time. In this context, data are collected systematically during normal operation, capturing comprehensive observations that reflect the battery's condition under different scenarios.

In addition to operational data, environmental factors such as temperature and humidity are also collected. These factors can influence battery performance from an external perspective, affecting aspects like thermal stability and degradation rates. Integrating this multi-source data into the Physical End of the DT framework enables a comprehensive representation of the BESS. By systematically capturing and transmitting high-quality data, the Physical End provides the foundational layer for constructing the DT, facilitating accurate modelling and analysis in subsequent stages.

In complex system environments like BESS, constructing the backbone of a DT is challenging without collaboration from domain experts. In domain-specific data representation, each data element is described using standardised formats and models, utilising open-source platforms. These platforms facilitate the building and storage of domain-specific data repositories. The DT model is developed based on refining the hierarchical structure and establishing relationships among various data parameters. Studies related to battery degradation and fault analysis can be categorised into four different facets: electrochemical degradation, mechanical stresses, thermal issues and electrical anomalies.

3.2.2 Data Preprocessing and Integration

After obtaining the data from various sources it is necessary to process and combine it carefully for better reliability in future modelling. As emphasised by domain experts, the heterogeneity of battery data presents significant challenges in data integration. For example, data collected from various sensors may differ in formats, sampling rates, and measurement units. It is necessary to standardise these data into a common framework to facilitate accurate analysis (Rathore et al., 2021).

In this context, data preprocessing involves several critical steps, including data cleaning, noise reduction, normalisation, and time synchronisation. Outliers and missing values are identified and addressed appropriately to maintain data integrity. Integrating the pre-processed data into a unified format enables the seamless development of the DT model on the digital end. Cloud computing resources and data management platforms are employed to store and manage large volumes of data efficiently (Wu et al., 2020). The utilisation of standard data representation formats and protocols enhances interoperability among different system components.

Constructing the backbone of the DT model relies significantly on the quality of the integrated data. In complex systems like BESS, achieving effective data integration is challenging without collaboration from domain experts. Standardised data representation and storage facilitate the development of robust DT (Lyu et al., 2020). The cloud end thus serves as an essential intermediary between the physical end and the digital end, providing high-quality data for accurate simulation and state estimation.

Studies related to data integration and preprocessing in battery systems often categorise challenges into four facets: data heterogeneity, data quality issues, scalability concerns, and security considerations (Li et al., 2019b). Addressing these challenges in the cloud end enhances the overall effectiveness of the DT-driven framework. The integrated and pre-processed data support advanced analysis and state estimation methods, which are discussed in Section 3.2.3.

The multi-source data collected from the Physical End differ in type and granularity. To utilise these data effectively for modelling, the initial step involves data mapping and harmonisation. For example, operational data such as current and voltage measurements may be recorded at high frequencies with sampling rates in milliseconds, whereas batch data like maintenance logs are recorded per event. Therefore, the data need to be aligned to the same granularity before being used.

Data repositories in battery management systems are often fragmented, with information distributed across various platforms, resulting in significant efforts in data integration and alignment from domain experts. In complex systems like BESS, processes are highly interdependent and complex. Processing such data using conventional approaches is typically time-consuming and labour-intensive. Moreover, it is essential that data cleaning and feature extraction are performed accurately for effective model development, but these tasks are often challenging when dealing with large-scale, multi-source. In this context, data are often incomplete and noisy, with missing values or inconsistencies. Consequently, the pre-processed data need to be refined or completed to be effectively utilised in the DT framework.

By integrating these pre-processed data into the cloud end of the DT framework, a unified and standardised data repository is established. This repository facilitates seamless data flow to the digital end, where advanced modelling and analysis are conducted. Addressing data quality and integration challenges enhances the reliability of the DT framework, enabling more accurate state estimation and predictive analytics, which are discussed in Section 3.2.3.

3.2.3 Advanced State Estimation

In the digital end of the DT framework, advanced state estimation methods are essential for accurately predicting the SOC and SOH. These metrics are fundamental to effective battery management, informing decisions related to charging cycles, maintenance schedules, and overall operational efficiency. By integrating model-driven and data-driven approaches, the DT achieves a comprehensive estimation process that leverages both real-time data and historical patterns of battery behaviour (Liu et al., 2023).

The SOC estimation process within the DT determines the remaining charge in the battery relative to its total capacity, a task complicated by varying operational conditions and battery degradation over time. The Equivalent Circuit Model (ECM) forms the foundation of SOC estimation in the model-driven approach. Using electrical components such as resistors and capacitors, the ECM represents the internal dynamics of the battery and its ability to store and deliver charge. Real-time sensor data from the Physical End, including voltage, current, and temperature measurements, continuously update the ECM (Farag et al., 2014). This real-time data integration allows the ECM to reflect the battery's current condition more accurately, enhancing the precision of SOC estimates under diverse operating scenarios.

Complementing the model-driven approach, the DT incorporates data-driven methods to further refine SOC estimation. Machine learning techniques process extensive amounts of operational data, enabling the DT to recognise patterns and account for nonlinearities in the battery's performance over time. By analysing both real-time data and historical records, the DT learns to predict SOC more accurately under conditions that may not be fully captured by physical models alone (Ma et al., 2016). This combination of model-driven and data-driven modelling results in a robust framework for SOC estimation, allowing the DT to adjust battery management strategies based on reliable state predictions.

SOH estimation, another key function within the DT, assesses the long-term health of the battery and predicts its future performance. As the battery degrades due to factors such as ageing, temperature variations, and repeated charge-discharge cycles, its ability to retain a full charge diminishes. The ECM plays a significant role in tracking these changes by accounting for internal resistance and capacity fade, which directly influence the battery's overall health (Chen et al., 2018). The model-driven approach enables the DT to simulate how these factors evolve as the battery ages, providing accurate SOH estimates that inform maintenance decisions and potentially extend the battery's usable life.

The data-driven approach complements the physical model by identifying patterns in the battery's performance data that may not be immediately apparent. By processing large datasets of historical battery behaviour, the DT can anticipate future degradation trends and predict when maintenance or replacement may be necessary (Chen et al., 2018). This enables a proactive approach to battery management, where potential issues are addressed before they lead to significant performance losses. The data-driven methodology thus enriches the SOH estimation process, offering a more holistic view of the battery's health.

A notable feature of advanced state estimation within the digital end is its hybrid nature, combining the strengths of model-driven and data-driven techniques. The ECM provides a physics-based foundation that captures the battery's internal characteristics, while data-driven models enhance predictive accuracy by incorporating operational data into the estimation process (Li et al., 2019b). This hybrid approach allows the DT to produce both real-time SOC and SOH estimations and long-term performance forecasts, improving overall battery management. The integration of real-time data from the physical end with the processing capabilities of cloud computing resources enables the DT to handle the high volume of data required for accurate predictions, offering valuable insights into battery performance under various conditions (Botta et al., 2016).

The continuous learning process embedded in the DT framework is further strengthened through rolling transfer learning. This method allows the DT to adapt its models as the battery's characteristics evolve. As new data become available, the DT updates its existing models to reflect the battery's current state without requiring complete retraining. This approach is particularly important for long-term battery management, as it maintains the DT's responsiveness to gradual changes in the battery's performance, such as capacity loss or increased internal resistance. By periodically integrating new data into the existing framework, the DT maintains a high level of accuracy in its SOC and SOH predictions over time.

Rolling transfer learning allows the DT to remain relevant throughout the battery's lifecycle, continuously refining its estimations as the battery ages. This process not only improves the immediate accuracy of SOC and SOH predictions but also enhances the long-term predictive capabilities of the DT. As a result, the system is better equipped to support informed decisions about maintenance, charging strategies, and operational adjustments, all of which contribute to optimising the battery's performance and extending its lifespan.

In summary, the advanced state estimation methods employed within the digital end of the DT framework provide a comprehensive solution for managing the performance of BESS. By combining model-driven and data-driven approaches, the DT delivers highly accurate SOC and SOH estimations that are continuously updated through rolling transfer learning. This hybrid methodology allows the DT to remain adaptive and capable of providing reliable, real-time insights into battery performance, supporting more efficient battery management and predictive maintenance strategies.

3.2.4 Decision Support for Battery Energy Storage Systems

The final component of the DT framework for BESS is the decision support mechanism, which leverages insights from advanced state estimation to optimise battery management strategies. This system integrates outputs from the digital end with user interfaces and analytical tools to facilitate informed decision-making regarding the operation, maintenance, and overall management of the BESS.

The primary function of the decision support system is to translate SOC and SOH estimations, along with other relevant performance metrics, into actionable recommendations. By providing a comprehensive view of the battery's current state and projected performance, the system enables operators to make data-driven decisions that enhance the efficiency, reliability, and longevity of the battery system. For example, accurate SOC estimations assist in scheduling charging and discharging cycles to optimise energy usage and prevent overcharging or deep discharging, which can adversely affect battery health (Teng et al., 2012).

Moreover, the decision support system facilitates predictive maintenance by utilising SOH estimations to anticipate potential failures or degradation trends. Identifying early signs of battery deterioration allows for proactive maintenance planning, reducing downtime and avoiding unexpected system failures (Meng and Li, 2019). This predictive approach contributes to cost savings by extending the battery's operational life and minimising maintenance expenses. The integration of user interfaces and visualisation tools enhances the usability of the decision support system. These interfaces present complex data and analytical results in an intuitive format, allowing operators and stakeholders to interpret information effectively (Yang et al., 2021b).

Overall, the decision support mechanism within the DT framework serves as a bridge between advanced state estimations and practical battery management actions. By providing accurate, timely, and actionable information, it enhances the effectiveness of BESS operations and contributes to the system's overall performance and sustainability.

3.3 Summary

With the advancement of connectivity and intelligence in modern energy systems, the integration of DT technology has become increasingly significant for battery management. In a data-rich environment, multi-source data and domain knowledge relevant to battery performance can be collected and utilised for enhanced state estimation and predictive maintenance. A framework has been designed for battery management based on the integration of model-driven and data-driven approaches within the DT framework.

This framework encompasses multi-source data acquisition from the physical battery system, data preprocessing and integration in a cloud-based environment, and the development of a DT model that accurately represents the battery's behaviour. Advanced state estimation methods are employed to estimate SOC, and SOH and predict the RUL by combining physical modelling with data analytics. Continuous learning through rolling transfer learning allows the model to adapt as new data becomes available, maintaining accuracy over the battery's operational lifecycle.

The decision support system utilises outputs from the DT to facilitate informed decision-making regarding the operation, maintenance, and overall management of the BESS. By providing timely and actionable information, the system contributes to optimising BESS operations and enhancing the sustainability of energy systems.

Chapter 4 Digital Twin-Supported Battery State Estimation

4.1 Introduction

BESS has now emerged as a fulcrum within the prevailing energy face, specifically amid the global shift towards renewable energy sources such as wind and photovoltaic (PV) generation. However, this shift is not just a technological development it is a response to increasingly urgent issues of universal nature such as climate change, energy security, and sustainable development. The urgent challenge of lowering carbon emissions leads countries to prioritise BESS for energy reliability and grid stability (Mahela and Shaik, 2016). The shift towards a carbon-neutral power system, a goal of paramount importance, is laden with a spectrum of technical challenges. BESS present a practical solution to address specific issues within this spectrum. The main challenges that the project is facing are controlling intermittent renewable energy resources, real-time supply-demand balance and preservation of reliability and stability of the power grid. BESS plays a critical role in overcoming these obstacles, thereby facilitating a smoother transition to carbon-neutral energy systems.

Lithium-ion batteries, among the array of emerging storage technologies, have been at the forefront due to their inherent technological attributes coupled with economic considerations. This versatility has been proven in the field as diverse as the portable issue mobile phones, online-pop-frass grid-scale energy storage, electric vehicles et al.

Using these attributes of the batteries i.e. quick charging capacity, long cycle life, high specific energy; high specific power, rechargeable and without a memory effect, both their large and wide set have wider applications and wide research on optimisation and safety (Hannan et al., 2017). Monitoring parameters such as SOC is not a mere operational requirement but a safety imperative. Furthermore, the derivation of health indicators, such as SOH and RUL, through capacity or resistance measurements, is of paramount importance (Li et al., 2019b). However, the landscape of direct online measurements for battery state estimation is complex. Achieving reliable and real-time estimation in this domain is an ongoing challenge and a key area of research focus. This complexity is primarily due to the dynamic nature of battery behaviours and the need for high-precision data for accurate estimation(Harris et al., 2017, Hu et al., 2018a). Our research specifically addresses this gap by developing methodologies that increase the accuracy and reliability of battery state estimation in real time, thereby contributing to the field.

In the domain of BMS, the accurate estimation of SOC and SOH is not only critical for operational efficiency but also for ensuring the longevity and safety of the battery systems. These metrics serve as vital indicators of the battery's operational status and its degradation trajectory, respectively. Over the years, a plethora of methodologies have been proposed for SOC estimation, encompassing traditional techniques and more recent computational approaches (Chang, 2013, Ng et al., 2009, Li et al., 2018, Ma et al., 2016, Zou et al., 2015, Farag et al., 2014, Pop et al., 2005, Lee et al., 2008). The indirect nature of SOC measurement presents significant challenges, which require advanced methodologies for accurate estimation. This complexity has driven substantial research into developing reliable and robust SOC estimation methods, encompassing look-up tables, ampere-hour integration, and strategies based on filtering, observation, and data analytics. While the simplicity of look-up table and ampere-hour integral methods is appealing, their accuracy and robustness are compromised by sensor inaccuracies (Wang et al., 2020b, Hu et al., 2019). In contrast, filter-based and observer-based methods offer high precision, self-correction, and noise resistance but require detailed battery testing for model calibration (Shrivastava et al., 2019, Wu et al., 2022). Data-driven methods utilise machine learning algorithms to reduce the necessity for deep knowledge of a battery's electrochemical properties, focusing on the correlation between input and output (Tian et al., 2021). However, these approaches contend with potential overfitting or underfitting, tied to the quality of training data and the algorithmic framework, which can hinder their practical application.

The intricacies associated with battery ageing mechanisms assess SOH as a complex endeavour. Direct capacity measurement, while being the most straightforward indicator of battery health, is challenging in real-world scenarios. This has led to a shift towards indirect measurements, with parameters like internal resistance emerging as potential indicators of degradation. The research community has been actively exploring these indirect measurements, with a focus on their potential for predicting SOH and RUL (Tang et al., 2017, Spillner et al., 2013). However, the dynamic nature of battery operations, influenced by a myriad of factors including environmental conditions, usage patterns, and manufacturing inconsistencies, often poses challenges to these methodologies. These challenges include the difficulty in accurately predicting battery life, variability in performance under different environmental conditions, and the need to constantly adapt to varying usage patterns. Additionally, manufacturing inconsistencies can lead to significant variations in battery behaviour, further complicating the task of developing universally applicable estimation methods.

In recent years, the development of DT has undergone transformative advancements, with the emergence of cloud computing (Botta et al., 2016) and the IoT (Grieves and Vickers, 2017) leading the way. These innovations have presented solutions to the challenges traditionally faced by the BMS. Among these solutions is the concept of cloud-based digital twins, which involves crafting digital replicas of physical battery systems. These replicas, serving as virtual mirrors of their physical counterparts, transmit real-time battery data to cloud platforms. The synergy between these digital twins and the robust data processing, analytics, and storage capabilities of cloud platforms unlocks a plethora of applications, ranging from real-time monitoring, diagnostics, and anomaly detection to predictive maintenance and optimisation (Li et al., 2020, Grieves, 2014). However, the journey to seamlessly integrate digital twins into BMS is not without hurdles. Assembling precise digital models of batteries requires a diverse range of full-scale real-world datasets that are rarely available. Additionally, battery degradation, which is highly variable due to many factors, creates additional layers of complexity in the modelling process. Despite these challenges, the potential benefits of melding digital twins with BMS are manifold. They promise enhanced battery performance, bolstered safety measures, and an extended battery lifespan (Wu et al., 2020), heralding a promising future for BMS augmented by digital innovations.

In this study, a DT for battery systems is introduced, encompassing its structure, operational mechanisms, modelling, and state estimation. The TCN-LSTM network, as delineated herein, has been developed for the SOC estimation, SOH monitoring and RUL prediction of lithium-ion batteries. Its effectiveness is corroborated through comprehensive validation. The notable work of this research encompasses: 1) Established DT for computing SOC, SOH, and RUL across diverse operational conditions, obviating the requirement for multiple models or reference tables. 2) Established the TCN-LSTM network which directly captures measurements from the battery, thus facilitating streamlined SOC estimation. 3) Introduced an approach that considers the impact of local regeneration on SOH monitoring, utilising the LSTM-TCN network for enhanced battery performance prediction. 4) The incorporation of transfer learning, allows the DT to be configured for various battery conditions, thereby mitigating modelling costs and dataset prerequisites.

The remainder of this chapter is structured as follows. Section 4.2 outlines the brief review of battery state estimation. Section 4.3 articulates the proposed framework and relevant algorithms associated with battery digital twins. In Section 4.4, the SOC and

SOH estimation, as well as RUL prediction using the TCN-LSTM network, are detailed, followed by results analysis and discussion in Section 4.5. Section 4.6 summarises this chapter.

4.2 Battery State Estimation

The management of batteries is critical for the optimal operation, safety, reliability, and cost efficiency of prevalent battery-powered energy systems, including electrified transportation and renewable-integrated smart grids (Hu et al., 2017). Given the intricate electrochemical dynamics and multi-physics interactions, a simplistic, black-box approximation of batteries, which solely measures voltage, current, and surface temperature, is insufficient for developing high-calibre battery management systems. A central technological advancement for advanced battery management lies in the precise and consistent estimation and monitoring of vital internal states. Reliable data on SOC and SOH are essential for proficient charging, thermal regulation, and overall health upkeep of batteries. Fundamental battery behaviours are typically delineated by a synergised electrochemical-thermal-aging framework, with each subcomponent of the multi-physics model operating on its distinct timescale. Notably, certain battery states, such as SOC, fluctuate contemporaneously due to rapidly evolving microscopic electrochemical attributes. The macroscopic temperature distribution undergoes adjustments at a median timescale, influenced by the battery's physical configuration and thermal transference properties. Conversely, the battery's SOH, associated with gradual variations in parameters like internal impedance augmentation and capacity degradation, exhibits minor shifts over brief durations. The overarching safety state of a battery can be ascertained through the assessment of the states previously mentioned. Figure 4.1 shows a general procedure of DT-supported battery state estimation that by data, mechanism and semi-empirical model, the dynamic model of the complex coupling system of battery and environment was accurately identified and evaluated.

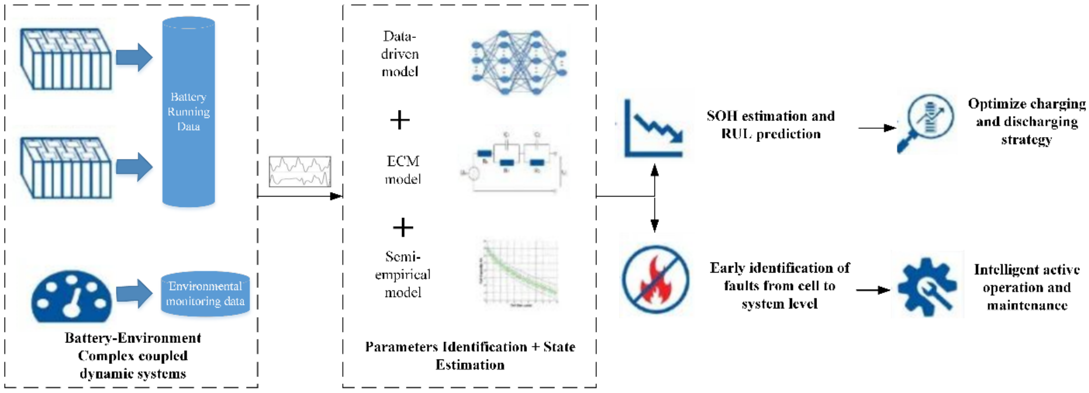


Figure 4.1 State estimation for the battery-environment coupled systems.

4.3 Technical Method

In this section, we delve into the virtual aspect of the framework, which integrates both model-driven and data-driven algorithms. These algorithms work in tandem, and their combined operation is central to the framework. As battery capacity decreases, an iterative learning methodology is employed to update the model parameters, enabling the continuous updating of the digital twin.

The DT framework is distinguished by its hierarchical structure, bidirectional interaction capability, and inherent ability to evolve autonomously. Within this structure, specific models are designed for various objectives, including state estimation, RUL prediction, and energy management. It is essential that data, regardless of its multi-dimensional nature, can flow smoothly across these hierarchical divisions.

Our research's primary objective is to leverage the DT to uncover the underlying relationship between the SOC and the variables measured. Figure 4.2 presents a detailed battery DT framework, which forms the backbone of our entire system. This system is organised into four key segments:

Physical End: This pertains to the real-world components of the system, such as battery packs, motors, BMS, and sensors. It enables real-time monitoring of parameters like open-circuit voltage, current, and temperature.

Digital End: This is the digital reflection of the physical components, designed to emulate real-world systems to meet specific objectives. At its core, it employs a mix of algorithms, both model-driven and data-driven, to integrate objectives from different hierarchical levels and timeframes.

Cloud End: This segment is reserved for storing both the system's initial data and its historical records. Additionally, it sets the optimisation objectives and defines the time scales for the entire digital twin.

Output: This end provides essential outputs like cell status monitoring, SOC estimation, and reliability recommendations, aiding technicians in making well-informed decisions.

In the proposed experimental framework, the DT of the BESS is conceived as a dynamic, multi-dimensional entity. This entity continuously evolves through the integration of data from its physical, virtual, and cloud-based components. Central to this system is the Information Flow mechanism, which enables a bidirectional exchange of data among these components. Such an exchange is critical for the autonomous evolution of the digital twin, allowing it to adapt and enhance its performance progressively. The virtual segment of the system is of paramount importance. It employs a combination of model-driven and data-driven algorithms to accurately predict and simulate the system's future states. This predictive modelling is vital for developing pre-emptive maintenance strategies, optimising operational efficiency, and extending the lifespan of the BESS. The virtual component, by integrating both real-time and historical data from the cloud, conducts a thorough analysis of the system's performance and health. This integration significantly improves the efficiency and adaptability of the BESS. Moreover, the output from this system is not limited to data collection; it provides actionable insights. These insights are essential for technicians and engineers, enabling them to make informed decisions and drive innovation in battery storage technologies. In summary, this paper highlights the synergistic effect of the virtual component within the DT framework, emphasising its critical role in enhancing the BESS's overall functionality and resilience.

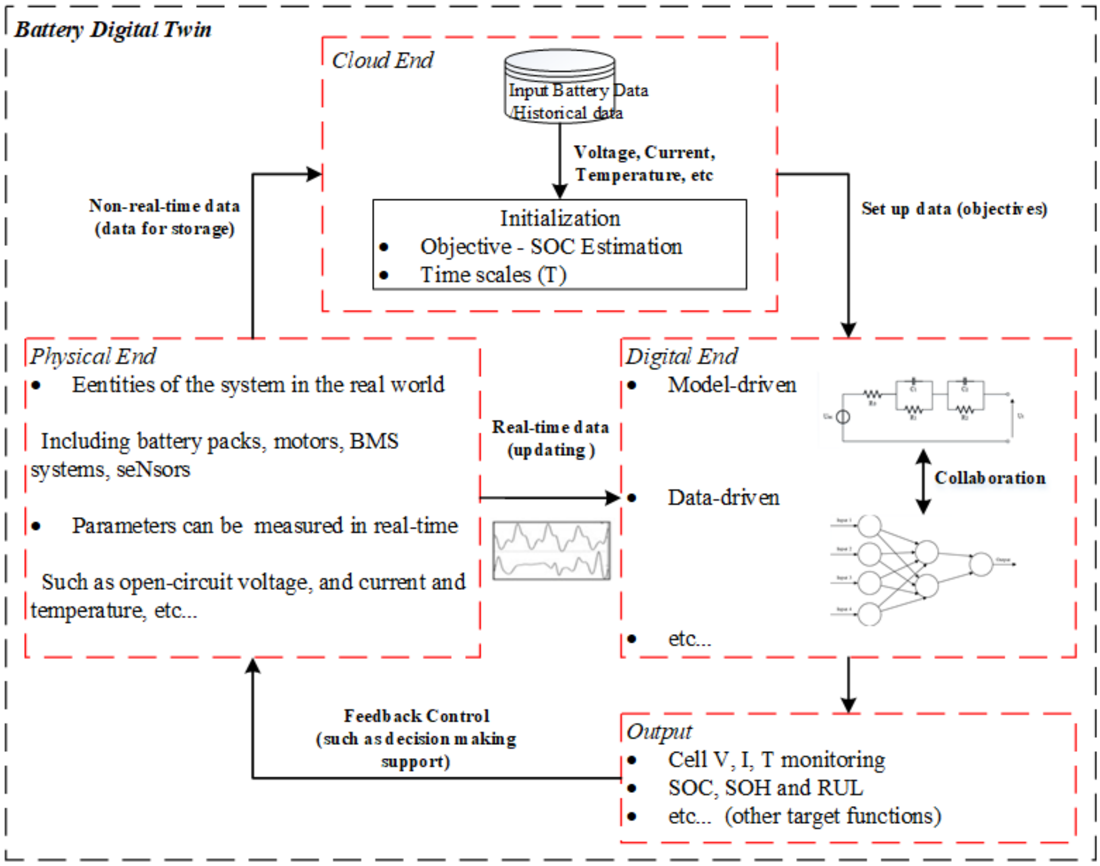


Figure 4.2 The battery digital twin framework for the proposed method.

4.3.1 Battery Modelling

Several model-driven methodologies are available, such as the internal resistance model, the n-RC model, the PNGV model, and the GNL model (Thiruvonasundari and Deepa, 2020, Salameh et al., 1992). In this study, we have chosen the Thevenin model, commonly known as the 2-RC model, for its adeptness at simulating both the steady-state and transient behaviours of the battery (Johnson, 2002). While more complex models might increase computational demands, their selection becomes redundant. This is because the TCN-LSTM (Shin et al., 2021) can effectively mitigate errors arising from model uncertainties.

Figure 4.3 illustrates the 2-RC equivalent circuit model. In this representation, U_{oc} denotes the open-circuit voltage, while R0 is indicative of the ohmic resistance. The circuits R_1 and C_1, which represent electrochemical polarisation resistance and capacitance, capture the rapid increase in discharge voltage. On the other hand, the R_2 and C_2 circuits, symbolising concentration polarisation resistance and capacitance, depict the slow stabilisation phase of the discharge voltage. Notably, the elements R_1, R_2, C_1, and C_2 together reflect the battery's polarisation, with U_t representing the terminal voltage.

In a theoretical context, these parameters undergo dynamic changes influenced by factors like SOC state, temperature, and ageing state, leading to potential estimation errors. However, within the digital twin paradigm, such errors are adeptly rectified by the TCN-LSTM neural network.

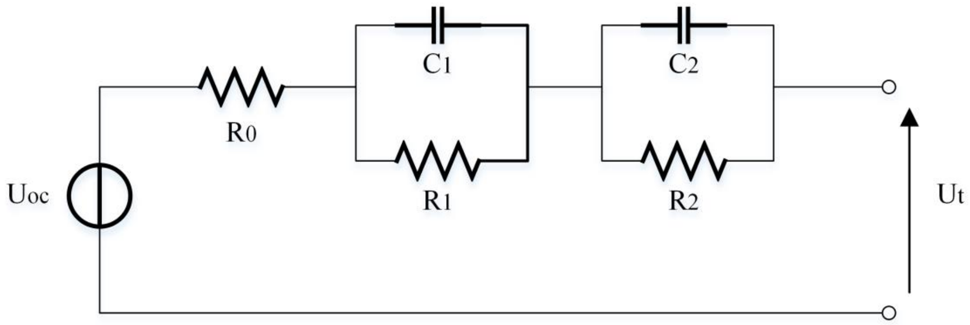


Figure 4. 3 The 2nd-order ECM structure

4.3.2 TCN-LSTM for SOC Estimation

Within the purview of BMSs, the SOC stands as a pivotal parameter and can be represented through diverse mathematical formulations (Hannan et al., 2017). Fundamentally, SOC delineates the available capacity Q_{a} as a fraction of the nominal capacity Q_{n}, with Q_{n} denoting the peak charge a battery can retain. Drawing a parallel to vehicular fuel tanks, SOC assumes an analogous role to that of a fuel indicator. Given a current I that is positive during charging and negative during discharging, a standard formulation for SOC is:

$$SOC(t) = SOC(t_0) + \int_{t_0}^{t} \frac{I(t)-\eta}{Q_n} dt \tag{4.1}$$

Here, $SOC(t)$ and $SOC(t_0)$ represent the SOC values at instances t and the commencement time t_0, respectively. The parameter η signifies the coulombic efficiency, mirroring the quotient of energy discharged fully to the requisite energy for restoring original capacity.

From an electrochemical perspective concerning batteries, SOC denotes the charge encompassed within both the anode and cathode electrode constituents. More precisely, the flux in SOC epitomises the lithium concentration distribution amidst the electrode components. Given that the quantum of accessible charge is intrinsically linked to the lithium reserve within the electrodes, SOC can be explicitly ascertained in relation to the average lithium concentration Cs as:

$$SOC(t) = \frac{(C_s(t) - C_{s,min})}{C_{s,max} - C_{s,min}} \tag{4.2}$$

In this equation, $C_s(t)$ symbolises the mean surface lithium-ion concentration at instance t, while $C_{s,min}$ and $C_{s,max}$ denote surface lithium-ion concentrations at battery states of full depletion and full charge, respectively.

For BMSs, precise SOC data is imperative, signifying the residual accessible energy within a battery during operational phases. State intelligence provides essential knowledge for the charging and discharging methods of the battery. Under controlled lab environments, post-ascertainment of the initial SOC, the benchmark SOC values are predominantly derived through a rigorously managed coulomb counting technique that aggregates the transmitted charge (Chang, 2013). Nonetheless, owing to multifaceted electrochemical interplays and pronounced interactive traits, direct measurement of battery SOC in practical settings proves challenging. As such, real-time SOC estimation emerges as an essential competency within BMSs, thereby garnering significant scholarly attention.

The EKF method for SOC estimation, due to its merits of expediency and swift response, aligns well with the real-time demands of DT systems (Shin et al., 2021). However, its accuracy is heavily influenced by the initial SOC and the impedance model, highlighting the need for accurate initial SOC values and precise sensors. Addressing this, the LSTM algorithm is used to adjust the initial SOC before the EKF estimation stages. The LSTM algorithm, while adept at estimating the battery's charge state amidst initial state uncertainties (Liu et al., 2021c), encounters a significant drawback due to its computational intensity, leading to time inefficiencies. To address this, the TCN emerges as a viable alternative. TCN's primary advantage lies in its flexibility to adjust the receptive field size, coupled with its effective management of the model's memory duration. This combination not only preserves accuracy in charge state estimation but also significantly enhances computational efficiency. One of its key advantages is the ability to address issues such as gradient explosion or vanishing gradients, often seen in RNN. Additionally, TCN requires less memory during training, especially with long input sequences. This efficiency is credited to its unique dilated causal convolution and the inclusion of the residual model. Combining the strengths of both TCN and LSTM can potentially optimise input parameters and reduce training time.

Figure 4.4 depicts the process for SOC estimation. A combined TCN-LSTM network is designed to capture the non-linear relationship between SOC, current, voltage and temperature, allowing accurate initial SOC values for real-time EKF-based SOC estimation. The raw data refers to the historical data collected from the sensor, including parameters such as battery terminal voltage, charge/discharge current, and temperature readings collected over time. To further adapt to varying environments, a rolling learning approach (Guo et al., 2021a) is implemented to continuously adjust the TCN-LSTM model parameters.

Selecting the right inputs for an estimation algorithm is a complex task. It's worth noting that current, temperature, and voltage, as directly measurable parameters, have been proven to significantly influence battery state estimations (Hannan et al., 2017). As a result, these parameters serve as inputs for both the ECM and TCN-LSTM in this study. To enhance accuracy, the TCN-LSTM is first initialised and trained using data from the battery's early operational cycles. The EKF then provides the final adjustment for SOC. This methodology, in comparison to traditional EKF estimation, delivers improved SOC estimation and reduces the uncertainties in initial battery state data.

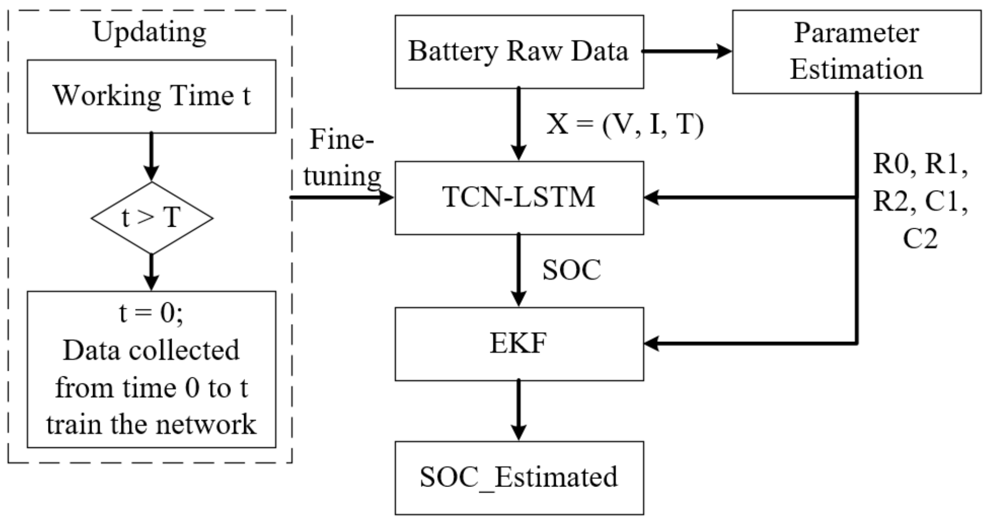


Figure 4.4 Flowchart of the SOC estimation in Digital End.

4.3.3 TCN-LSTM for SOH Estimation and RUL Prediction

During their operational lifespan, electrochemical batteries invariably undergo incremental performance attrition due to side reactions (Li et al., 2019a). This leads to the ageing phenomenon characterised by the depletion of lithium inventory and loss of active materials (Berecibar et al., 2016). The SOH is a pivotal metric, quantitatively assessing battery ageing, specifically about capacity diminution and internal resistance alterations (Zheng et al., 2016). Mathematically, SOH is articulated as:

$$SOH = \frac{C_a}{C_r} \times 100\% \quad \text{or} \quad SOH = \frac{R_a - R_r}{R_r} \times 100\% \tag{4.3}$$

In this equation, C_a and C_r present internal and nominal capacity values. R_a and R_r present internal and nominal resistances.

For automotive battery applications, demarcations for a battery's End-of-Life (EOL) typically include a 20% capacity reduction or a 100% surge in internal resistance. SOH of a battery underscores its safety, reliability, and operational efficacy (Hu et al., 2018b). It's of utmost importance to have a precise and timely SOH gauge during vehicular operations, which aids in battery anomaly detection, and SOC estimations and dictates maintenance or replacement schedules. Both the capacity and internal resistance parameters evade direct measurements with conventional sensors. Thus, the quest is on for pioneering estimation algorithms that facilitate real-time SOH determinations through an affordable sensor suite. This has spurred a plethora of academic endeavours, resulting in a vast repository of scholarly insights. It's critical to note that to assess these estimation algorithms, a benchmark SOH must be accurately determined. Standard practice dictates conducting battery ageing tests under meticulously regulated settings. During these tests, a battery's actual capacity or internal resistance is intermittently gauged with precision instruments. Data procured from these empirical endeavours become the gold-standard SOH for validating estimation methodologies.

The RUL is defined as:

$$RUL(t) = t - t_{EOL} \tag{4.4}$$

where t_{EOL} Denotes the cycle count upon the battery's EOL and t represents the ongoing cycle iteration. Thus, the difference between these two values represents the RUL, essentially quantifying the remaining cycles before the battery is expected to fail or degrade beyond acceptable performance thresholds. Equation (4.4) conceptually illustrates the definition and relationship of RUL, while the practical determination of RUL within our digital twin system is conducted directly by the deep learning algorithm. The overarching challenge is to devise strategies that enable multi-step

RUL forecasts utilising archived datasets (Dong et al., 2014).

The TCN model employs 1-D causal convolution for the extraction of historical data and provides the preservation of temporal sequences. This model benefits from the inclusion of residual connections, promoting faster convergence. Additionally, its utilisation of dilated convolution is pivotal for temporal feature extraction. In parallel, the LSTM model, characterised by its nonlinear nature, functions as a complex component within a comprehensive deep neural network. This characteristic empowers the LSTM to exhibit robust nonlinear fitting capabilities, thereby optimising its feature extraction proficiency. As illustrated in Figure 4.5, during the feature extraction procedure, data features are conveyed to the TCN layer for convolutional computations. After these calculations, parameters are normalised across each layer. The Rectified Linear Unit (ReLU) function is then employed to map these normalised features. Post-computation, the derived sequence features are further refined in the TCN layer by combining expansion and causal convolution techniques. This combination allows a more exhaustive extraction of sequence features, tapping into a wider spectrum of information dependencies. Following this, the TCN layer's output feeds into the LSTM network layer. Here, an additional layer of feature extraction takes place, consolidating features from both the TCN and LSTM. This combined methodology aids in preventing potential feature degradation. The amalgamated features are then channelled into the fully connected layer. To make the model remain generalised and avoid overfitting, a Dropout mechanism is integrated. The TCN-LSTM estimation process can be categorised into two phases: offline training and online estimation. In the offline training phase, the network is inundated with an extensive set of battery data, equipping it to identify the nonlinear associations between battery metrics and the corresponding SOH and RUL. Here, the offline training data refers to historical battery data collected from sensors, including current, voltage, and temperature. From these historical datasets, capacity data is derived through calculation. Meanwhile, the online test data denotes the real-time sensor measurements collected directly from the battery system during operation, similarly including current, voltage, and temperature.

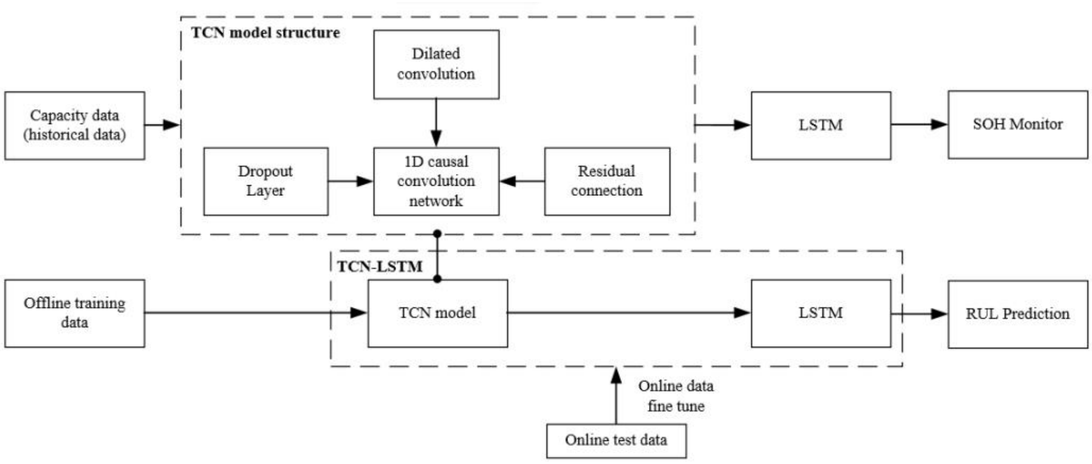


Figure 4. 5 The framework for battery health prognostics.

4.3.4 Rolling Transfer Learning

Regular updates are critical for a battery digital twin, particularly given the impact of battery ageing on SOC estimation. Therefore, a rolling transfer learning method is introduced, focusing on updating the TCN-LSTM model parameters to address ageing effects. Transfer learning involves adapting a model trained for one application to another. Given that lithium-ion battery measurement parameters exhibit varied but related spatial features, a primary TCN-LSTM model is trained for SOC estimation. This model then acts as the base for training another SOC estimation model. During transfer learning, network parameters are adjustable, allowing for updates during the training phase. Figure 4.6 illustrates this transfer learning approach. Both models have congruent structures, with the target model initialised using the source model's parameters and subsequently trained with a new dataset. As the battery DT functions, it consistently collects data. When the cumulative operational time surpasses a set duration T, a secondary TCN-LSTM network undergoes retraining and recalibration remotely. The main TCN-LSTM combines these updated parameters to enable continuous changes and the use of past information in the digital twin.

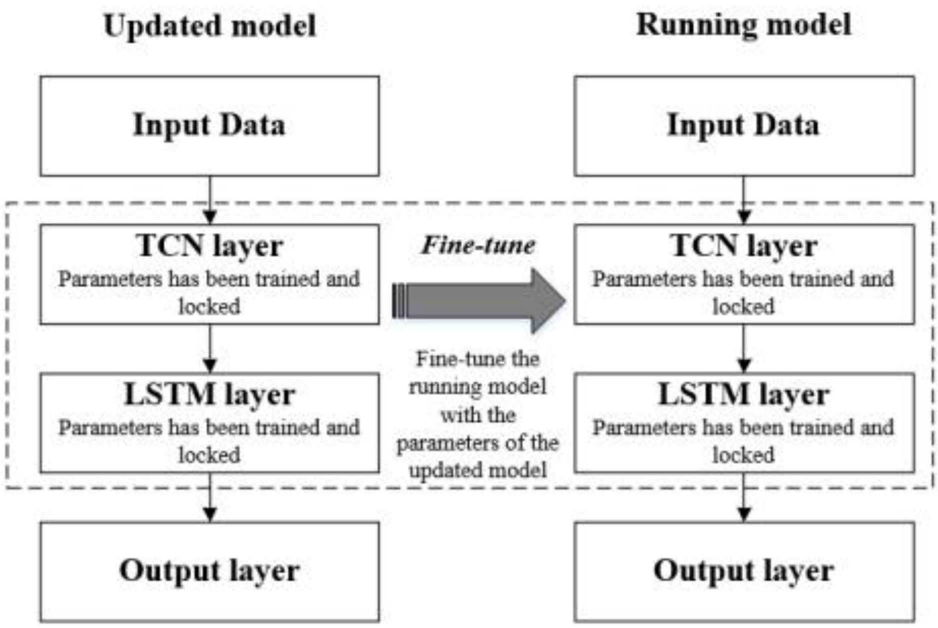


Figure 4. 6 The rolling transfer learning approach.

4.4 Case Study

In this section, we present experimental validations and engage in discussions to validate the effectiveness of the proposed framework. Our case study leverages data from the National Aeronautics and Space Administration's (NASA) dataset on lithium-ion battery charge and discharge experiments to verify the DT model (Saha and Goebel, 2007). An observation was made regarding the battery tester's logging mechanism: due to its inconsistencies, several drive cycles were consolidated into a single extensive file, causing some data repetition. For data integrity, it is critical to remove the redundancy, which could be indicative of data-logging anomalies. Notably, within the framework of supervised learning, the TCN-LSTM's capacity loss is quantified by Ah, serving as the foundation for the reference SOC.

Drawing from the calibrated battery DT model detailed earlier, we can incorporate a range of state estimation algorithms, distinguished by their accuracy and resilience, into the digital endpoint. The process commences with the input of parameters such as voltage, current, and temperature, followed by the extraction of ECM parameters like R0, R1, R2, C1, and C2. Thereafter, both the state equation and the measurement equation for the equivalent circuit model are formulated. To refine the estimation, the TCN-LSTM algorithm is applied for error adjustments, while the final SOC estimation is realised through the EKF. As part of this cyclical mechanism, the TCN-LSTM network is periodically retrained and refined, assimilating real-time data at predefined intervals T. Figure 4.7 is the schematic diagram of DT running. The three models, SOC estimation, SOH monitoring and RUL prediction, are intricately linked, working collaboratively to provide real-time updates and comprehensive insights throughout the battery's operational phase. This collaboration creates a comprehensive view and enhances the control of the battery system.

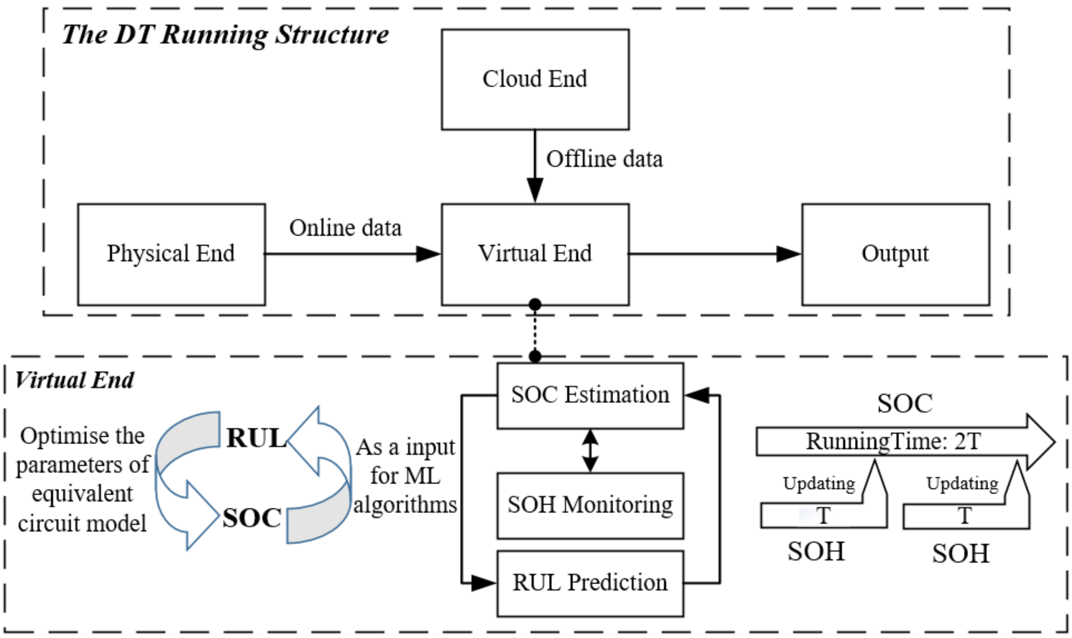


Figure 4. 7 Schematic diagram of DT running.

4.4.1 Evaluation Metrics

At the physical end, the evaluation of the digital twin and battery state estimation algorithm will be conducted experimentally using lithium-ion batteries. This approach aims to validate the precision and robustness of both the model and algorithm within the DT framework.

For the cloud end, the Mean Absolute Error (MAE) and the Root Mean Square Error (RMSE) have been selected as the primary metrics to assess estimation accuracy. It is defined as:

$$MAE = \frac{1}{K}\sum_{k=1}^{K}\left|l(k) - \dot{l}(k)\right| \tag{4.5}$$

$$RMSE = \sqrt{\frac{1}{K}\sum_{k=1}^{K}(l(k) - \hat{l}(k))^2} \tag{4.6}$$

The RMSE serves as an indicator of the disparity between predicted and actual values. It is expressed as:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(SOC_{ei} - SOC_{ti})^2} \tag{4.7}$$

In this equation, n signifies the total number of observations, while SOC_{ei} and SOC_{ti} correspond to the ith estimated SOC and true SOC, respectively.

4.4.2 SOC Estimation in the Digital Twin

Utilising the Jupyter Notebook platform, equipped with a deep learning environment, this investigation was centred on the development and assessment of the TCN-LSTM network. This network comprises an input layer with a single time series and three specific features: voltage, current, and temperature. After conducting a series of repeated tests and verifications, the relatively optimal parameter is selected based on both the operating time and the test results. This method enables a more precise and effective approach to parameter optimisation. While the output layer is for SOC estimation, the hidden layer integrates 150 nodes. For refining the model, we adopted the MAE loss function and the Adam optimiser, with an operational batch size of 32. The primary role of both the loss function and the optimiser is to hone the model, driving the loss closer to 0. As presented in Figure 4.8, post 20 epochs, the model's loss during training and testing phases converges, not surpassing 0.04. The training set exhibits a particularly low loss of under 0.005, indicative of the model's robust performance. However, a slight elevation in the validation loss compared to the training loss points to a potential overfitting issue.

Figure 4.9 provides a comparative analysis of the SOC, as determined by the EKF after the TCN-LSTM correction, against a reference SOC. The graphical representation includes three distinct lines symbolising the reference value, estimated value during training, and estimated value during testing. While the model aligns well with the training data, there are discernible deviations in the SOC estimation when processing new data. The RMSE is recorded at 1.1% for training and 2.7% for testing. It is generally understood that a model with a lower RMSE is indicative of better SOC estimation precision.

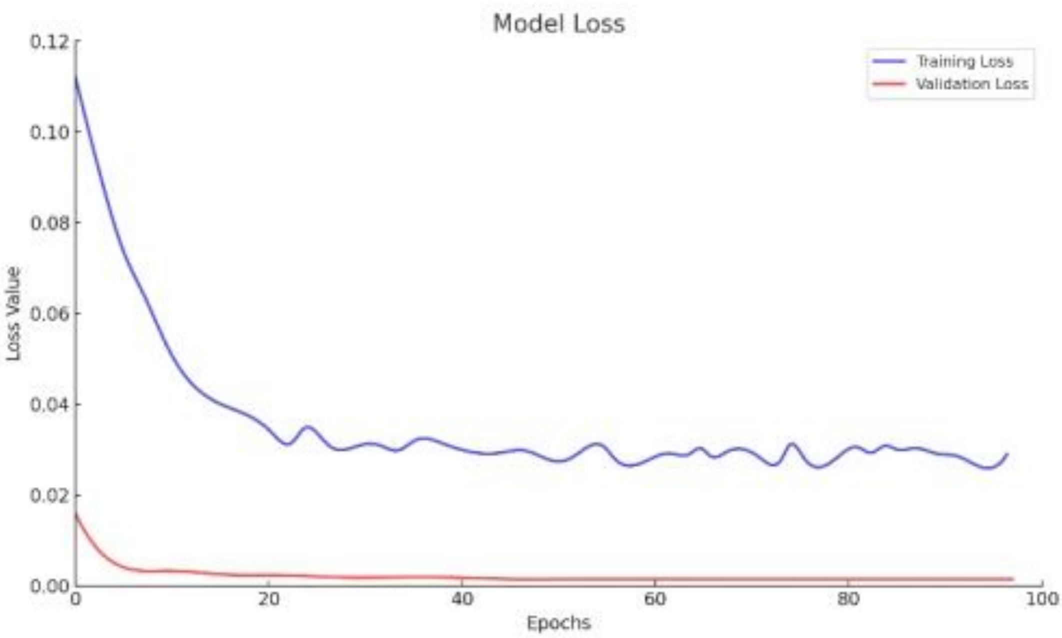


Figure 4.8 The model loss of TCN-LSTM at training and test

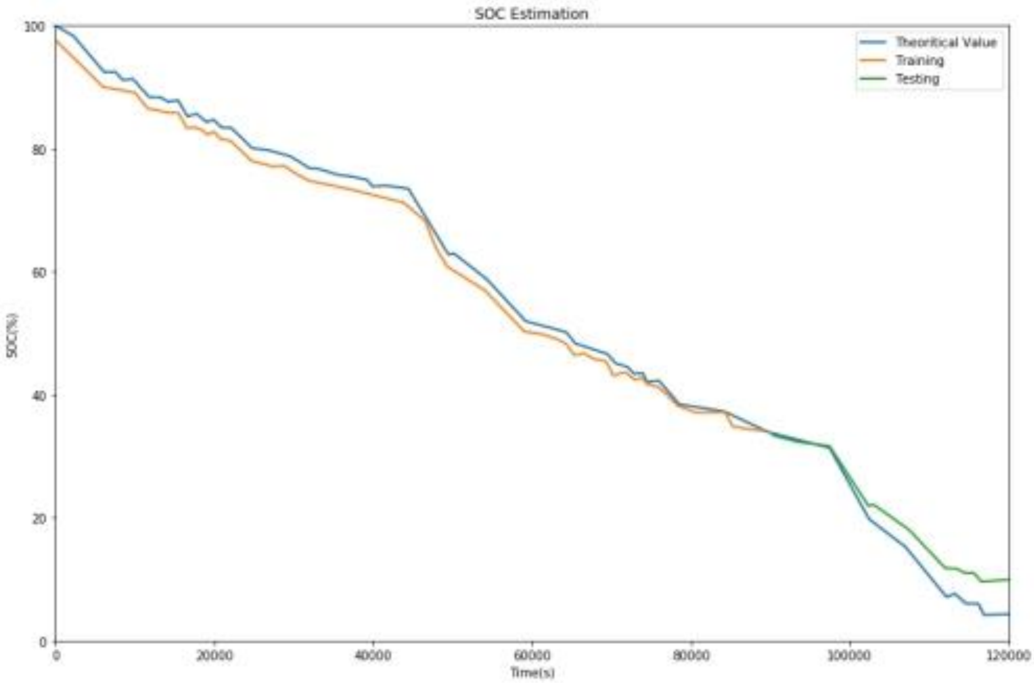


Figure 4. 9 The SOC estimation by TCN-LSTM

Table 4.1 The comparison of SOC estimation for different methods

Methods	RMSE
EKF	3.9%
SVM	3.2 %
CNN	2.2 %
LSTM-EKF	1.7%
TCN-LSTM	1.1 %

The observed discrepancy in RMSE values between the training and testing data in our study can be attributed to overfitting, which might affect the model's handling of previously unseen data. The RMSE values mentioned in the Table 4.1 were calculated based on a dataset using the pervasive network structures. This dataset was also the basis for the reference methods introduced in the analysis. When benchmarked against other algorithms in Table 4.1, the proposed method showcases the least RMSE across the four algorithms evaluated. This underscores the algorithm's enhanced accuracy, particularly once overfitting issues are rectified. The introduction of the reference methods for the same dataset further supports the reliability and robustness of our findings.

4.4.3 SOH Monitoring in the Digital Twin

Using the capacity series data outlined in the manuscript, this study subjected the model's parameters and structure to an intensive experimental analysis. The study focuses on the SOH of battery B0005, starting from its nth (30th, 60th and 90th) cycle. The first n cycles are thus treated as the training set, and the cycles that follow are the prediction set. By adopting the method, which is similar to the sliding window technique, the model systematically incorporates predicted values. This process aids in predicting the SOH value, leveraging the aggregated SOH data until the complete test set is covered. The choice of parameters mainly draws from the control variable method, a standard practice in neural networks to ascertain optimal parameters. Such a method requires the modification of only one parameter during each tuning phase. The model's core parameters include 1000 iterations, a mini-batch size of 128, a 3×1 kernel dimension, 256 convolution kernels, dilation factors of [1, 2, 4, 8, 16, 32, 64], and it utilises the Adam optimiser.

Accurate SOH monitoring, marked by a minimal error in predicting subsequent SOH values, is critical for dependable RUL prediction. Such precise estimations further facilitate proactive battery maintenance. Therefore, to closely emulate real-world scenarios, monitoring commenced from the 30th cycle. In addition, the SOH was assessed at various starting points to validate the predictive precision and resilience of the model. Table 4.2 provides a comparison of the TCN-LSTM model's prediction capabilities for three specific battery cycles (30th, 60th, and 90th) against established methods. For a fair comparison, models like LSTM, TCN, and CNN were all designed with two hidden layers. The model maintained a consistent parameter setup throughout the prediction stage, having been fine-tuned through multiple experiments.

Table 4.2 affirms the model's consistent performance, regardless of the prediction start point. For complex neural networks, an ample amount of training data typically bolsters prediction accuracy. Figure 4.10 visually represents battery cells B0005 under different models and starting points. These visuals emphasise the TCN-LSTM model's proficiency in tracking the degradation trend of the capacity series, surpassing current models, and adeptly highlighting local regeneration instances.

Table 4.2 Performance of SOH monitoring

Training cycle	RMSE				MAE			
	CNN	LSTM	TCN	TCN-LSTM	CNN	LSTM	TCN	TCN-LSTM
30C	4.8%	12.3%	10.1%	1.4%	4.6%	11.1%	9.2%	0.9%
60C	3.1%	12.0%	8.7%	1.3%	2.8%	11.4%	8.3%	0.8%
90C	2.0%	4.4%	1.9%	0.8%	1.5%	4.0%	1.5%	0.6%

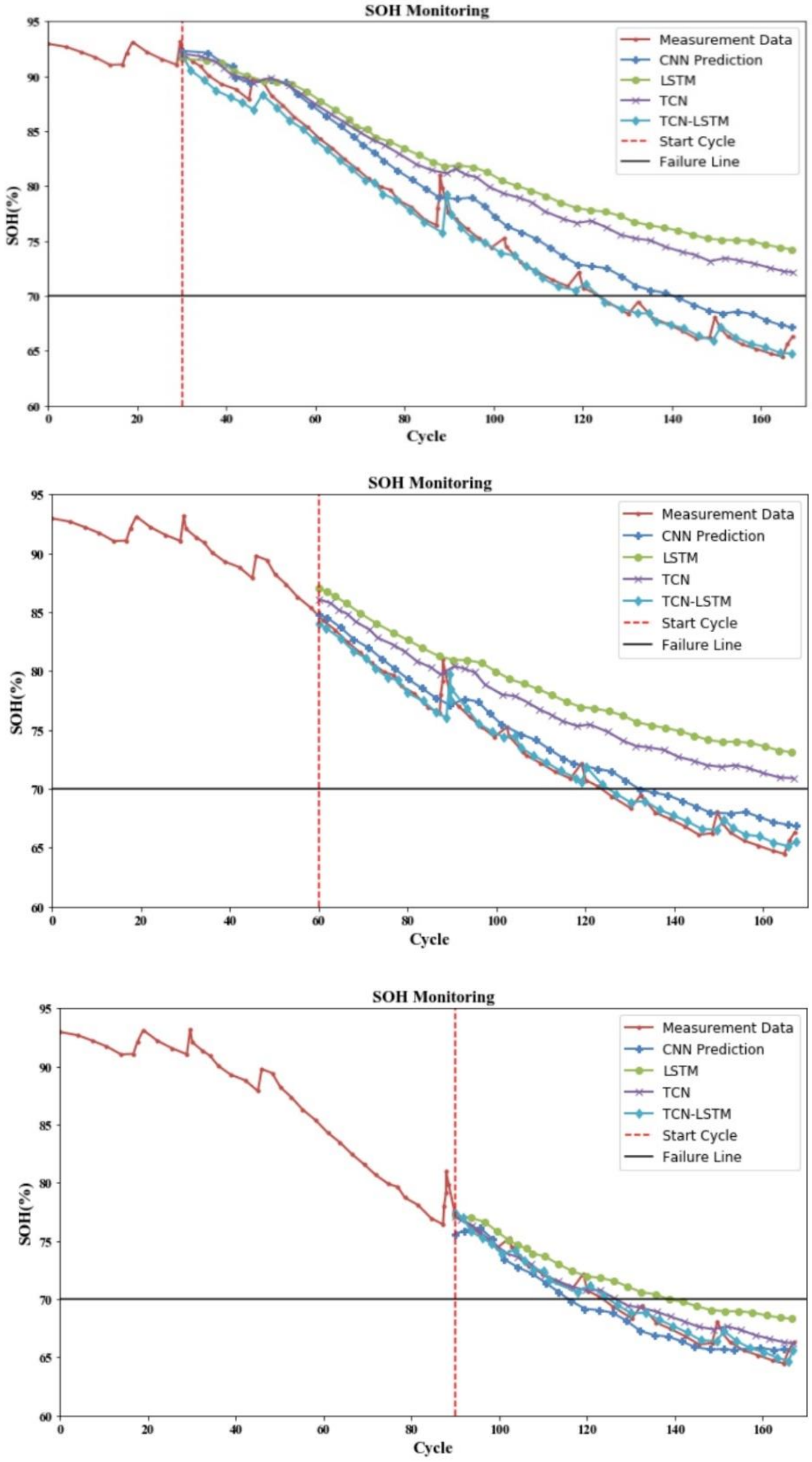


Figure 4. 10 The SOH monitoring of B0005 with 30th, 60th and 90th start cycle

4.4.4 RUL Prediction in the Digital Twin

This section evaluates the TCN-LSTM model's performance in RUL prediction using offline data, comparing it with other models. Accurate RUL prediction is essential not only for timely battery replacement but also for maintaining system stability and safety. In the context of this analysis, batteries B0006 and B0018 were used for offline training, while battery B0005 was designated as the test data. To gauge the accuracy of the TCN-LSTM model, we defined several starting points and compared the results with those from different models. During the prediction process, the model, already trained with offline data, was further refined using a selected portion of available online data, aiming to bolster its predictive precision. The presented results encapsulate the best outcomes from multiple experimental iterations. Table 4.3 indicates that the LSTM model outperforms the CNN model in terms of RUL prediction. While the TCN model—an enhanced iteration of CNN—might not excel in early prediction stages, its integration with LSTM consistently delivers optimal RUL outcomes. It's noteworthy that the accuracy of predictions increases as they draw closer to the battery's failure point. In real-world scenarios, the accuracy of predictions made closer to the end of the battery's life is of paramount importance. The TCN-LSTM model's prediction accuracy for the 90th cycle reaches an impressive 0.9%, highlighting the model's effectiveness. Figure 4.11 corroborates this, showing the TCN-LSTM model's alignment with the degradation trend of the volume sequence during the 90th cycle. Finally, Table 4.3 contrasts the prediction accuracies, underlining the proficiency of

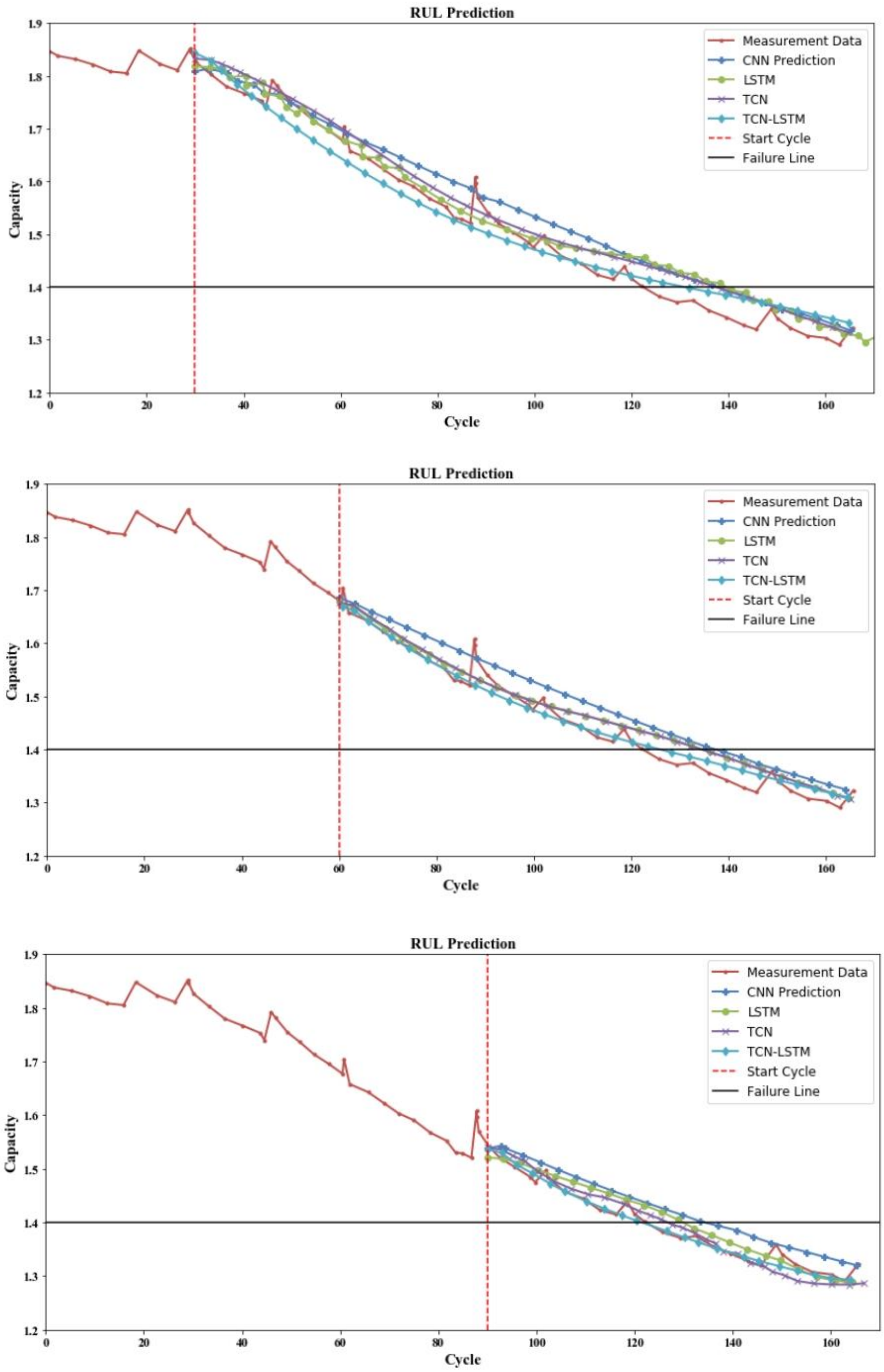


Figure 4.11 The RUL prediction of B0005 with a) 30th, b) 60th and c) 90th start cycle

our model in reliably predicting the RUL of lithium batteries.

Table 4.3 Comparison of evaluation RUL prediction among different methods

Training cycle	RMSE				MAE			
	CNN	LSTM	TCN	TCN-LSTM	CNN	LSTM	TCN	TCN-LSTM
30C	3.7%	2.9%	3.0%	2.0%	3.3%	2.3%	2.3%	1.7%
60C	4.4%	2.7%	1.8%	1.5%	4.2%	2.4%	2.5%	1.2%
90C	3.6%	2.4%	1.5%	0.9%	3.4%	2.1%	1.3%	1.6%

4.4.5 Validation of Transfer Learning Model

In this section, we conduct a detailed comparative analysis using two distinct TCN-LSTM models, with the primary distinction being the application of transfer learning, to validate the real-time updating ability. We use the NASA dataset to train both models by the first 30th cycles, with subsequent data reserved for the validation. The analysis revealed RMSE for SOH predictions at 1.4% for the model incorporating transfer learning and 1.42% for its counterpart, indicating a slight difference. However, as Figure 4.12 demonstrates, initial assessments of both TCN-LSTM algorithms during the early battery cycle tests showed significant consistency. As the study progressed beyond 105 cycles, a clear disparity emerged: the model without transfer learning displayed notable jitter in its SOH estimations—a contrast to the model that employed transfer learning. This performance gap underscores the models' varying adaptation to the complex, evolving nature of battery data through successive cycles and highlights transfer learning's critical role in enhancing battery state estimation stability. The transfer learning-augmented model's ability to dynamically adjust its parameters and neural networks in reaction to real-time data showcases its exceptional adaptability and resilience, important for accurate state estimation.

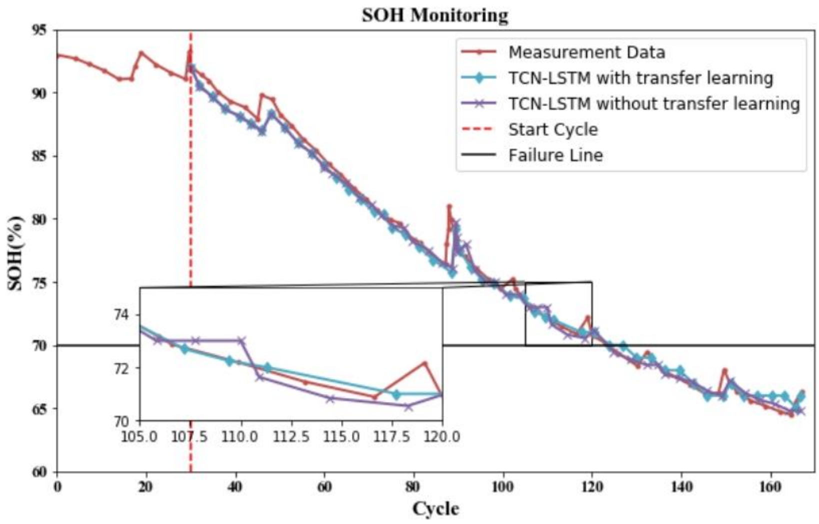


Figure 4.12 The SOH prediction of B0005 with the 30th start cycle

4.5 Discussion

This chapter introduces a DT-supported battery state estimation framework that employs a combination of TCN and LSTM networks. The discussion emphasises the importance of incorporating deep learning techniques into DT frameworks for battery management systems. The proposed DT framework is notable for its adaptability to diverse battery operating conditions and its capability to accurately estimate battery states, including SOC, SOH and RUL.

The primary contribution of this research is its innovative application of TCN and LSTM networks, which significantly enhance the robustness and accuracy of battery state estimation. The proposed model leverages the hierarchical DT structure and the strengths of both TCN and LSTM to overcome the limitations of conventional battery management systems. Specifically, combining TCN's sequence modelling capabilities with LSTM's memory retention properties enables precise feature extraction from battery data, even under diverse operating conditions. Additionally, incorporating transfer learning into the BDT enables dynamic model updates using real-time data.

The experimental results further validate the effectiveness of the proposed method.

The TCN-LSTM model consistently outperformed traditional methods based on RMSE and MAE. The model demonstrates exceptional adaptability and superiority in battery digital twins, achieving average RMSE values of 1.1%, and maximum errors of 0.8% and 0.9% in these respective areas. This enhanced performance can be attributed to the model's capability to capture temporal dependencies in battery data and adjust to new operating conditions through transfer learning. The proposed method provides accurate real-time insights into battery health and performance, thereby contributing to the optimisation of battery utilisation and extending the lifespan of energy storage systems.

In conclusion, this study significantly advances the field of battery management by proposing a robust DT framework supported by TCN-LSTM models for state estimation. The findings provide a strong foundation for future advancements in battery management systems and the development of more efficient and reliable energy storage solutions. Future research should aim to address the current limitations and explore integrating DT with emerging technologies to enhance its applicability and scalability.

4.6 Summary

In conclusion, this study has presented a methodology for battery state estimation and RUL prediction. Utilising an equivalent circuit as its foundational basis, a DT model has been developed, integrating factors such as voltage, current, and ambient temperature. Recognising the complexities of battery state estimation, we introduced the TCN-LSTM approach. This innovative method is specifically designed to reduce dependence on initial values, especially in scenarios with limited training data. The study included the battery digital twin framework and applied transfer learning methods to maintain model improvements throughout the operational phases using rolling learning.

This research offers a comprehensive analysis of the digital twin framework, focusing on its complex structure and key stages in the learning process. The empirical results confirm the efficiency of combining online SOC estimation, SOH monitoring, and RUL prediction. Underlining the practical implementation aspect of the method, the formation of a multi-layered digital twin structure enables the integration of SOC estimation, SOH monitoring, and RUL prediction. This consolidated approach offers profound insights into battery health and operational performance, laying the groundwork for advanced battery management strategies. Consequently, battery operations are minimised, thereby improving the life cycle of the battery and also elevating system efficacy. The integration of TCN-LSTM techniques with the digital twin paradigm is an innovative combination that contributes to breakthroughs in battery management and storage system optimisation in a variety of applications.

Chapter 5 Multi-faceted Situational Awareness of Digital Twin-driven Battery Storage

5.1 Introduction

The estimation of accurate battery states is important in energy storage technology owing to the inherent complexity and non-linearity of these systems. Multi-faceted modelling has drawn increasing research attention over a diverse range of research domains, including energy storage because it can reflect real-world problems from multiple perspectives (Che et al., 2021, Hu et al., 2020). For example, a variety of material composition, operating conditions and environmental factors can influence the performance of a battery (Ren et al., 2022). Considering these multiple facets allows for a better understanding of the behaviour of a battery, which in turn improves BESS decision-support in battery management systems. Traditional techniques for monitoring and managing battery systems do not fully capture the multifaceted nature of battery behaviour. These methods employ single source data or models which are not capable of fully representing the dynamic changes of a battery system. Because of the limitation, situational awareness of the battery system is poor, and there are risks to battery management, including over-charging/discharging, and thermal runaway (Qin et al., 2021). Therefore, there is a need for an advanced method to estimate multiple battery states, to combine various estimation techniques, to provide decision support based on different battery states, and to achieve continuous and accurate monitoring and management of the battery.

Recent advancements in battery state estimation have introduced sophisticated approaches that leverage deep neural networks and multi-timescale feature extraction to enhance predictive accuracy. Fan et al. proposed a SOC and SOH co-estimation framework that utilises convolutional filters of varying sizes to extract multi-timescale features, improving estimation accuracy across both laboratory and real-world scenarios (Fan et al., 2023). Similarly, Zhou et al. developed a novel capacity estimation method based on singular value decomposition (SVD) and information energy theory, which demonstrated strong robustness against environmental variations and driving conditions (Zhou et al., 2022). These studies underscore the potential of advanced data-driven methodologies in battery management while also highlighting persistent challenges in achieving reliable real-world implementation. Many existing models, despite their success in controlled environments, lack the flexibility to adapt to dynamic operational conditions. Furthermore, they often overlook the interconnected nature of battery states, which is crucial for accurate long-term monitoring and predictive maintenance. By incorporating these insights, our study strengthens the understanding of battery management challenges and emphasises the necessity of an adaptive and intelligent framework for state estimation and decision support.

In the last decade, Digital Twin (DT) has become an important technique across many industries as a dynamic digital replica of physical assets with the ability to collect real-time data and incorporate advanced simulation models. Michael Grieves first conceptualised Digital twins in 2002, and their use has become common due to their ability to improve operational efficiency, optimise performance, and predict the future behaviour of physical assets (Drath and Horch, 2014, Dubarry et al., 2023).

The complexity of battery systems makes DT valuable. Renewable energy relies heavily on batteries, whose complicated performance is influenced by many factors (Grieves, 2005, Tuegel et al., 2011, Semeraro et al., 2023a). However, the multi-facets of these systems are overlooked by the traditional monitoring methods leading to inefficiencies and safety risks (Naguib et al., 2021). Combining multi-faceted modelling and real-time updating of system performance, DT provides a general solution. This capability allows the remaining useful life of the battery to be extended, provides safety guarantees, and improves the overall energy storage system efficiency.

A robust DT for battery management includes several key components: physical battery and sensors, data acquisition systems, computational models, and user interfaces. Real-time data of various parameters (temperature, voltage, current etc.) are collected by the physical battery and its associated sensors. Computational models are then used to process this data to simulate battery behaviour (e.g., state of charge (SOC), state of health (SOH), and thermal dynamics). Predictive maintenance comes with a digital twin which enables real-time monitoring of equipment and predictive fault detection. Chen et al. (Chen et al., 2023) have done a comprehensive review of DT-based PdM that integrates different sources of sensor data and machine learning techniques to improve prediction accuracy. The DT can be interacted with by its user interfaces where stakeholders can pass on DT insights on battery performance and make informed decisions (Tang et al., 2022, Qu et al., 2020). Through interacting with these components, a detailed and dynamic view of the battery system can be continuously monitored and optimised.

Preliminary research on DT in battery management systems shows promising results. The accuracy in SOC and SOH estimates is improved and the risk of overcharging or over-discharging is minimised while system reliability is improved (Panwar et al., 2021). For instance, case studies have shown that DT can effectively monitor and manage the performance of lithium-ion batteries in electric vehicles and results in longer battery useful life and better overall performance (Zhu et al., 2022). This research shows the potential that DT has to revolutionise battery management through a more sophisticated and more reliable approach to monitoring and maintenance.

However, there are many challenges and limitations to the use of DT. A major problem is the high cost and complexity involved with developing and maintaining accurate digital models. The process of producing a DT is expensive in terms of data collection and processing. Moreover, technical challenges include the integration of different data sources and the requirement for continuous real-time updates (Naseri et al., 2023). Another concern is the reliability of the data used; inaccurate or incomplete data can lead to erroneous predictions and suboptimal decision-making (Wang et al., 2022). In addition, the systems must be interconnected so that integrity and confidentiality of the data can be enforced, and the cybersecurity risks involved. As a result, there is an urgent need for more cost-effective, reliable, and secure DT solutions that can be easily integrated into existing systems.

To address these challenges, we present a hierarchical and self-evolving digital twin (HSE-DT) specifically designed for battery management systems. This method utilises transformer and convolutional neural network (CNN) models to improve predictive accuracy and flexibility. The data used in this paper was pre-processed to get the quality and reliability of the input data. The method comprises data acquisition, storage, processing and real-time update mechanisms to keep the digital twin up to date. Moreover, we have added some extra advanced cybersecurity measures which will help us maintain the data integrity and have a secure link between the physical and the virtual ends (Li et al., 2020, Wang et al., 2021a).

Traditional battery monitoring approaches primarily rely on single-source data and static models, limiting their ability to comprehensively capture the dynamic and multifaceted nature of battery behaviour. Integration of multi-source data plays a very important role in efficient predictive modelling of a complex system. In the work by Qin et al. (Qin et al., 2018), they proposed a hybrid approach to combine deep learning and clustering techniques with IoT data in order to optimise energy consumption in Additive Manufacturing (AM). Deep learning has shown significant promise in predictive maintenance applications, particularly when integrating diverse data sources. Chen et al. (Chen et al., 2021a) introduced a Merged Long Short-Term Memory (M-LSTM) network to model both sequential and spatial data for predictive maintenance. Inspired by these methodologies, our work applies similar multi-source data analytics principles to improve digital twin-driven situation awareness for battery management. The HSE-DT method enhances real-time adaptability by integrating diverse data streams and dynamically updating system models to reflect the evolving state of the battery. Furthermore, it provides predictive insights that enable proactive maintenance and optimised battery control strategies. By leveraging a multi-layered structure, HSE-DT ensures that decision-making is informed by accurate and up-to-date information. This approach not only improves battery longevity but also enhances the overall efficiency and reliability of battery energy storage systems.

The HSE-DT method is developed and implemented in this paper as a method for battery management systems. The framework simulation models and mechanism are detailed and the components and functionalities of the method are described. The results from the case study show that the method is effective for battery monitoring and state estimation. We also discuss broader potential applications of DT to other complex systems and future research directions for improving and validating this new method.

The remainder of this chapter is structured as follows. In Section 5.2, the components and functions of the method are introduced in detail, including physical modelling, deep learning algorithms, integration mechanisms and self-renewal mechanisms. Section 5.3 reports the experimental setup using data from the real world. The results are discussed in Section 5.4. Finally, Section 5.5 summarises this chapter.

5.2 Technical Approach

As discussed in the preceding sections, the complexities and dynamic nature of battery systems necessitate a robust and adaptive approach to enable effective battery management. Traditional methods often fall short in addressing the multifaceted aspects of battery state estimation and management.

Firstly, data relevant to the battery's state, such as current, voltage and temperature, is collected from various sensors embedded in the physical battery system. This data is then processed and integrated into a unified framework, forming the foundation for the digital twin. The integrated data is utilised to develop the digital model, which replicates the physical battery's electrochemical, thermal, and ageing behaviours. Secondly, advanced machine learning algorithms, specifically CNN and Transformer models, are employed to analyse both historical and real-time data. These models work in tandem to provide accurate predictions and estimations of SOC and SOH. Thirdly, the self-evolving mechanism of the HSE-DT framework leverages continuous learning techniques to adapt the DT models based on new data. This allows the models to remain relevant and accurate over time, accounting for changes in battery conditions and usage patterns. Finally, the insights derived from the digital twin are used for predictive maintenance and optimisation of battery performance. This comprehensive method enhances battery situation awareness, improves safety, and extends the life of the battery system.

The HSE-DT method is designed to integrate multi-faceted layers within a structured digital twin architecture. It consists of multiple layers, each responsible for specific aspects of battery management, enabling a comprehensive method for battery situation awareness.

Physical end: The actual battery system, with sensors to collect real-time data of parameters. These sensors deliver the requisite data for state estimation.

Cloud end: This end integrates, and preprocesses data collected at the physical layer. This includes noise filtering, data normalising, and having consistency over various data resources.

Digital end: The DT models that mimic the physical battery's behaviour are served on this end. The models include electrochemical models, thermal models, and ageing models that are coupled to give a complete representation of the state of the battery. Real-time data is used to keep the models updated and accurate. On the digital end, advanced algorithms (CNN and Transformer models) are used to estimate SOC and SOH. These models use machine learning to analyse historical and real-time data predict future states and detect anomalies.

Output end: Critical outputs such as cell status monitoring, SOC estimation, and reliability recommendations are delivered at this end, to help technicians make informed decisions.

Decision Support end: The estimations and predictions are used to provide insights and recommendations on the topmost end. The user interfaces for stakeholders to interact with the digital twin, visualise data and make informed decisions on battery management are part of this layer.

5.2.1 Battery Modelling

There are three commonly used approaches for battery modelling, each offering distinct advantages and limitations: the electrochemical model, the equivalent circuit model (ECM), and the data-driven model (Wang et al., 2021b). This study adopts the ECM approach, as depicted in Figure 2. The ECM is a grey-box model that represents the dynamic behaviour of a battery by integrating resistors, capacitors, and voltage sources. The model's parameters are refined using collected data.

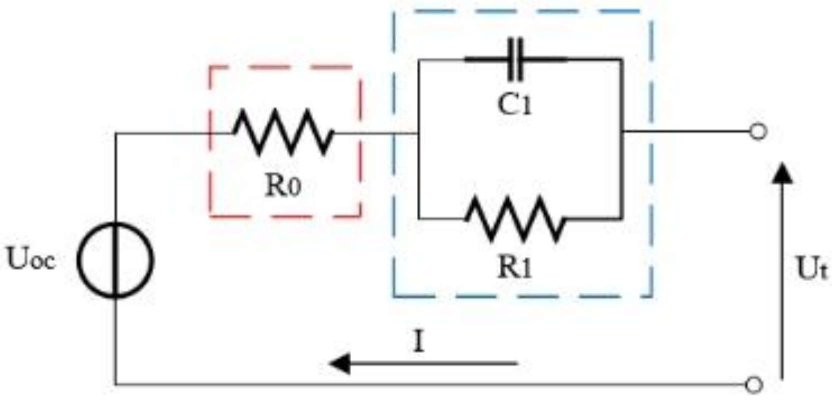


Figure 5.1 The first-order ECM for a lithium-ion cell.

The electrochemical model offers a detailed representation of internal battery mechanisms, including ion transport and electrode reactions. While highly accurate, this model requires an extensive understanding of battery chemistry and relies on computationally intensive numerical solutions. Consequently, its application in real-time battery management is limited. Instead, it is primarily utilized for in-depth electrochemical analysis and long-term degradation studies, where precision in capturing microscopic processes is paramount.

The data-driven model, in contrast, utilizes machine learning techniques to establish correlations between input features and battery behaviour without incorporating explicit physical relationships. This approach is particularly advantageous when substantial historical data is available, as it enables adaptive learning and predictive capabilities. However, data-driven models often demand significant computational resources and may suffer from limited generalizability when applied to unseen conditions, restricting their effectiveness in real-time embedded systems.

By comparison, the ECM provides a well-balanced solution, making it the most suitable choice for this study. It achieves an optimal trade-off between modelling accuracy and computational feasibility, offering a sufficiently precise representation of battery dynamics while enabling real-time implementation. Its straightforward parameterization, low computational complexity, and ease of integration facilitate seamless deployment in digital twin environments for battery management applications (Du et al., 2021). By adopting the ECM, this study ensures an efficient and reliable modelling framework that captures essential battery characteristics without imposing the computational burden associated with more complex models.

The ECM is defined by a simple mathematical formulation, in which the dynamics of the charging and discharging processes are governed by the following set of equations:

$$\frac{dSOC^n}{dt} = -\eta \frac{I^n}{E^n} + \omega_1 \tag{5.1}$$

$$\frac{dU_1^n}{dt} = -\frac{U_1^n}{R_1^n C_1^n} + \frac{I^n}{C_1^n} + \omega_2 \tag{5.2}$$

$$U_L^N = U_{oc} SOC^n - U_1^n - I^n R_0^n + \beta \tag{5.3}$$

where the superscript n denotes the nth cell in the battery module, which consists of a total of N cells; η is the coulombic efficiency of the battery; I is the current and E is the battery capacity in Amp Hour; R_0 is the internal resistance; R_1 and C_1 are the polarisation resistance and capacitance, respectively; U_1 and U_L are terminal voltage of the polarisation capacitance and the battery cell, respectively; ω1 and ω2 are process noise, and β is measurement noise; U_{oc} is the open circuit voltage dependent on SOC.

To make the ECM more suitable for computer simulation and model-driven predictive control, the continuous-time model is discretised with a sampling time T, as shown in the following equation:

$$SOC_{k+1}^n = SOC_k^n - \eta \frac{I_k^n}{E^n} T + \omega_{1,k} \tag{5.4}$$

$$U_{1,k+1}^{n} = U_{1,k}^{n} e^{-\frac{T}{R_1^n C_1^n}} + R_1^n \left(1 - e^{-\frac{T}{R_1^n C_1^n}}\right) I_k^n + \omega_{2,k} \tag{5.5}$$

$$U_{L,k}^{n} = U_{oc} SOC_k^n - U_{1,k}^{n} - I_k^n R_{0,k}^n + \beta_k \tag{5.6}$$

5.2.2 Transformer-CNN Model

Accurate battery state estimation is vital for the effective management of battery systems, particularly given their inherent complexity and dynamic behaviour. Traditional estimation methods often fall short of capturing the nonlinear and temporal dependencies present in battery data. To address these challenges, CNN and Transformer models are used within the HSE-DT method.

CNN and Transformer models are selected for battery state estimation due to their demonstrated ability to deal with large-scale data with complex patterns and dependencies. CNN is suited for extracting spatial features from time series data and making them an optimal choice for processing sensor data such as battery voltage, current and temperature readings. CNN can effectively capture local patterns and correlations within the data with a convolutional filter, which is needed for accurate state estimation.

However, long-term dependencies and contextual relationships in sequential data are effectively learned by Transformers through their self-attention mechanism. In particular, this is important for understanding the temporal dynamics of battery states (e.g., SOC and SOH). Transformers have a self-attention mechanism that weighs the importance of different parts of the input sequence and thus gives you a complete picture of the data over time.

The strengths of CNN and Transformer models are utilised through the integration. CNN is designed to extract spatial features and Transformers are designed to extract temporal features of data. The HSE DT method combines this complementary combination to provide increased overall accuracy and robustness of battery state estimation.

While the use of Transformer-CNN models is not advanced in itself, they are effective in a wide variety of domains, including natural language processing and computer vision. The models could improve the reliability and accuracy of our battery management system to allow that battery systems perform and last better. The design, implementation, and integration of the Transformer-CNN model into the HSE DT method is elaborated in this section and how it improves battery state estimation accuracy and robustness is shown.

Several critical stages in the design and implementation of the CNN and Transformer model within the HSE-DT method are needed to take advantage of their complementary strengths for battery state estimation. The architecture, as well as the data processing pipeline and steps required to deploy the Transformer–CNN model, are presented in this section.

Transformer-CNN is also designed to accommodate the complex and dynamic nature of battery data, which includes spatial and temporal nature. The architecture comprises two primary modules: The CNN module and the Transformer module. The transformer-CNN model within the HSE-DT method is shown in Figure 5.2.

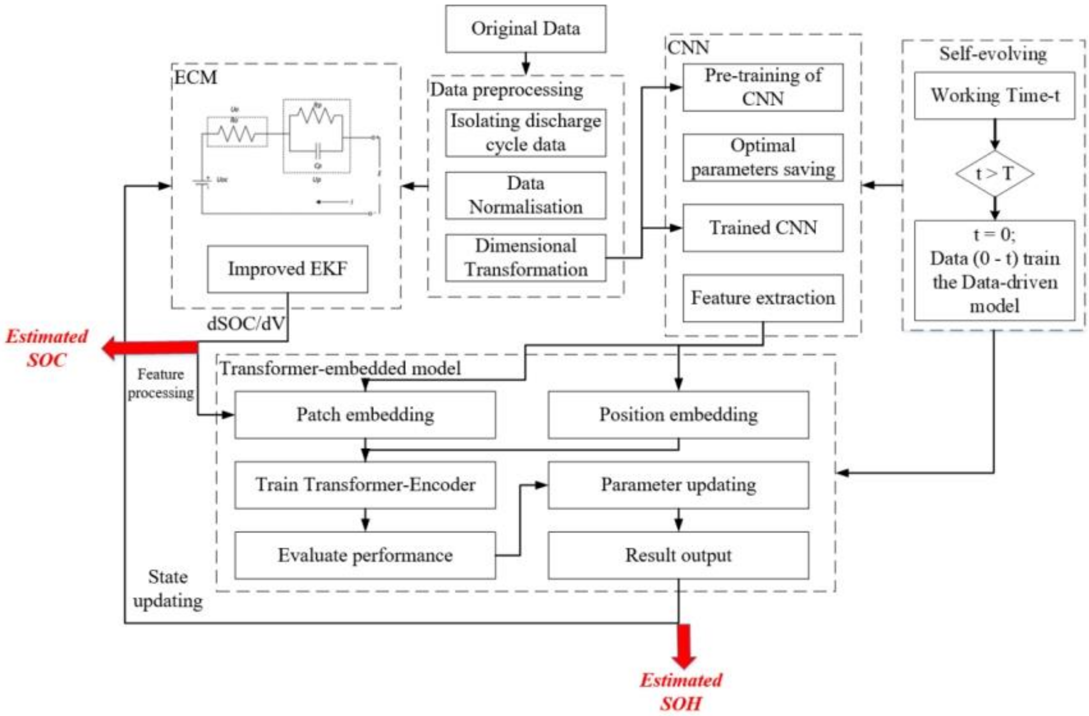


Figure 5. 2 The Transformer-CNN model within the HSE-DT method

The CNN module processes time series data coming from battery sensors such as voltage, current, and temperature. The CNN module takes in the input data and extracts spatial features by passing the data sequentially through a series of convolutional filters. After each convolutional layer comes down with an activation function, like ReLU and a set of pooling layers to reduce the dimensionality, retaining the important information. The output of the convolutional layers gives a set of feature maps that encode local patterns and correlations in the battery data, and explicitly have a spatial nature.

CNN is structured in three layers: the input layer, hidden layers, and output layer. The input layer receives the original data and forwards it to the hidden layers for feature extraction. The hidden layers include fully connected layers, max-pooling layers, and convolutional layers, which facilitate hierarchical representation learning. The output layer then generates the final predictions based on the learned features.

The CNN architecture is effective in capturing local features hierarchically through convolutional operations. It extracts spatial patterns from battery data, such as voltage, current, and temperature, by progressively refining localized representations. The CNN branch begins with an input layer that preprocesses and structures the incoming raw data. Convolutional layers extract local variables while preserving time-independent characteristics over long distances. Max-pooling layers enhance computational efficiency by reducing dimensionality while retaining essential spatial information. Finally, fully connected layers consolidate the hierarchical representations before passing the processed data to the Transformer module for further analysis.

This is further processed by the transformer module on top. The first thing is to add positional encoding to keep track of the relative positions of data points so that we can understand the sequence of events over time. The transformer module then applies self-attention to different parts of the input sequence to give different weights to parts of the sequence and learn about long-term dependencies and contextual relationships. Feedforward layers generate the final feature embeddings, and summarised battery data temporal dynamics.

The Transformer module combines pointwise layers with stacked self-attention layers and fully connected layers to support both encoding and decoding operations through its structured design. The self-attention mechanism eliminates both recurrence and convolutional dependencies through its components scaled-dot-product attention and multi-head attention to achieve global feature aggregation. The Transformer module incorporates positional encoding which maintains input data sequence order through value assignments between 0 and 1 to uphold temporal coherence.

Through its encoding process, the Transformer produces embedded representations that detect hidden relationships between sequential input segments to extract an extensive range of features. The decoder works with generated decoder outputs and these embeddings to create the sequence of final outputs. Through self-attention mechanisms, the Transformer can reweight importance according to changing battery states while focusing on vital fluctuations and long-term patterns. The adaptive weighting system improves predictive accuracy through its ability to model short-term changes and sustained patterns in battery activity which produces better state estimation results.

The transformer-CNN model is effective only if the data processing pipeline is designed carefully so that the input data is optimised for model performance. Real-time measurements of critical parameters are recorded by continuous data collection from battery sensors, which is the basis for subsequent processing steps. Normalisation in data preprocessing is critical for the consistency of different measurement scales and improves model performance. Then, we segment time-series data into smaller sequences of fixed time windows so that the CNN and Transformer modules can efficiently process the data.

Following the feature extraction, segmented and normalised data is first processed by the CNN module, where convolutional layers extract intricate spatial features from the battery data. Then, we feed them into the Transformer module, which comprises positional encoding, then performs self-attention and feed-forward layers to capture the temporal dependency and contextual relationships to yield an accurate estimation of the state.

The HSE-DT method seamlessly integrates the transformer-CNN model for real-time battery state estimation and management. In turn, the model is trained in a supervised learning way using labelled data with SOC and SOH known values. In the training process, the parameters of a model are optimised for a minimum loss function (e.g. Mean Squared Error that tells how far are predicted and actual values from each other). The trained transformer-CNN model receives real-time sensor data to estimate the state continuously. The SOC and SOH estimation is used by the HSE-DT method to monitor and manage the battery system. Transfer learning are used to update the model parameters with new data that was not present at training so that the model remains accurate and timely over time without necessitating full retraining.

The transformer-CNN module extracts local features progressively through its CNN branch which then passes enriched details to Transformer modules for global perception enhancement. All data structures undergo standardisation as a preprocessing step since CNN and Transformer exhibit possible discrepancies in data formats and feature patterns. Cross-entropy losses serve as training mechanisms which unite CNN-derived local features with Transformer-based global information during model learning. The predictive model produces its results through flattened layers which transform multidimensional outputs into a single-dimensional space for effortless model propagation. Dropout layers use random neuron selection to reduce model overfitting. Network density enables every neuron to gather information from all preceding neurons leading to a complete interconnected decision path. The transformer-CNN hybrid framework delivers reliable battery state estimation by maximizing local features and strengthening global dependencies to achieve better prediction outcomes.

The HSE-DT method with the transformer-CNN model provides a robust and efficient method for battery state estimation. This model combines the spatial feature extraction capability of CNNs with the temporal analysis strengths of transformers to significantly improve the accuracy and reliability of battery management systems. Further optimisations and real-world applications will be investigated in future work to validate the model's performance in various operational scenarios.

5.2.3 Synergistic Interaction within the Digital Twin

The synergistic interaction between the HSE and the DT method is critical to improving battery state estimation and management. The mechanisms by which different components of the HSE-DT method interact and collaborate to present a complete and accurate representation of the battery system state are discussed in this section.

1) Multi-faceted Integration

The battery management functions are organised into several multi-faceted components of the HSE-DT method. That seamless integration makes it so that the system can effectively take advantage of the strengths of each component to give a holistic view of the battery system. The first part of this is to acquire real-time data from sensors embedded within the battery system. This data covers important voltage, current, temperature and other relevant metrics. The data undergoes preprocessing to remove noise and get consistent so that the data is suitable for further analysis. The second component, modelling and simulation, uses the pre-processed data as input to digital twin models of electrochemical, thermal, and ageing processes. These models model the physical and chemical activities within the battery and hence provide insight into the battery's internal states such as SOC and SOH. The estimation and prediction component then makes use of advanced algorithms (including the Transformer-CNN model) to analyse the data and predict the future states of the battery. Using a combination of historical and real-time inputs, these predictions are based on dynamic state estimation. Finally, the estimation process provides insights and predictions that the decision support component uses to inform decision-making. Maintenance recommendations, charging strategies and operational adjustments are all provided for this component. Furthermore, available to stakeholders are also user interfaces, in the form of detailed reports and visualisations to support informed decision making.

2) Feedback Mechanisms

That digital twin can continuously adapt and evolve using new data and new conditions –or not– and it requires effective feedback mechanisms for it to be enabled. The HSE-DT method combines several feedback loops to improve its accuracy and reliability. This method relies heavily on real-time feedback to monitor the battery system continuously. This ongoing observation also allows for immediate changes to the digital twin models, so they stay accurate and current with the state of the battery. Also, real-time feedback allows our system to quickly discern anomalies and take corrective action before any failures occur.

In addition to real-time adjustment, the HSE-DT method also includes periodic updates of the models to provide further refinement. The Transformer–CNN has its internal parameters retrained on fresh data, causing an improvement in its predictive accuracy. Transfer learning techniques are used to update the model parameters in an efficient and adaptable manner without a full retraining process.

3) Collaborative Analysis

The HSE-DT method greatly improves the effectiveness of battery state estimation through the collaborative interaction between different models and algorithms. This collaboration is enabled through several important mechanisms that combine to increase accuracy and reliability.

This method relies on a critical mechanism of data fusion by which data from various sensors and models are fused to form a complete picture of the battery’s state. This procedure capitalises the strong point of every information source in a great estimation. The refined predictions of the Transformer CNN model are then further improved using the fused data.

However, another important mechanism is cross-validation by which we can make sure all predictions and the insights drawn from different models are accurate and consistent. In this, we compare the outputs of various models and algorithms to determine inconsistencies and reconcile conflicts. Cross validation strengthens the robustness of the digital twin, and provides reliable and trustworthy information derived from said digital twin.

The HSE-DT method contains adaptive learning: the models get infused with new data and new knowledge. That process requires a continuous learning structure to keep the digital twin relevant and accurate over time. Moreover, the digital twin can adapt to changes in the operating conditions of the battery system, e.g., temperature, load, or usage pattern, through adaptive learning.

To provide accurate and complete battery state estimations, the synergistic interaction within the HSE-DT method is required. The HSE-DT method integrates multiple facets, includes effective feedback mechanisms, and enables collaborative analysis to improve the management and performance of battery systems overall.

4) The Self-Evolving Mechanism

A key part of the HSE-DT method is the self-evolution mechanism. Models in digital twin are dynamically adapted to remain relevant and effective to the changing conditions and user patterns of the battery as it updates. The self-evolution mechanism consists of three key elements: transfer learning, continuous learning, and adaptive algorithms. Taken together, these elements enable the digital twin models to remain robust and truthful as these react to new data and changing operational conditions.

To minimise the need for full retraining, new data is used to update digital twin models using transfer learning. With this we only apply this technique to pre-trained models and adapt them to new tasks or datasets, saving us from the computational prerequisites and making it more efficient. In the HSE–DT method, transfer learning enables the digital twin to learn new battery data such as temperature, voltage and current changes without having to start from scratch. Variations in battery chemistry, ageing effects and different operational environments are particularly useful for this.

This leads to fresh data updating and refining the DT. It is supervised and unsupervised learning. To improve the accuracy of the models for the mentioned tasks of SOC and SOH estimation, models are trained under supervised learning in the labelled data. One technique, however, unsupervised learning, discovers patterns and anomalies in the data using features inside the dataset without any labels previously added, making it better suited for the model to adjust to unexpected changes in battery behaviour. The

HSE-DT method can be continually learned and thus becomes more accurate and more reliable with time.

They are adaptive algorithms, which means that they will change their behaviour upon detecting anomalies or shifts in the operational environment of the battery. The feedback mechanisms of this algorithm adaptively refine model parameters to achieve near-optimal performance despite changes in the environment. As an example, if the adaptive algorithm detects a sudden change in temperature, it can update its thermal model. The adaptability is important for real-time monitoring and management such as electric vehicles and renewable energy storage systems where the operating conditions vary greatly.

5.3 Experimental Setup

In this section, experimental validations and discussions are conducted to validate the feasibility of the proposed method.

5.3.1 Data Description and Pre-processing

In this section, experimental validation of the HSE-DT method is presented using data from NASA lithium-ion battery charge and discharge experiments. We use this dataset as a robust testbed to demonstrate the effectiveness of our digital twin model. The NASA dataset comprises many charge and discharge cycles of lithium-ion batteries under different conditions with critical parameters like voltage, current, temperature and capacity. Accurate models for battery state estimation require these parameters. The dataset is highly comprehensive and of high quality, making it suitable for our study, offering a rich set of time series data which characterises the dynamic behaviour of batteries. In the data collection phase, we observed inconsistencies with the battery tester logging mechanism. Data was repeated as several drive cycles were consolidated into a single extensive file. However, this consolidation introduced redundancy and possible anomalies, which had to be resolved to allow the integrity of data used in training and validating the models.

Redundant entries indicative of data-logging anomalies were removed to allow data integrity. Data cleaning process consisted of identifying and removing duplicated entries and implementing algorithms to philtre out spurious data points that did not follow expected battery behaviour. To improve the performance of machine learning models used in the HSE-DT method, normalisation was applied to scale the data to a standard range. To make them consistent across different measurement scales, we scaled parameters like voltage, current, and temperature to a range of 0 to 1, and transformed the data to have a mean of 0 and a standard deviation of 1.

The CNN and Transformer models were trained over small, manageable sequences of continuous time series data to allow efficient processing. To capture complete cycles of battery charge and discharge, the data was segmented into segments of equal length, and to capture transitional behaviours and improve model robustness, the overlap between segments was introduced. The preprocessed data was further extracted to extract key features to feed in the Transformer-CNN model. To do this, the time-dependent characteristics like the slope of voltage and current versus time and measures like mean, variance, and skewness were calculated for each segment to give a complete picture of the battery state.

Several advantages of the NASA dataset for our study are provided. It covers a broad range of operating conditions and thus allows robust models to be built which can generalise across different situations. The data is meticulously recorded, well documented and thus reliable and suitable for research purposes. In addition, the NASA dataset is widely used in the battery research community, and, as such, enables meaningful comparisons with other studies and methods. Using this dataset, our results are comparable to existing research, which confirms the efficiency of our HSE-DT method.

In the next section, the above data preprocessing steps are necessary to prepare the NASA dataset for the use of the HSE-DT method. Data redundancy is addressed, data is normalised, time–series sequences are segmented, and relevant features are extracted to allow that the input data is of high quality and usable for accurate battery state estimation. The objective is to demonstrate the effectiveness in enhancing battery situational awareness, which includes not only an accurate estimation of battery states such as SOC and SOH but also a comprehensive understanding of battery conditions and behaviours under various scenarios. We performed a series of experiments using the transformer-CNN model to assess the performance of the HSE-DT method. The purpose of these experiments was to validate the accuracy, robustness and overall situational awareness capabilities provided by the method.

5.3.2 Evaluation Metrics

We evaluate the performance of the HSE-DT method using the pre-processed NASA dataset. The objective is to demonstrate the effectiveness in enhancing battery situational awareness, which includes not only an accurate estimation of battery states such as SOC and SOH but also a comprehensive understanding of battery conditions and behaviours under various scenarios. To assess the performance of the HSE-DT method, we conducted a series of experiments utilising the Transformer-CNN model. These experiments were designed to validate the accuracy, robustness, and overall situational awareness capabilities provided by the method.

The evaluation process began with training the Transformer-CNN model using the pre-processed NASA dataset. Supervised learning techniques were employed, utilising labelled data with known SOC and SOH values to optimise the model parameters. The mean squared error (MSE) was used as the loss function to measure the discrepancy between the predicted and actual values, guiding the optimisation process. This training phase allows the model could learn from historical data and develop accurate predictive capabilities.

Following the training phase, the model's performance was evaluated on a separate test dataset that was not used during training. This test dataset included various battery cycles under different operating conditions to assess the model's generalisation capabilities. The key metrics used for performance evaluation included MAE and RMSE, which quantified the accuracy of the SOC and SOH estimation mentioned in previous sections. Furthermore, other metrics such as R^2 are computed as:

$$R^2 = 1 - \frac{\sum_{k=1}^{K} (l(k) - \hat{l}(k))^2}{\sum_{k=1}^{K} (\overline{l(k)} - \hat{l}(k))^2} \tag{5.7}$$

Here, $l(k)$ denotes the actual capacity, $\hat{l}(k)$ represents the estimated value, and K is the total number of cycles.

5.3.3 Collective Situation Awareness

1) Battery State Monitoring and SOC Estimation

The HSE-DT method proposed in this study was validated using public datasets. Due to the absence of specific conditions required for battery model parameter identification, the SOC was provisionally estimated using the EKF as a reliable alternative. The estimation results of the proposed model, along with comparisons to three well-established superior algorithms, are detailed in Figure 5.3 and Table 5.1. Overall, all four methods demonstrated strong estimation performance across the NASA battery datasets.

Figure 5.3 provides voltage, current, temperature and a comparative analysis of SOC determined by the EKF, measured against a reference SOC. The graph illustrates SOC, current, voltage, and temperature over time during each cycle for batteries B0005, B0006, B0007, and B0018. Although the model aligns well with the training data, noticeable deviations are observed in SOC estimation when processing new data. These deviations are reflected in the RMSE values, which are 0.9% for training and 2.5% for testing. Generally, a lower RMSE signifies better SOC estimation accuracy, but the discrepancy between training and testing RMSE suggests potential overfitting, which may affect the model's performance on previously unseen data. These RMSE values were computed using a dataset that employed pervasive network structures, the same dataset used for the reference methods introduced in the analysis. When compared to other algorithms in Table 5.1, the proposed method demonstrated the lowest RMSE among the four algorithms evaluated, underscoring its superior accuracy. This accuracy is anticipated to improve further as overfitting issues are addressed. The consistent use of reference methods with the same dataset further supports the reliability and robustness of these findings.

Table 5.1 The comparison of SOC estimation for different methods USING the B5 dataset

Methods	RMSE
HSE-DT	0.009
LSTM	0.032
CNN-LSTM	0.011
Transformer	0.017

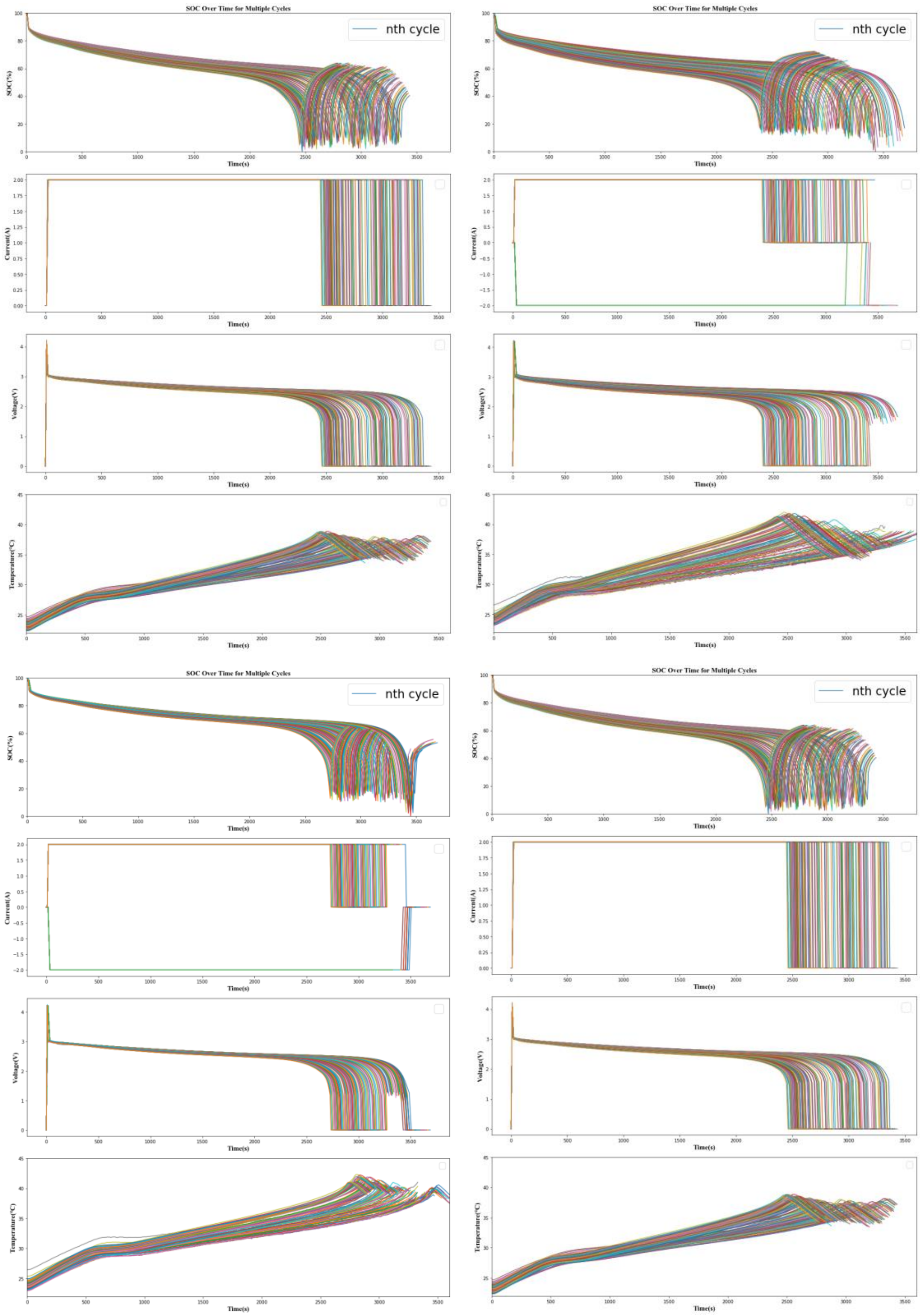


Figure 5. 3 SOC, current, voltage and temperature over time during each cycle of B0005, B0006, B0007 and B0018.

2) **SOH Estimation**

Pearson correlation coefficient (PCC) analysis measures the linear relationship between two variables. It is defined as the ratio of the covariance of the two variables to the product of their standard deviations (Kong et al., 2021). The PCC is calculated as follows:

$$PCC = \frac{\sum_{i=1}^{n}(z_i-\bar{z})(q_i-\bar{q})}{\sqrt{\sum_{i=1}^{n}(z_i-\bar{z})^2}\sqrt{\sum_{i=1}^{n}(q_i-\bar{q})^2}} \tag{5.8}$$

where z_i is the values of the x-variable in a sample, z is the mean of the values of the x-variable, q_i is the values of the y-variable in a sample, and $\bar{q}$ is the mean of the values of the y-variable (Jebli et al., 2021).

PCC is a statistical metric used to determine the linear relationship between two variables and it is in the range from -1.0 to 1.0. An absolute value of 1.0 means a perfect linear relationship, that is all data points lie exactly on a straight line in either positive or negative direction. A value of zero for the PCC indicates no linear dependency of the variables and positive or negative values indicate direct or inverse linear dependences, respectively. In the framework of battery SOH modelling, PCC analysis is employed to choose input features from each discharging cycle: capacity (Ah), output current (A), terminal voltage (V), sampling time (s), and temperature (°C). These features are quantitatively evaluated based on their linear dependencies, which are categorised into five levels of strength: Correlations were extremely strong (0.9-1), strong (0.7-0.89), moderate (0.4-0.69), weak (0.1-0.39), or negligible (0-0.1) (Benesty et al., 2008). By categorising these correlations, we can find out which features are most relevant for accurate SOH prediction.

It is necessary to evaluate these features to understand the relationships between battery characteristics and how they affect SOH estimation. Battery capacity, the primary target of prediction, has a moderate correlation with temperature (0.15), weak correlations with current (0.13) and voltage (-0.14), and a negligible correlation with sampling time, according to PCC analysis. According to this analysis, terminal voltage, output current, temperature and capacity are chosen as the input features for the prediction model. Correlation diagrams further visualise these relationships as measures of correlation strength and direction between battery characteristics, to facilitate the identification of major factors that will impact performance of battery life and performance. Figure 5.5 shows a strong negative correlation (-0.92) between cycles and capacity, meaning as the number of cycles increases the capacity decreases and better battery health is associated with higher capacity. On the other hand, a strong negative correlation is observed between cycles and SOH, meaning that battery health decreases as the cycles increase. Knowing these correlations is necessary to estimate battery life and performance correctly, and it identifies important features—number of cycles, capacity, and SOH—for battery lifetime. Through detailed diagrams of these correlations, these interrelationships of the battery characteristics are visualised and enable effective feature selection and model development of SOH estimation.

As discussed in previous sections, data from four batteries labelled B5, B6, B7, and B18, sourced from NASA, were utilised to validate the prediction performance of the HSE-DT method. In our experiment, the complete dataset starting from the 30th, 60th, and 90th cycles were used for offline training, while the remaining data were employed for online testing. To further evaluate the robustness and effectiveness of the CNN-Transformer model, three additional methods—LSTM, Transformer, and CNN-LSTM—were also employed to estimate battery SOH using the same offline training strategy.

Figure 5.6 presents the SOH estimation from the proposed model along with the relative errors for each cycle of B0005. As depicted in Figures 5.6(a)-(c), the predicted SOH values align closely with the reference SOH values, clearly demonstrating the effectiveness of the HSE-DT method.

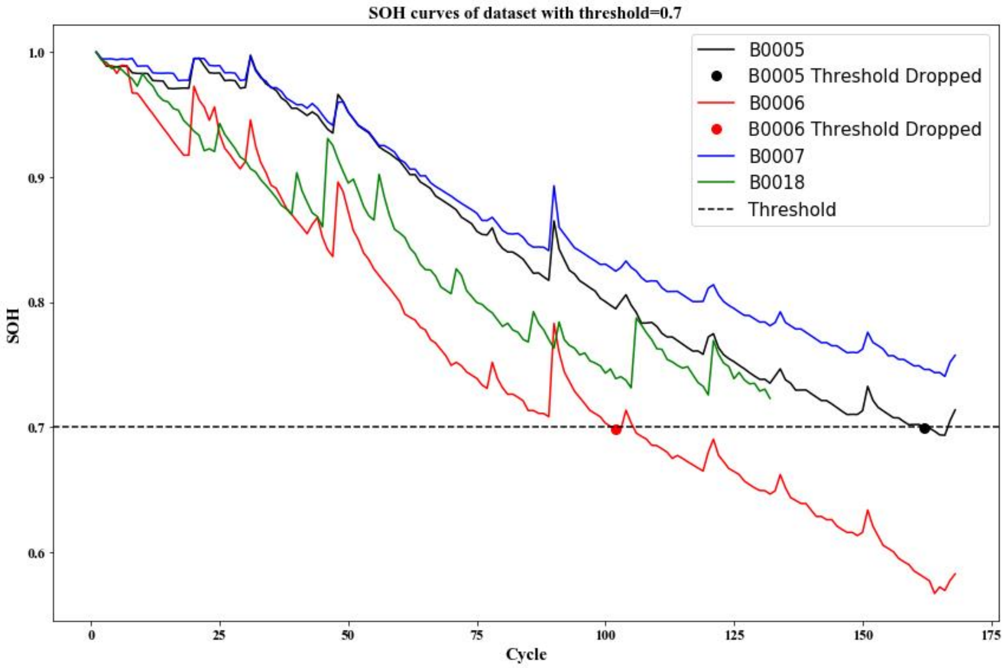


Figure 5. 4 The theoretical SOH of the NASA dataset

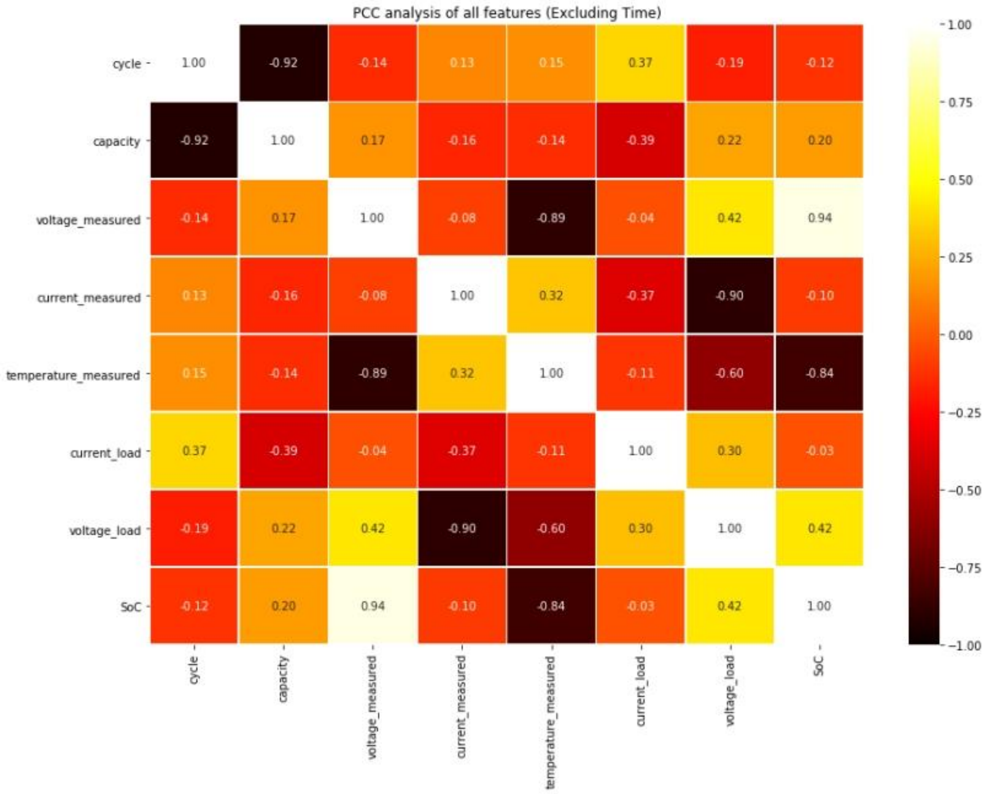
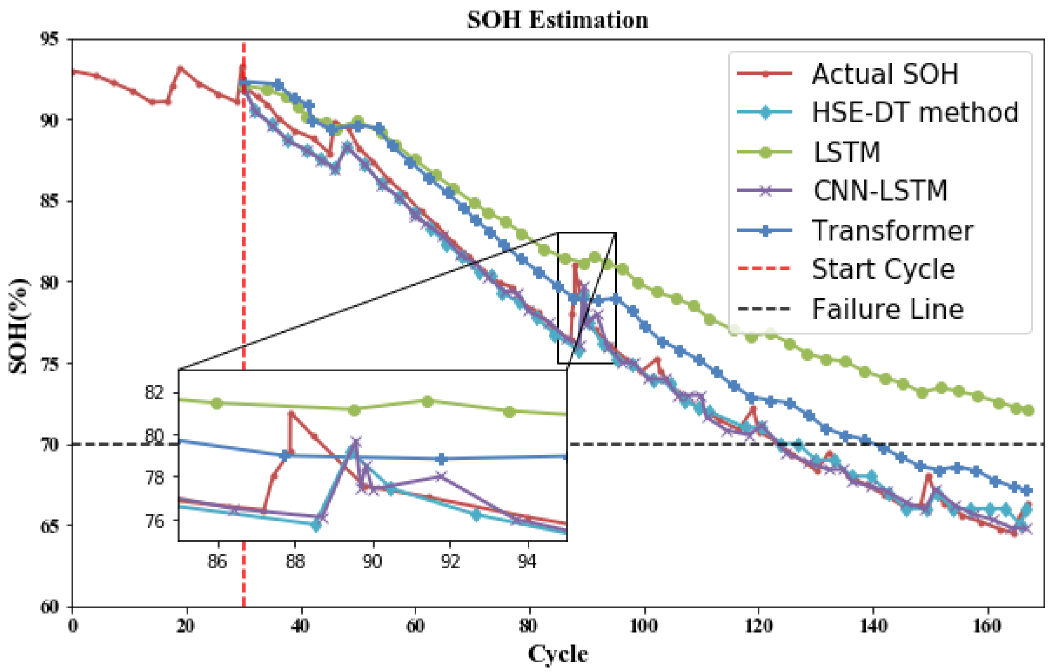
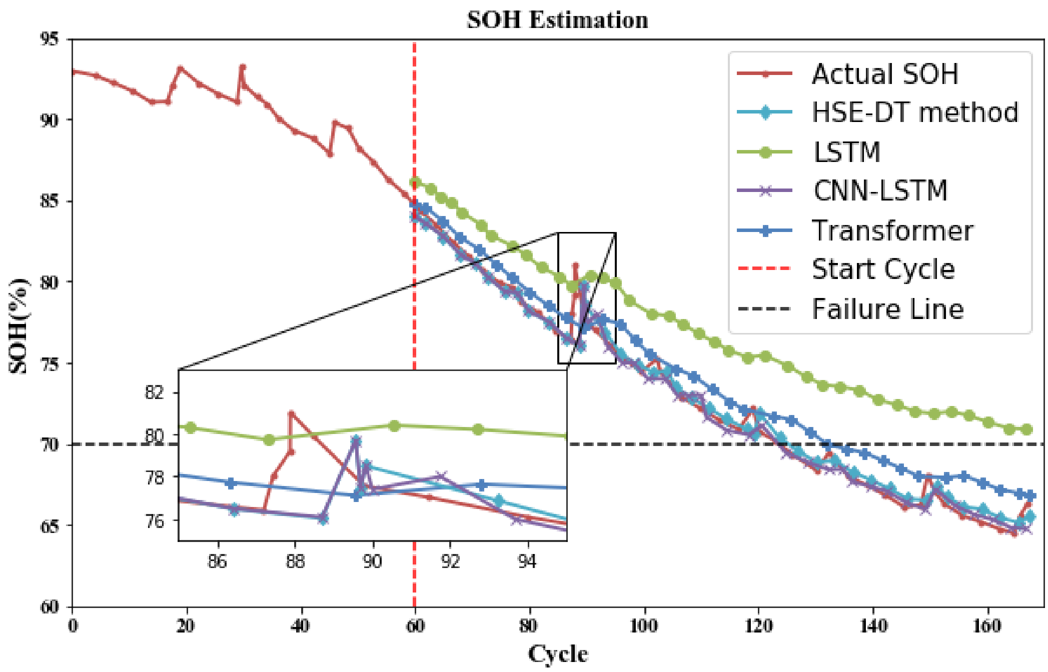


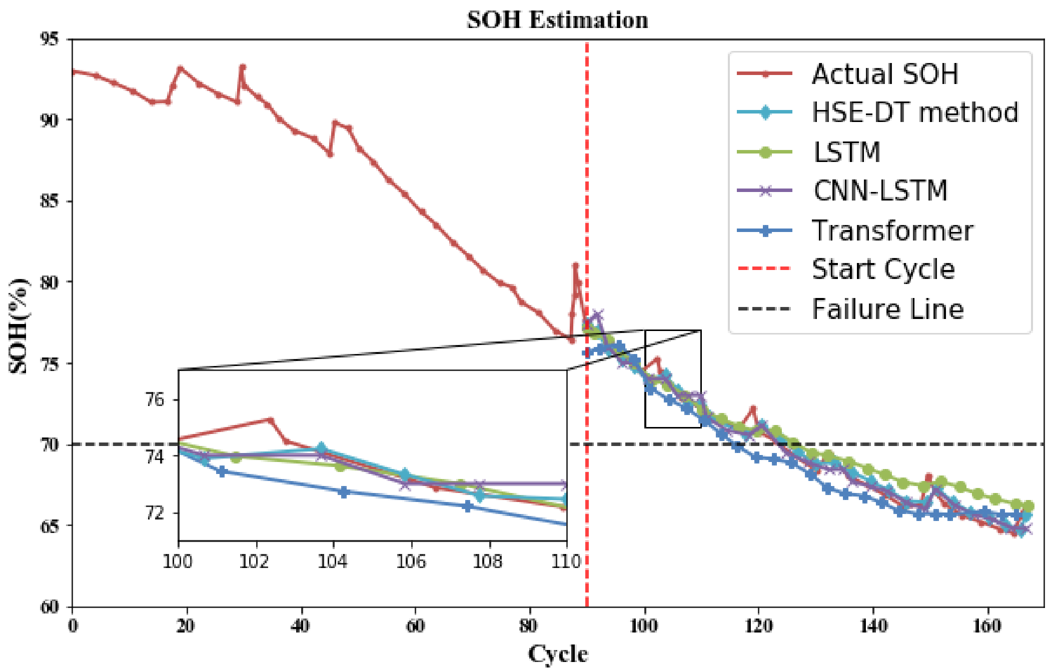
Figure 5. 5 PCC analysis of all features


SOH Estimation
SOH(%)
Cycle
Actual SOH
HSE-DT method
LSTM
CNN-LSTM
Transformer
Start Cycle
Failure Line

(a)


SOH Estimation
SOH(%)
Cycle
Actual SOH
HSE-DT method
LSTM
CNN-LSTM
Transformer
Start Cycle
Failure Line

(b)



(c)

Figure 5. 6 The SOH estimation regarding B5 by training at (a), 30th cycle (b), 60th cycle (c), 90th cycle

A summary of the results of the first 90 cycles for pre-training across all four datasets is given in Table II. As can be seen, the MAEs, MAPEs and RMSEs of the proposed model are less than 0.5% while the R^2 value exceeds 99%, which means the transformer-CNN model outperforms the others in SOH estimation. Additionally, these results show a substantial reduction of SOH estimation error for lithium-ion batteries using the HSE-DT method.

The results indicated that the HSE-DT method achieved high accuracy in estimating battery states. The MAE, MAPE, RMSE and R^2 values for SOC and SOH estimation were significantly lower compared to traditional methods, demonstrating the model's effectiveness in capturing complex relationships and dependencies within the battery data. These metrics confirmed the model's ability to provide reliable and precise estimations, which are important for comprehensive situational awareness.

Table 5.2 The comparison of SOH estimation for different methods

Dataset	Methods	MAE	MAPE	RMSE	R^2
B5(90th)	Transformer-CNN	0.0024	0.0031	0.0029	0.9901
	LSTM	0.0043	0.0624	0.0071	0.8981
	CNN-LSTM	0.0029	0.0160	0.0041	0.9721
	Transformer	0.0035	0.0740	0.0045	0.9610
B6(90th)	Transformer-CNN	0.0024	0.0038	0.0028	0.9938
	LSTM	0.0105	0.0575	0.0135	0.8425
	CNN-LSTM	0.0030	0.0168	0.0045	0.9848
	Transformer	0.0035	0.0752	0.0051	0.9816
B7(90th)	Transformer-CNN	0.0018	0.0050	0.0022	0.9908
	LSTM	0.0037	0.0520	0.0056	0.9215
	CNN-LSTM	0.0017	0.0335	0.0025	0.9869
	Transformer	0.0021	0.0711	0.0029	0.9809
B18(90th)	Transformer-CNN	0.0024	0.0038	0.0029	0.9981
	LSTM	0.0569	0.0768	0.0666	0.8491
	CNN-LSTM	0.0204	0.0394	0.0283	0.9330
	Transformer	0.0425	0.0712	0.0498	0.7885

Additionally, the self-evolving mechanism of the HSE DT method enhances its situational awareness capability by leveraging the transfer learning technique, which periodically updates the model with new data, such that predictions are accurate and up to date. This continuous learning process results in the method being able to adjust to changing battery behaviours over time and to improve estimation accuracy and lead time of the battery condition and operational status information.

In addition to state estimation, the HSE-DT method provides a broader understanding of the battery's health and operational context, which is important for optimising performance, enabling safety, and extending the battery's lifespan. The integration of the Transformer-CNN model with the self-evolving mechanism further enhances the method's ability to monitor and manage battery systems effectively by enabling more precise analysis and decision-making.

Finally, the performance evaluation using the NASA dataset shows that the HSE-DT method can improve the situational awareness of battery systems. Finally, the performance evaluation using the NASA dataset shows that the HSE-DT method can improve the situational awareness of battery systems under typical operating conditions. However, real-world applications often present more challenging environments, such as extreme temperatures which can influence the accuracy and reliability of state estimations. The dataset used in this study was limited in scope resulting in an evaluation of the model’s performance across a wider range of temperature variations that was not feasible. Nevertheless, the results show that the HSE-DT method can accurately and reliably monitor and manage under typical conditions, thus providing accurate condition estimates.

5.4 Discussion

In this chapter, the HSE-DT method is proposed and integrates advanced machine learning models with a structured digital twin framework to address the complexities of battery state estimation and management. The methodology employed a Transformer-CNN model within a multi-layered architecture that includes real-time data acquisition, continuous learning, and dynamic model adaptation. This systematic approach enhances the accuracy and reliability of the estimations, enabling effective battery management and optimisation.

A critical component of the HSE-DT method is its self-evolving mechanism, which utilises transfer learning to update the model parameters based on newly acquired data.

This process allows the model to refine its predictions incrementally without the need for complete retraining, significantly reducing computational overhead. The HSE-DT framework's adaptability allows it to remain effective in capturing the nonlinear and dynamic behaviours of batteries, particularly as they age or operate under varying environmental conditions. By incorporating real-time data and historical records, the method can accurately estimate key battery states, such as SOC and SOH, thereby providing timely and actionable insights.

The integration of the Transformer-CNN model within the HSE-DT framework serves a pivotal role in feature extraction and prediction. The CNN component captures intricate spatial features within the time-series data, while the Transformer component models long-term dependencies and contextual relationships. This hybrid approach leverages the strengths of both models, allowing for precise estimation of battery states even in the presence of noise or irregularities in the data. The unique combination of CNN and Transformer models not only enhances the robustness of the method but also enables it to provide a holistic understanding of battery health and performance.

The experimental results presented in this study validate the proposed methodology, demonstrating its effectiveness in various scenarios. The HSE-DT method consistently outperformed conventional models, such as LSTM, CNN-LSTM, and standalone Transformer models, in terms of SOC and SOH estimation accuracy. The superior performance of the HSE-DT method can be attributed to its hierarchical structure, which systematically integrates multiple estimation layers and continuously refines predictions based on real-time observations. This systematic approach enables the HSE-DT framework to capture complex relationships within the data and adapt to changing battery conditions dynamically.

The integration of real-time feedback mechanisms within the HSE-DT framework further enhances its capability to monitor and manage battery systems. By incorporating both predictive and diagnostic elements, the method not only provides accurate estimations of SOC and SOH but also identifies potential anomalies and performance deviations. This proactive approach to battery management minimises the risk of unexpected failures and optimises battery utilisation, ultimately extending the lifespan of the energy storage system.

In conclusion, the HSE-DT method proposed in this study provides a robust and scalable solution for battery state estimation and management. The innovative combination of the Transformer-CNN model within a hierarchical digital twin framework, coupled with the self-evolving mechanism, offers significant improvements over conventional methods. The experimental validation using the NASA dataset demonstrates the method's high accuracy and adaptability, confirming its potential for real-time battery management and predictive maintenance. Future research should explore additional methodological enhancements, such as incorporating more advanced feature extraction techniques and expanding the framework's applicability to other battery chemistries and configurations.

5.5 Summary

In summary, this study introduced the HSE-DT method, designed to enhance battery situational awareness. Utilising a structured DT model, the method integrates critical parameters such as voltage, current, and temperature, alongside advanced estimation techniques. Recognising the complexities of battery situational awareness, the HSE-DT method employs the Transformer-CNN model to effectively capture spatial and temporal dynamics, providing a comprehensive understanding of battery conditions and behaviours.

The HSE-DT method incorporates a self-evolving mechanism that leverages transfer learning and continuous learning techniques. This approach allows the model to remain adaptive and relevant over time, capable of refining its insights with new data through rolling learning. Our research provides a detailed analysis of the HSE-DT method, describing its complex structure and key stages in the learning process. Empirical results indicate the efficiency of the method in combining online situational awareness, including real-time monitoring of battery states and prediction of future conditions. The Transformer-CNN model demonstrated high accuracy, achieving low RMSE and MAE values, supporting the utility of the HSE-DT method in enhancing battery situational awareness.

The HSE-DT method is underscored by its multi-layered structure, which integrates various aspects of battery monitoring and analysis. This approach offers insights into battery health and operational performance, laying the groundwork for advanced battery management strategies. Consequently, battery operations can be optimised, enhancing the battery's lifecycle and overall system efficacy. The integration of advanced machine learning techniques with the digital twin paradigm represents a promising combination, contributing to improvements in battery management and situational awareness across various applications.

Looking ahead, our research will focus on addressing key challenges to further refine the HSE-DT method for battery situational awareness. This involves developing a fully integrated digital twin that combines dynamic and static models and tries to integrate historical and real-time data to enrich situational awareness. Also, future studies will examine the model’s performance under extreme temperatures, varying battery health states, and different usage patterns. Additionally, optimising the digital twin to minimise latency will be key to its capability for real-time synchronous updates and adaptive feedback control. Exploring these research dimensions will augment the capabilities and impact of battery digital twin technologies.

Chapter 6 RUL-Based DT-Supported Optimisation for Operational Decision Support in BESS

6.1 Introduction

DT technology integrated with battery energy storage systems (BESS) is increasingly recognised as a way to improve operational decision support (Semeraro et al., 2023b). However, traditional maintenance strategies, either reactive or following predefined schedules, typically fail to capture the real-time health state of BESS components (Singh et al., 2021b). The use of these strategies may lead to suboptimal performance, higher costs and unexpected failures. Therefore, there is a need for advanced methods, which use real-time data and sophisticated analytical models to enable continuous monitoring and predictive maintenance of BESS for improved system reliability and longevity. The Digital Twins are a promising solution providing a complete digital replica of physical systems, able to collect real-time data, monitor health status and make operational decisions (Chen et al., 2023).

Integrating DT technology into BESS is generally regarded as a very effective way to enhance operational decision support. Unlike DT-supported maintenance, reactive response or schedule-based approaches cannot capture the real-time health status of BESS components. Therefore, such approaches often lead to suboptimal performance, higher costs, and unexpected failures because they are based on fixed maintenance intervals and lack predictive ability (You et al., 2022).

To address these challenges, this chapter presents a DT-supported decision support system that employs advanced predictive maintenance and fault analysis methodologies. The proposed system incorporates two innovative strategies. First, an RUL-based maintenance approach integrates RUL estimates with equipment availability to optimise maintenance decisions dynamically (Ahmad and Kamaruddin, 2012). Second, a large language model (LLM) based fault analysis framework enhances decision-making by offering contextually relevant recommendations based on unstructured textual data (Tao et al., 2025), such as maintenance logs and technical manuals.

The RUL-based maintenance strategy significantly improves traditional approaches by integrating real-time health status data with equipment availability metrics (Alaswad and Xiang, 2017a). Unlike conventional methods that solely rely on RUL predictions, this approach incorporates both remaining lifespan and real-time equipment availability to determine optimal maintenance timing (Alaswad and Xiang, 2017b). By balancing these two critical factors, the strategy minimises maintenance costs while maximising system availability and reliability. Additionally, integrating RUL with availability allows for more precise scheduling of maintenance activities and spare parts management, thereby reducing the risk of unexpected failures and stockouts (Prajapati et al., 2012).

With the development of sensor technology, the use of real-time equipment health status information to predict the RUL and then use it for equipment health management decisions has become the core content of fault prediction and health management (Si et al., 2013, Mosallam et al., 2016, Zhang et al., 2018, Roemer et al., 2006). Based on RUL, scholars have developed a joint optimisation of maintenance and spare parts ordering decisions, and the sequential joint optimisation strategy model proposed by Wang (Wang et al., 2013) firstly determines the optimal time for equipment replacement and then optimises the ordering point. Based on this study, Jiang (JIANG et al., 2015) optimised both the equipment replacement time and the spare parts ordering time and compared them with the results of the sequential joint strategy optimisation, which ultimately showed that the joint decision was more effective. However, none of them considered the costs associated with ordering spare parts (Wang et al., 2013, JIANG et al., 2015). Wang (Wang et al., 2014) proposed a joint spare parts ordering and replacement strategy for unrepairable systems, under which historical state information is used to predict the remaining life at any monitoring moment, and various scenarios that may occur at the ordering point, the time of preventive replacement, and the time of the next monitoring moment are combined to construct an objective function that minimises the expected cost per unit of time while optimising the ordering point and the replacement time. The objective function is constructed to minimise the expected cost per unit of time by combining various scenarios that may occur at the ordering point, the preventive replacement moment, and the next monitoring moment, while optimising the ordering point and preventive replacement moment. Although the above studies consider the remaining life of the equipment, they are mainly used in maintenance decisions, where the ordering decision for spare parts is based on the degradation level or the moment of equipment replacement. However, the decision maker will judge whether to order or not by comparing the length of the remaining useful life of the equipment with the length of the lead time for spare parts (Sikorska et al., 2011).

These methodologies collectively establish a robust framework to enhance the operational decision-support capabilities of BESS (Lo Franco et al., 2021). By integrating diverse data sources—including real-time sensor data, historical operational records, and expert insights—the DT-supported system dynamically assesses the health state of BESS components and offers actionable maintenance strategies (Rathore et al., 2021). The RUL-based optimisation addresses the limitations of conventional maintenance strategies while extending the lifespan of BESS components, reducing operational costs, and improving system reliability (Wang et al., 2009).

At the same time, the LLM-based fault analysis framework applies advanced natural language processing techniques to interpret and analyse complex maintenance records and operational manuals (Zheng et al., 2024). Specifically, through domain-specific fine-tuning of the LLM for energy storage systems, the framework extracts valuable insights that traditional analytical methods cannot easily obtain. Integrating LLM-based insights with real-time monitoring and prognostic capabilities, the system offers comprehensive decision support that includes data-driven predictions and context-aware recommendations.

These methodologies collectively establish a robust framework to enhance the operational decision-support capabilities of BESS. By integrating diverse data sources—including real-time sensor data, historical operational records, and expert insights—the DT-supported system dynamically assesses the health state of BESS components and offers actionable maintenance strategies. The integration of RUL-based optimisation and LLM-based fault analysis addresses the limitations of conventional maintenance strategies while extending the lifespan of BESS components, reducing operational costs, and improving system reliability.

The remainder of this chapter is organised as follows: Section 6.2 outlines the methodology for the DT-supported operational decision support approach. Section 6.3 describes the experimental setup used to validate the proposed approach, while Section 6.4 presents the results and their implications, followed by a summary and future research directions in Section 6.5.

6.2 Technical Method

This section outlines the methodological framework for developing the DT-supported operational decision support system for BESS. The approach is built on two key strategies: (1) optimised maintenance strategy based on RUL prediction and battery availability, and (2) LLM-based fault diagnosis and operational decision support. These strategies are integrated within the DT-supported system to enable real-time monitoring, RUL prediction and advanced fault diagnosis.

The first method utilises real-time operational data and equipment availability metrics to optimise maintenance scheduling, thereby minimising maintenance costs and reducing system downtime. Concurrently, the LLM-based method applies natural language processing techniques to analyse unstructured textual data, such as maintenance logs and technical manuals, providing context-aware insights that support maintenance planning and decision-making. Together, these approaches form a robust foundation for enhancing the operational performance and reliability of BESS.

The subsequent sections describe each methodological component in detail. Section 6.2.1 covers data acquisition and preprocessing, followed by Section 6.2.2, which discusses the DT model for fault diagnosis and prognostics. Section 6.2.3 details the predictive maintenance strategy based on RUL estimation, and Section 6.2.4 introduces the LLM-based decision support model for maintenance optimisation.

6.2.1 Data Acquisition and Pre-processing

The reliable performance of the DT-supported operational decision support system hinges upon effective data gathering and preliminary processing. The dataset consists of real-time sensor data capturing key parameters such as voltage, current and temperature. These measurements offer detailed insights into the operational conditions and performance of BESS components. The data obtained from monitoring systems is used not only to assess the current health status of the physical asset but also to predict the RUL. By analysing RUL predictions and battery availability, the DT determines optimal maintenance scheduling and the necessity of ordering spare parts at specific monitoring points. This proactive approach minimises unexpected failures and reduces downtime by enabling the timely availability of replacement parts.

Additionally, historical maintenance records and failure logs are incorporated to enhance the dataset, enabling accurate prognostics and fault analysis. Unstructured textual data, including technical manuals and maintenance reports, are processed using natural language processing techniques to extract relevant contextual information for the LLM-based fault diagnosis model. This holistic integration of structured and unstructured data supports comprehensive decision-making for maintenance and spare parts management.

The data pre-processing includes several steps. First, data cleaning is performed to eliminate errors and address missing values that could compromise model performance. This involves detecting and removing outliers, imputing missing values through statistical methods, and normalising sensor readings to a standard scale. Next, data transformation techniques such as feature engineering and dimensionality reduction are applied to improve data quality and relevance. These transformations involve extracting essential features from sensor readings, aggregating historical maintenance information, and reducing noise in textual data through tokenisation and removal of irrelevant terms.

For unstructured textual data, a specialised preprocessing pipeline is implemented. This pipeline includes text cleaning, tokenisation, and vectorisation to convert unstructured text into structured numerical representations suitable for input into the LLM-based model. The resulting textual features are integrated with structured sensor data, creating a unified dataset that supports both RUL and battery availability-based predictive maintenance and LLM-based fault diagnosis.

By combining multiple data sources and employing rigorous preprocessing techniques, the resulting dataset is optimised for real-time health state estimation, RUL prediction, and spare parts management. This comprehensive approach enables the DT-supported system to capture the dynamic behaviour of BESS components accurately, thereby effective decision support and maintenance strategy optimisation.

6.2.2 Integration of Digital Twin to Decision Support System

The integration of DT into decision support systems enhances the ability of BESS to monitor, diagnose, and predict the health status of its components. By leveraging real-time operational data and historical maintenance records, the DT framework enables precise fault diagnosis and facilitates informed decision-making. This integration supports a comprehensive approach to maintenance optimisation and system reliability.

In this section, the DT serves as a pivotal element that bridges fault diagnosis and decision support. Through continuous monitoring, the DT identifies anomalies and deviations from normal operating conditions, assesses the severity of emerging faults, and provides a dynamic health state estimation of BESS components. This real-time fault analysis enables the decision support system to proactively determine the necessity for maintenance actions, reducing the risk of unexpected failures.

The insights generated through DT-supported fault diagnosis feed directly into the decision-support framework. This fusion guarantees that maintenance choices like best scheduling and part management rely on a precise and thorough grasp of the system's existing and future health. Consequently, the DT’s role in fault diagnosis is not isolated but is an integral part of the broader decision-making process, guiding maintenance strategies that enhance system availability and minimise operational costs.

By establishing a seamless link between predictive maintenance strategy and decision support, the DT allows for dynamic adaptation to changing operational conditions. This capability is essential for the effective implementation of advanced maintenance strategies, including RUL and battery availability-based optimisation and context-aware fault diagnosis using LLM.

6.2.3 RUL and Availability-based Decision Support

Maintenance strategies based solely on RUL predictions are often influenced by the accuracy of the estimation models, which may lead to discrepancies between the predicted and actual service life. Such inaccuracies can result in increased maintenance costs and reduced system reliability.

In contrast, operational availability offers a more comprehensive measure of the battery's ability to perform its intended functions. Availability reflects the proportion of time the battery is operational, considering factors such as downtime due to maintenance or failures. By integrating RUL and availability, maintenance decisions can be made based on both the component's health status and the system's overall operational readiness.

This section presents a predictive maintenance strategy that optimises maintenance decisions by considering both RUL and availability. The proposed method establishes a unified model that combines these two indicators to evaluate maintenance needs, prioritising actions that minimise maintenance costs and maximise battery life.

A combined maintenance index is calculated using RUL predictions and availability metrics to assess the urgency and timing of maintenance activities. Maintenance is prioritised for batteries with lower index values, indicating a higher likelihood of imminent failure and a greater impact on system performance. This prioritisation allows maintenance to be performed at the most appropriate time, reducing unplanned downtime and preventing unnecessary replacements.

Furthermore, the strategy incorporates a proactive spare parts ordering policy based on RUL predictions. Predicting when each part might fail allows ordering spare parts ahead of time to guarantee they are ready when required. This forward-thinking method decreases interruptions caused by insufficient stock and improves the way inventory is managed while lowering total operational expenses.

Integrating RUL predictions and availability provides a method for measuring battery performance and optimising maintenance strategies. This approach supports rational and data-driven decision-making, enhancing the reliability and efficiency of BESS.

6.2.4 LLM-based Fault Analysis

The integration of LLMs into fault analysis and maintenance decision-making frameworks offers a powerful tool for enhancing the operational decision-support capabilities of energy storage systems. As an approach to processing and understanding complex data, LLMs provide advanced natural language processing (NLP) techniques that enable the extraction of valuable insights from vast amounts of textual information, such as maintenance records, operation manuals, and historical reports. This capability is particularly beneficial when combined with DT technology, which provides a dynamic digital representation of physical systems, allowing for real-time monitoring, simulation, and predictive analytics. This section introduces an LLM-based decision support system that integrates with DT, providing a structured approach to maintenance optimisation for energy storage systems.

The integration of LLMs with DT frameworks involves leveraging the language model's capacity to process and interpret domain-specific knowledge, thereby enhancing the DT's ability to support decision-making processes. In the context of energy storage systems, LLMs are used to analyse maintenance logs and operational documents, identifying patterns and correlations that may not be evident through conventional analytical methods. The LLM-based decision support system begins with the preprocessing of textual data, which includes cleaning, formatting, and augmenting the data to create a high-quality dataset for model training. This dataset serves as the foundation for fine-tuning the LLM, enabling it to specialise in understanding and generating maintenance-related insights.

The fine-tuning process adapts the LLM to the specific domain of energy storage systems, where it learns to associate fault patterns with potential failure modes and recommended maintenance actions. This domain adaptation is achieved through transfer learning techniques, such as LoRA (Low-Rank Adaptation), which modify the base model's weights to capture the nuances of energy storage system operations. As a result, the fine-tuned LLM becomes proficient in providing contextually relevant recommendations, such as suggesting maintenance schedules based on detected fault trends or proposing corrective actions based on historical failure data.

Once integrated into the DT framework, the LLM-based decision support system functions as an intelligent assistant that complements the DT's real-time monitoring and predictive maintenance capabilities. While the DT provides a real-time overview of the system's operational state and health status, the LLM enhances this capability by offering in-depth analysis and interpretation of historical and contextual data. For example, when an anomaly is detected in the DT, the LLM can be queried to provide possible causes based on similar historical events, suggest preventive measures, or recommend spare parts provisioning strategies. This synergy between LLM and DT technologies enables a more comprehensive approach to maintenance decision-making, combining data-driven insights with contextual knowledge for optimised maintenance outcomes.

The integration of LLMs into DT-supported maintenance optimisation frameworks offers several distinct advantages. First, it reduces the dependency on human expertise for interpreting complex maintenance documentation and historical records. By automating the extraction and analysis of knowledge from these sources, the LLM-based system can identify relevant information more efficiently and consistently than manual methods. Second, the ability of LLMs to understand and generate natural language allows for intuitive interaction between the system and operators. This capability facilitates seamless communication, enabling operators to query the LLM for explanations, recommendations, or clarifications in a conversational manner. Third, the integration of LLMs enhances the DT's ability to simulate and predict maintenance scenarios, supporting proactive maintenance planning and reducing downtime.

Furthermore, the LLM-based decision support system contributes to the overall operational efficiency and reliability of energy storage systems by enabling predictive maintenance strategies that are closely aligned with the system's real-time and historical data. The combination of LLM and DT technologies provides a holistic view of the system's condition, incorporating both real-time sensor data and contextual knowledge derived from textual sources. This approach improves the accuracy and relevance of maintenance recommendations, ultimately leading to more effective resource utilisation and extended equipment lifespan.

In summary, the integration of LLM-based decision support with DT frameworks creates a synergistic relationship that enhances the capabilities of both technologies. By leveraging the advanced NLP capabilities of LLMs to interpret and analyse domain-specific knowledge, the DT's monitoring and predictive maintenance functions are significantly augmented. This integration offers a comprehensive solution for optimising maintenance strategies, reducing operational costs, and improving the overall reliability and sustainability of energy storage systems. The methodologies presented in this section demonstrate the potential of combining LLMs and DTs to create an intelligent and adaptive decision support system, paving the way for more efficient and resilient energy storage operations.

6.3 Experimental Setup

This section outlines the experimental setup used to evaluate the effectiveness of the proposed DT-supported decision support system for BESS. The experiments focus on assessing the performance of predictive maintenance strategies based on RUL predictions and battery availability, as well as the integration of LLM-based fault diagnosis and decision support.

Real-world operational data and domain-specific textual information are used to validate the system's capability to enhance fault diagnosis, optimise maintenance decisions, and improve overall system performance. The following subsections detail the data sources, experimental procedures, and evaluation metrics used to analyse the proposed methodologies.

6.3.1 Data Integration and Digital Twin Configuration

Effective integration of diverse data sources is essential for configuring the DT to accurately represent the health status and dynamic behaviour of BESS. This integration combines real-time sensor measurements, historical maintenance logs, and technical documentation into a unified dataset that offers a holistic view of system performance and operational conditions.

Real-time sensor data, including voltage, current and temperature enables continuous monitoring of the battery's operating state. Historical maintenance records supplement this data by capturing long-term degradation trends and failure patterns of individual components. Moreover, unstructured textual data from maintenance reports and technical manuals are processed using natural language processing techniques to extract valuable insights, further enriching the structured dataset.

After merging the data sets they receive preprocessing actions like normalisation and feature engineering to guarantee fit with the DT's analysis tools. Sensor information undergoes normalisation to correct discrepancies and align measurement metrics; at the same time, critical attributes are pulled out to accentuate the influencing factors on system health. By tokenising and vectorising textual data we create numerical forms that can be analysed. The DT receives superior input from these preprocessing actions that allow for exact fault detection and the estimation of RUL.

The final configuration of the DT involves defining relationships between physical components and their digital replica and setting parameters for real-time monitoring and state estimation. Leveraging this configuration, the DT continuously assesses the health status of the battery system, detects anomalies, and generates actionable insights to support predictive maintenance and decision.

6.3.2 Predictive Maintenance Strategy Optimisation Based on RUL and Availability

Using health state information obtained from monitoring, the RUL is predicted, and it is determined whether spare parts should be ordered at the current monitoring point. At this point, an average repair or preventive maintenance time q, is introduced, representing the upper limit of the difference between the RUL and the lead time. If, at monitoring time t_k, the difference between the equipment's remaining life t_k and the L satisfies the condition $RUL_k - L \leq q$then spare parts are ordered, with the order point recorded as $t_0 - t$and the spare parts will arrive after the lead time L. Otherwise, no order is placed until the decision is reassessed at the next monitoring point.

If, a time t, the equipment's health state is monitored and its RUL is predicted as , and the average repair or preventive maintenance time is q_1, then if the condition $RUL_k - L \leq q_1$ holds, the spare parts are ordered at time t_k , and they will arrive at the inventory after the lead time L. If the spare parts have arrived before the lead time, i.e., they have entered storage at time t_{k+3}, and the average repair or preventive maintenance time is q_2, then if $RUL_k - L < q_2$, no order is placed at time t_k.

In this joint strategy, the average repair or preventive maintenance time q reflects the relationship between the remaining useful life and the lead time. When the RUL is longer than the lead time, no order is placed. Conversely, if the RUL is shorter than the lead time, spare parts are ordered. The value of the average repair or preventive maintenance time q is determined through the joint strategy model and serves as a decision variable.

1) **Energy Storage Equipment Availability**

In practical use, the steady-state availability can be divided into inherent availability A_i, achieved availability A_a, and operational availability A_0. At the equipment usage stage, operational availability is the most effective indicator of actual equipment utilisation and maintenance support conditions (Ahmad and Kamaruddin, 2012). It represents the proportion of time the equipment or system is capable of performing its intended function, indicating the relationship between reliability and maintainability.

The size of operational availability is primarily influenced by three factors: Mean Time Between Maintenance (MTBM), Mean Corrective Maintenance Time (MCMT), and Mean Logistic Delay Time (MLDT). The magnitude of MLDT is determined by the system's support capability. Spare parts supply capability is critical for supportability, as it significantly impacts the frequency of maintenance cycles and overall system operational availability.

In spare parts management, operational availability is calculated as shown in Equation 6.1:

$$A_0 = \frac{MTBM}{MTBM+MCMT+MPMT+MSD} \tag{6.1}$$

Spare parts availability:

$$A_a = \frac{MTBM}{MTBM+MCMT+MPMT} \tag{6.2}$$

Supply availability:

$$A_s = \frac{MTBM}{MTBM+MSD} \tag{6.3}$$

Therefore, the operational availability can be derived as:

$$A_0 = \frac{1}{1/A_a + 1/A_s} \tag{6.4}$$

This model calculates availability by dividing it into two parts: achievable availability and spare parts supply availability. Compared with the updated Markov renewal theory for calculating system availability, this method simplifies the calculation by making certain assumptions. However, when there is a constraint on spare parts supply, the model has limitations. Thus, many studies on inventory issues have been conducted to expand the model's applicability (Ahmad and Kamaruddin, 2012).

The method proposed in this text optimises the spare parts supply strategy by integrating operational availability with spare parts availability. The optimisation equation is given as:

$$A = \frac{T}{T+q} \tag{6.5}$$

Where T refers to the mean maintenance time interval and q average repair or preventive maintenance time, including corrective or preventive maintenance intervals.

The RUL of the equipment is RUL_k and the spare parts lead time is L, where q satisfies: $RUL_k = L + q$, thereby combining availability with the spare parts supply process to achieve joint strategy optimisation.

2) Joint Maintenance Strategy Optimisation Modelling

Each time, the cost C_i is used to monitor the system status. If $l_p \leq RUL(t_k) \leq L_c$, the cost C_R will initiate preventive maintenance; otherwise, if $RUL(t_k) \geq L_c$, the cost C_R will initiate corrective maintenance, which will result in losses C_F. The system availability and spare parts supply are comprehensively analysed to establish a joint strategy considering six potential updating events which is shown in Table 6.1. Among them, if a more critical system fault occurs, the spare parts are ordered immediately, leading to urgent replacement (E1 and E4). When the availability is q_1, spare parts are ordered at time t_k and the system may be maintained at time t_k, t_{k+2}, while the spare parts have not arrived and one has to wait for the spare parts to arrive for replacement (E2 and E5). Typically, the cost of placing an emergency order, C_{eo}, is higher than the cost of placing a normal order, C_0. If the ordered spare part does not arrive, it incurs a shortage cost; if the spare part arrives and is not immediately replaced, it goes into storage and incurs a holding cost; where the shortage cost per unit of time is C_s; and the holding cost per unit of time is C_h.

Table 6.1 All possible renewal scenarios of the joint policy modelling

Events	Status	Spare parts status	Decision
E1	$l_p \leq RUL(t_k) \leq l_c$ Preventive Maintenance	Not Ordered	Urgent order and immediate maintenance
E2		Ordered but not arrived	Wait for spare parts to arrive for maintenance
E3		Arrived	Immediate maintenance
E4	$RUL(t_k) \geq l_c$ Fault maintenance	Not Ordered	Urgent order and immediate maintenance
E5		Ordered but not arrived	Wait for spare parts to arrive for maintenance
E6		Arrived	Immediate maintenance

Based on the expected cost and length of each update event, the update payoff theory is used to establish the objective function of minimising the expected cost per unit of time, and the optimal decision variables are obtained: the ordering threshold q^* and the preventive maintenance threshold L_p^*. The specific formulas are as follows:

$$\min E\left(C\left(L_p, q\right)\right) = \frac{\sum_{s=1}^{6} E\left(C_s\left(L_p, q\right)\right)}{\sum_{s=1}^{6} E\left(L_s\left(L_p, q\right)\right)}$$

$$s.t. \quad l_k - L \leq q;\ L_p < L_c \tag{6.6}$$

where $E(C_i(L_p, q))$ and $E(L_i(L_p, q))$ correspond to the expected cost and expected length.

The steps of the experiment are as follows:

Step 1: Set initial cost parameters $C_i, C_o, C_{eo}, C_R, C_F, C_s, C_h$ and maximum number of calculations $N_{max}, L_p = 0, A = \frac{T}{T+q}, q = \frac{T}{A} - T$.

Step 2: Setting preventive maintenance thresholds $L_p = L_p + 1, q = 0$.

Step 3: Average repair/preventive maintenance time $q = q + 1$.

Step 4: Total expected cost $TC = 0$; total expected duration $TL = 0$ and number of runs $i = 0$.

Step 5: With L_p and A fixed, the number of runs $i = i + 1$.

Step 6: Updated the $RUL(t)$ of the system every T period, at time t, if $l_k - L \leq q$, then if $t_0 \geq 0$, if it has been ordered, if not, order spare parts, otherwise go to step 7.

Step 7: If the RUL at time t, if $RUL(t) \leq L_p$, then return to step 5. If $L_p \leq RUL(t) \leq L_c$, then perform preventive maintenance; and make the following decisions: when $t_0 = 0$, spare parts have not been ordered, E1 occurs; when $t_0 \leq t \leq t_0 + L$, spare parts have been ordered but not arrived, E2 occurs; when $t_0 + L \leq t$, spare parts have arrived, E3 occurs. If $RUL(t) \geq L_c$, then perform fault maintenance, similarly, according to the various states of spare parts, E4, 5, and 6 may occur.

Step 8: If the number of operations under the current q, L_p has reached the maximum number $i = N_{max}$, if satisfied, calculate and record $C(A, l_p)$, otherwise return to step 5.

Step 9: If $C(A, L_p) > C(A-1, L_p)$ is satisfied, find the minimum objective function value and availability under fixed L_p, record it as $C(A^*, L_p)$, and return to step 2; otherwise, return to step 3.

Step 10: If $C(A^*, L_p) > C(A^*, L_p - 1)$ is satisfied, it means find the minimum objective function value, $minC(A^*, {L_p}^*)$,, the optimal preventive replacement threshold ${L_p}^*$ and availability A^*; otherwise, return to step 2.

3) Experimental Results

To verify the model, the previously calculated RUL is used for the case study. The RUL is updated every T charge and discharge cycle, the fault threshold $L_c = 0$, and the cost parameters are shown in Table 6.2.

Table 6.2 Cost parameters

C_i	C_o	C_{eo}	C_R	C_F	C_s	C_h
500	100	4000	12000	50000	25	5

Based on the above parameters, Python is used to program the discrete event simulation algorithm, and the minimum objective function value is $EC(A^*, {L_p}^*) = 5.35$, where the optimal availability $A^* = 0.11$ and the preventive maintenance threshold ${L_p}^* = 16$. Figure 6.1 shows the trend of the expected cost per unit time with the ordering threshold and the availability under different periods T. When L_p is fixed, the expected cost per unit time shows a trend of first decreasing and then increasing with the increase of A. Because if A is too small, ordering spare parts will easily lead to no spare parts available when the system fails, increasing downtime losses and costs; but a larger A will increase the holding cost of spare parts. Similarly, when A is fixed, the expected cost per unit time first decreases and then increases with the increase of

L_p. This is because an excessively large L_p increases the possibility of preventive replacement and reduces the expected length, resulting in a higher expected cost per unit time; a small L_p is prone to failures, and failure to prevent them increases the expected cost per unit time.

Table 6.3 The influence of the order lead time L on the optimal decisions

L	A^*	L_p^*	$EC(A^*, L_p{}^*)$
100	0.14	15	6.03
300	0.16	10	6.28
500	0.19	10	6.49
1000	0.17	9	7.14

Figure 6.2 shows the impact of order lead time on the optimal decision, and Table 6.3 shows that the expected cost per unit time $EC(A^*, L_p{}^*)$ gradually increases with the increase of L. The reason is the system degradation process does not change. As L increases, it is necessary to start ordering when the remaining life is longer, that is, A^* gradually increases; and once the system needs preventive replacement or fault replacement if the spare parts have been ordered but have not arrived, the out-of-stock loss caused by the long wait for spare parts will increase, which increases the expected cost per unit time, so $L_p$decreases, making the preventive maintenance time closer to the arrival point.

A joint maintenance and spare parts ordering strategy based on RUL is proposed for single-component systems. The maintenance strategy adopts a control limit strategy to determine the system degradation at each monitoring point to determine whether to perform preventive replacement or fault maintenance; at the same time, the predicted RUL is used to compare the difference between the remaining service life and the lead time of the monitoring point with the size of the availability to determine whether to order spare parts, thereby integrating the spare parts ordering strategy with the real-time health status of the system. A model for minimising the expected cost per unit time is constructed, and a discrete event simulation algorithm is designed to optimise the preventive replacement threshold and the availability threshold. The optimal solution is given through case analysis, and the influence of the monitoring cycle and the ordering lead time on the optimal decision is analysed.

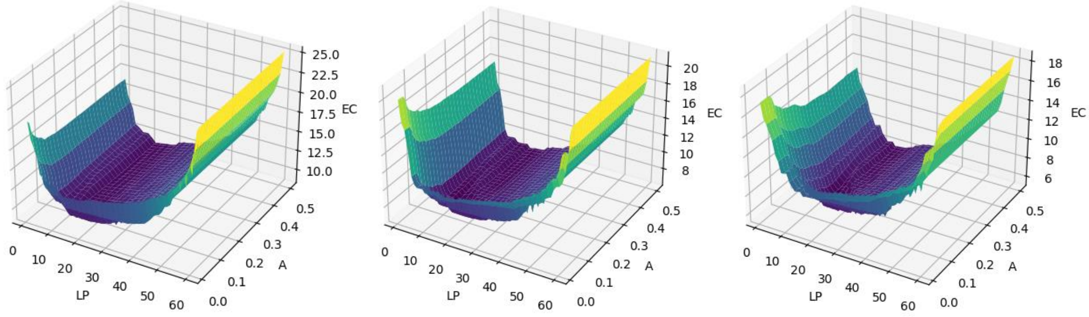


Figure 6. 1 The expected cost per unit time in terms of the preventive maintenance threshold L_p and the availability A with different period T (T=100, 200, 300)

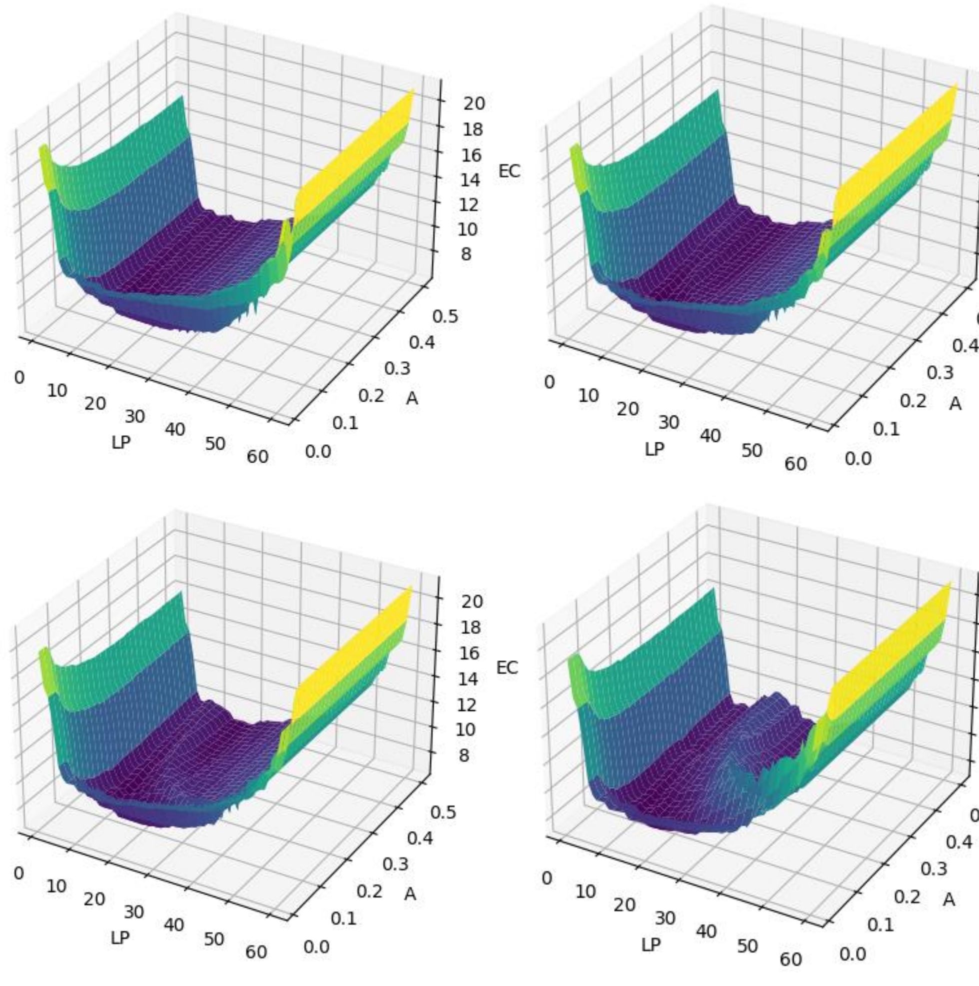


Figure 6. 2 The expected cost per unit time with different leading time L (=100, 300, 500 and 1000)

6.3.3 LLM-based Fault Analysis and Operational Decision Support

With the application of cloud computing, big data analysis, the Internet of Things, digital twins and other technologies in industrial production processes, data is being generated at an unprecedented rate. Artificial intelligence technologies represented by LLM can mine and analyse data such as industrial documents, maintenance records, and standard manuals with their zero-sample learning and generalised answer capabilities and provide insights for fault analysis and maintenance decisions based on previous cases (Naqvi et al., 2024). The LLM large model fine-tuning process for energy storage system fault analysis and maintenance decision-making is shown in Figure 6.3. Its main process can be divided into four steps, including data preprocessing, model fine-tuning, evaluation and testing, and deployment and use.

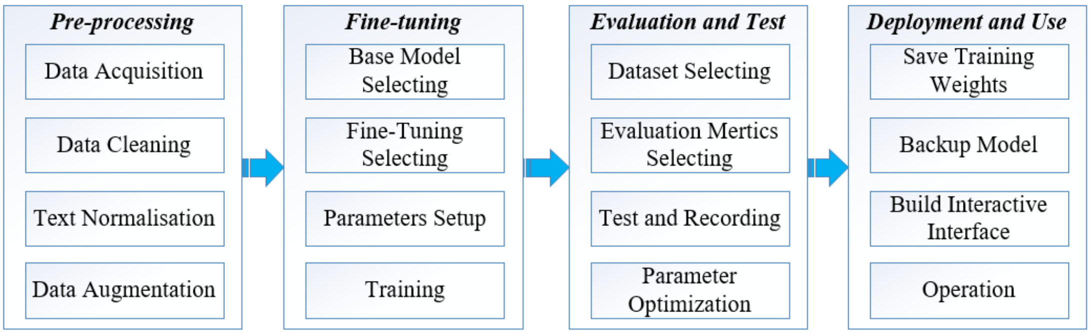


Figure 6. 3 LLM model construction process

The conducted experiment serves as an initial demonstration of the LLM-based Q&A system integrated within a DT environment, designed to validate its practical feasibility and operational utility rather than provide exhaustive validation. The system demonstrates its capacity to enhance battery management by delivering rapid, context-aware responses to maintenance inquiries, significantly reducing diagnostic time and enabling efficient decision-making under dynamic operational conditions. By leveraging intuitive, dialogue-based interactions, the system improves accessibility for non-expert operators, allowing them to address technical issues with minimal training while maintaining operational flexibility. Furthermore, the LLM-based Q&A system facilitates predictive maintenance by identifying anomalies and generating targeted recommendations, thereby supporting preventive actions to extend battery lifespan and improve system reliability. The system's knowledge integration capability is demonstrated through its ability to synthesize diverse data sources including historical maintenance records and technical standards, to deliver timely and contextually relevant guidance. Collectively, these results underscore the LLM-based Q&A system's potential to complement DT-driven BESS management by bridging data analytics with actionable insights, ultimately contributing to enhanced operational efficiency and reliability in renewable energy systems.

1) Data Preprocessing and Fine-tuning

Data preprocessing refers to the process that takes place before LLM fine-tuning, where original data is acquired from application scenarios and then processed through a series of steps to improve model training efficiency. These steps typically include data collection, data cleaning, text formatting, and data augmentation. Data collection involves extracting relevant information from various industrial documents related to fault diagnosis and operational decision-making. Once the data is collected, it undergoes a data cleaning procedure, which focuses on removing noise and irrelevant information, such as extra spaces, special characters, and HTML tags, to ensure data quality and consistency. The cleaned data is then subjected to text formatting, where the structure and representation of the data are standardised according to the requirements of the LLM training framework, requiring that all data is uniformly represented. After the data has been cleaned and formatted, it may be necessary to perform data augmentation, particularly when the existing data is insufficient for certain training scenarios. Data augmentation techniques include synonym replacement, linguistic transformations, and the use of generative language models to produce additional data that maintains contextual relevance and diversity. These augmentation strategies not only expand the dataset but also improve the generalisation capability of the model by increasing the volume and variability of the training data.

Fine-tuning is further training based on a conventional base model through vertical domain datasets to enable its ability to accomplish specific tasks in specific environments and scenarios. The process of model fine-tuning can be roughly divided into several stages, such as selecting a base model, choosing a fine-tuning method, setting the fine-tuning parameters, and starting the fine-tuning training. Due to the huge number of parameters of large models, cutting-edge researchers have designed a variety of fine-tuning methods for large models, and the mainstream supervised fine-tuning methods mainly include but are not limited to, Adapter Tuning, Prefix-Tuning, Prompt Tuning, LoRA and so on. Among them, the Adapter Tuning method mainly refers to a fine-tuning method that introduces an adapter based on the original model framework without changing the overall structure of the original model and realises the training under specific tasks by adjusting the adapter parameters. The Prefix-Tuning fine-tuning method is a kind of fine-tuning method by adding a prefix layer in the input layer of the model, and in the Attention mechanism computation, the prefix layer is involved in the computation together with the original input to realise the fine-tuning method. The advantage is that the model can be adapted to a specific task quickly and with less computational resources. Prompt Tuning is a type of command fine-tuning approach, which is centred on providing the model with given commands or prompts to improve the efficiency of the model's answer to a question and is characterised by the fact that there is no need to fine-tune the model structurally. LORA fine-tuning is a type of fine-tuning approach that freezes some of the weights of the base model and adds trainable low-rank matrices to the structure of the model. The fine-tuning training method with a low-rank matrix is characterised by efficiently tuning the neural network layer of the model to achieve parameter optimisation through a flexible low-rank matrix. The LoRA low-rank parameter update matrix is shown in Equation 6.7, A and B are trainable matrices, W_0 is the pre-trained weight matrix, ΔW represents the parameter update during fine-tuning, x is the word embedding vector input, and h is the output.

$$h = W_0 x + \Delta W x = W_0 x + BAx \tag{6.7}$$

Setting up the fine-tuning model mainly refers to setting up the relevant parameters of fine-tuning in the process of fine-tuning, such as the learning rate, iteration number, maximum gradient paradigm, maximum number of samples, and truncation length. After completing the previous steps, fine-tuning training can be carried out for the fault analysis and maintenance decision-making model of the energy storage system.

2) Evaluation Metrics

The evaluation and testing of the model is carried out in terms of test data set selection, evaluation method selection, testing and recording, and feedback and optimisation. First of all, the fine-tuned model needs to provide a test dataset including questions and answers, and the model will answer the questions and compare the answers with the standard answers to measure the model's capability, for example, to ask about the cause of a component failure and how to deal with it to check whether the model's answer is in line with the standard answer given in the technical manual. According to the application scenarios of the model, the common evaluation indexes of the model capability mainly include BLEU-4, ROUGE-1 and ROUGE-2, etc. BLEU-4 is an index based on n-gram to measure the quality of machine translation, and the formula for BLEU algorithm accuracy is shown in Equation 6.8, and the formula of the length penalty factor BP is shown in Equation 6.9, and the BLEU formula is shown in Equation 6.10. ROUGE-1 and ROUGE-2 focus on the recall of a single word in a single sentence and the recall of two consecutive word groups in a sentence, respectively, and the formula for ROUGE-N is shown in Equation 6.11. The testing and recording phase mainly involves testing the model performance based on the test data set and evaluation metrics and recording the test results. Finally, the model is optimised based on the test results.

$$p_n = \frac{\sum_{C\in(Candidate)} \sum_{n-gram\in C} Count_{clip}(n-gram)}{\sum_{C\in(Candidate)} \sum_{n-gram\prime\in C\prime} Count_{clip}(n-gram\prime)} \tag{6.8}$$

Where the numerator represents the number of matched $n-grams$ and the denominator represents the total number of $n-grams$ in the candidate sentence.

$$BP=\begin{cases}1, if\ c>r\\ \exp\left(1-\frac{r}{c}\right), if\ c\le r\end{cases} \tag{6.9}$$

Where c represents the number of characters in the candidate translation sentence; r represents the number of characters in the reference translation sentence.

$$BLEU=BP\times\exp\left(\sum_{N=1}^{4}w_n\log(p_n)\right) \tag{6.10}$$

where $w_n=1/N$, and when $N=4$, Equation (4) is the expression for BLEU-4.

$$ROUGE-N=\frac{\sum_{S\in(ReferenceSummaries)}\sum_{gram_n\in S}Count_{match}(gram_n)}{\sum_{S\in(ReferenceSummaries)}\sum_{gram_n\in S}Count(gram_n)} \tag{6.11}$$

Where the denominator represents the total number of $n-gram$ in the standard answer and the numerator represents the number of $n-gram$ generated by the model.

3) Deployment and Use

The deployment and use phase is the application phase after the model has been fine-tuned. Existing model training requires a large memory of GPU, so most of the training process needs to be deployed on the cloud platform. Therefore, the deployment and use of the model can be roughly divided into the steps of training weight saving, local backup of the model, interactive interface construction and running use. Training weight preservation refers to the preservation of the parameters of the fine-tuned model. The conventional base model makes it difficult to provide professional advice on failure analysis and maintenance decisions of energy storage systems, but after fine-tuning with domain knowledge and data, it can answer questions on failure analysis and operation and maintenance advice of energy storage systems, so it is necessary to preserve the weights for subsequent reloading and recalling. Model local backup mainly refers to the process of downloading the model from the training platform to local backup after training the model in the cloud service platform. Finally, the interface for interacting with the model in terms of questions and answers needs to be constructed for operational use.

4) Experimental Results

This section presents the experimental results of the LLM-based fault diagnosis and maintenance decision support model for BESS. The experiments were conducted to evaluate the effectiveness and robustness of the proposed methodology, using a dataset constructed from two primary technical resources: the ‘GB/T 40090-2021 national standard’ and the ‘PowerTitan Operation and Maintenance Guide’. These documents contain detailed information regarding the standard operating procedures, fault diagnostics, and maintenance strategies for energy storage systems. The dataset includes information on fault categories, troubleshooting methods, component-level repair instructions, and decision-making strategies for optimal maintenance planning.

Documentation Description			
Serial Number	**Fault Name**	**Common Causes**	**Solutions**
3	Total voltage overvoltage fault	The **RACK** voltage consistently exceeds the set fault threshold.	• Check whether the BSC parameters setting are correct. • Check whether battery cell voltage is abnormal. • Check whether the voltage sampling line is abnormal.

Normalised Data Format


```
[
{
"instruction": "What are the common causes of total voltage overvoltage faults?",
"input": "",
"output": "The RACK voltage consistently exceeds the set fault threshold."
"system": ""
"history": []
},
{
"instruction": "What are the solutions for total voltage overvoltage faults?",
"input": "",
"output": "1. Check whether the BSC parameters setting are correct; 2. Check whether battery cell voltage is abnormal; 3. Check whether the voltage sampling line is abnormal.
"system": ""
"history": []
},
]
```


Figure 6. 4 Text normalisation

After data cleaning, the two technical documents were converted from PDF type format to text format, and the corresponding question-answer(Q&A) dataset was constructed according to the descriptions in the technical documents, and the process of text formatting is shown in Figure 6.4. A total of 585 Q&A pairs were constructed, covering a wide range of fault scenarios, maintenance procedures, and decision-making strategies specific to energy storage systems. The dataset included a diverse set of faults and their corresponding solutions, with a total length of 52,996 characters, allowing both common and rare fault scenarios to be represented.

The LLM used in this study was the Qwen1.5-14B-Chat model, a large-scale language model known for its capability to handle complex language tasks and domain-specific knowledge. The fine-tuning process was carried out on the Llama factory platform, leveraging GPU acceleration to expedite the process. The model has 14B parameters, and the specific basic requirements of the training environment are shown in Table 6.4.

Table 6 4 Basic requirements of dependency

Dependency	**Require**
python	3.11
torch	2.4.0
transformers	4.43.4
datasets	2.20.0
accelerate	0.32.0
peft	0.12.0
trl	0.9.6
CUDA	12.2
deepspeed	0.14.0
bitsandbytes	0.43.1
vllm	0.5.0
flash-attn	2.6.3

After completing the construction of the basic training environment, enter the llama-factory platform. The platform interface layout is shown in Figure 6.5. Select the constructed dataset and complete the setting of the corresponding parameters to start fine-tuning training. The specific fine-tuning algorithm used is the LoRA algorithm, and the specific fine-tuning parameters are shown in Table 6.5.

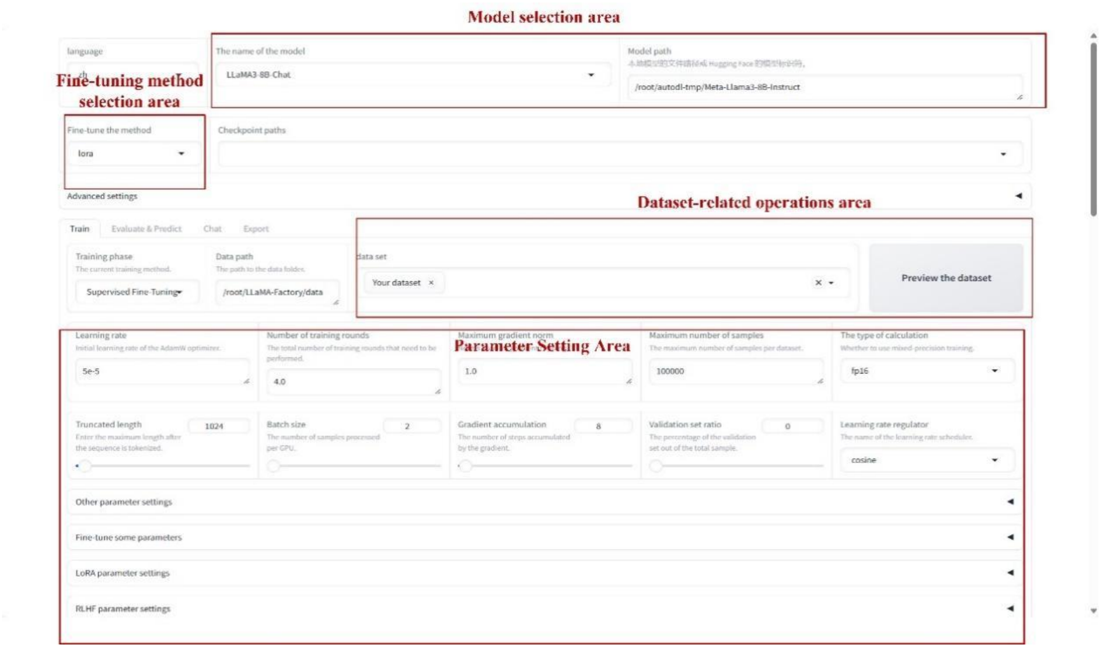


Figure 6. 5 Llama-factory platform interface

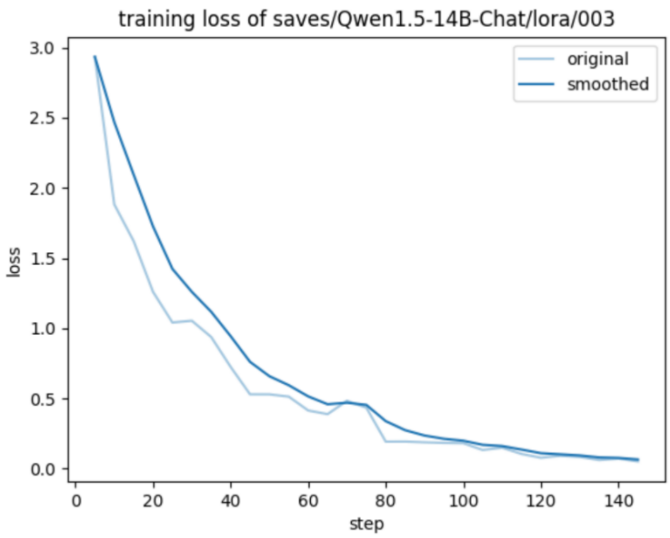


Figure 6. 6 Loss function of the LLM

Table 6.5 Fine-tuning parameters setup

Parameter	Value
stage	ft
model_name_or_path	/root/autodl-tmp/Qwen1.5-14B-Chat
preprocessing_num_workers	16
finetuning_type	LoRA
learning_rate	5e-5
num_train_epochs	4
template	Qwen
flash_attn	auto
dataset_dir	/root/LaMA-Factory/data
cutoff_len	1024
max_samples	100000
per_device_eval_batch_size	2
gradient_accumulation_steps	8
lr_scheduler_type	cosine
LoRA_rank	8
LoRA _alpha	16
LoRA_dropout	0.1
LoRAplus_lr_ratio	16

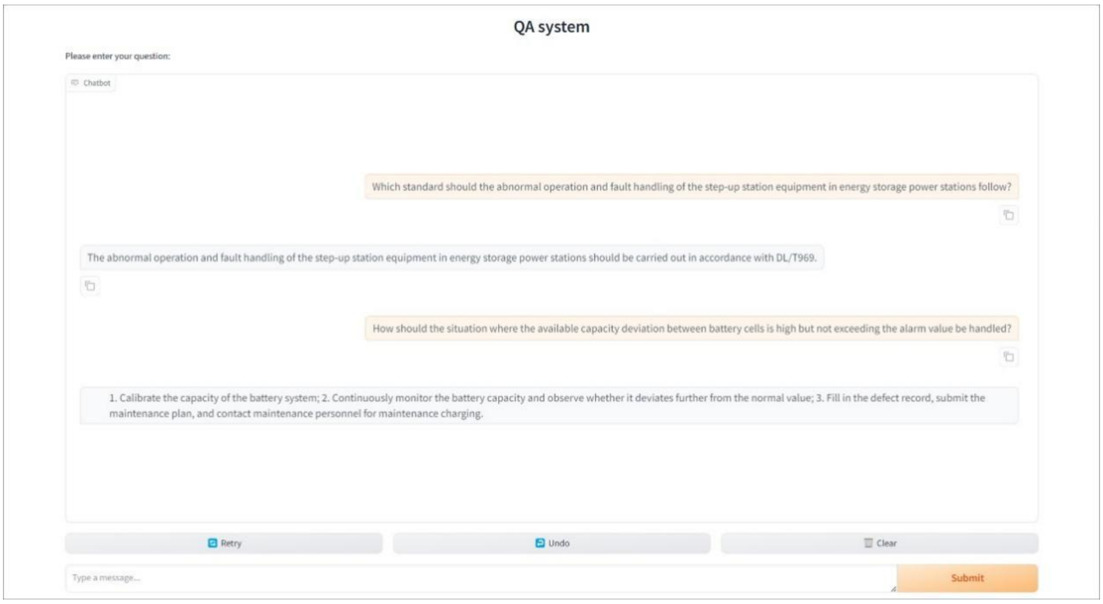


Figure 6.7 Question and answer interactive system based on gradio

Table 6.6 Evaluation scores

BLEU-4	ROUGE-1	ROUGE-2
86.28	88.97	84.57

Finally, the safe tensors format file generated by platform training was saved, and an interactive question-and-answer interface was built based on gradio [15]. The model was tested in this interactive interface. The specific interface is shown in Figure 6.7 The results show that after fine-tuning the knowledge data related to energy storage system fault diagnosis and maintenance recommendations, the model can quickly provide fault analysis causes, and standardised maintenance strategies based on the questions. Compared with the standard answers, it is found that the answers of the model are correct and can provide reasonable guidance for the maintenance of energy storage systems during use.

Table 6.7 Examples of the specific questions of the cold rolling process for user inquiries

Inquiries	Descriptions
Q1	How should operators urgently handle serious faults in the energy storage system, such as smoking or fire?
Q2	What standards should be met before an energy storage power station is put into operation through grid connection debugging and acceptance?
Q3	What operational modes can an energy storage power station be divided into?
Q4	What are the operating conditions of the energy storage system in an energy storage power station?
Q5	How should faults occurring during shift change be handled?
Q6	What reporting and cooperation work should operators do after handling equipment failures?
Q7	What are the requirements for the inspection items of the battery room or battery compartment?
Q8	What are the methods to handle the situation where the communication of the energy storage converter is abnormal and the remote measurement and remote signalling data are not refreshed in time?
Q9	How should the situation where the available capacity deviation between battery cells is high but not exceeding the alarm value be handled?
Q10	What are the methods to handle the undervoltage and overvoltage alarms of the battery cells?

6.4 Discussion

The experimental results presented in the previous sections demonstrate the effectiveness of integrating predictive maintenance strategies and LLM-based fault diagnosis into BESS. This discussion synthesises the findings from both experiments, highlighting their significance, potential applications, and implications for future research and industrial implementation.

The first experiment focused on optimising predictive maintenance strategies based on the integration of RUL prediction and battery availability. The findings illustrate that incorporating both RUL and availability information significantly improves maintenance decision-making, leading to a more efficient allocation of resources and reduction of unnecessary maintenance actions. By using RUL as a primary indicator, the model could identify the optimal timing for preventive maintenance, thus avoiding premature replacement and excessive downtime. Additionally, considering battery availability allowed the strategy to account for external factors such as component supply and system availability, which are critical in practical scenarios. This integrated approach outperformed traditional maintenance strategies, as evidenced by the reduced overall maintenance costs and improved system uptime achieved during the experimental evaluation.

The second experiment, which employed an LLM-based model for fault diagnosis and operational decision support, further validates the feasibility and advantages of integrating advanced AI technologies into BESS maintenance frameworks. The LLM model demonstrated high accuracy in fault identification and decision support, achieving BLEU-4, ROUGE-1, and ROUGE-2 scores that indicate a strong alignment with expert-verified reference answers. The model's ability to interpret complex queries and generate context-aware responses shows its potential to assist maintenance personnel in diagnosing faults and making informed decisions in real-time. Furthermore, the qualitative analysis revealed that the LLM could understand nuanced language and provide detailed recommendations that extend beyond predefined rules, highlighting its potential to serve as a flexible and intelligent support tool in maintenance operations.

When comparing the two experiments, several complementary strengths can be observed. The RUL-based predictive maintenance model excels at optimising the timing and frequency of maintenance activities based on quantitative metrics, thus enhancing operational efficiency and resource utilisation. In contrast, the LLM-based model adds qualitative value by providing detailed fault analysis and decision support, leveraging domain-specific knowledge to handle unstructured data and complex scenarios. Together, these approaches provide a holistic maintenance framework that combines data-driven optimisation with AI-based interpretability and support.

The integration of these two models within a DT framework creates a synergistic effect, where the strengths of both approaches are leveraged to enhance the overall reliability and efficiency of BESS operations. The RUL-based model can inform the LLM model about potential failure modes and maintenance schedules, while the LLM model can provide context-aware recommendations and insights that complement the quantitative predictions. This dynamic interaction enables the system to adapt to changing conditions, continuously improve maintenance strategies, and provide real-time decision support that aligns with operational needs.

6.5 Summary

In summary, this chapter explores the integration of advanced data-driven approaches into DT to enhance maintenance decision support for BESS. Experimental results show that combining spare parts ordering strategy combining RUL prediction and availability with LLM-enabled insights can significantly improve maintenance planning, fault detection, and operational decisions. This chapter highlights the complementary strengths of these models and suggests that integrating them into a DT framework can provide a more comprehensive and adaptive approach to BESS management, thereby improving system reliability and reducing maintenance costs.

Chapter 7 Achievements and Conclusions

7.1 Achievements

The thesis systematically presents the achievements of integrating DT technology into BESS through a series of research explorations and implementations. Each segment of the study contributes to different aspects of DT development, deployment, and evaluation, providing a comprehensive understanding of how DT can enhance BESS management. Firstly, the research begins by establishing the fundamental motivations, objectives, and research questions, which provide a solid foundation for the subsequent study. It introduces the necessity of a data-driven, real-time operational environment for BESS management, setting the context for the proposed DT-driven approach. The discussion emphasises the challenges and complexities associated with accurately estimating critical battery parameters such as SOC, SOH, and RUL. The limitations of conventional methods are highlighted, pointing out the need for advanced methodologies that can handle complex battery behaviours under varying conditions. The first chapter of this thesis contains four research questions. Based on the work achieved, the answers to the research questions are obtained. The first chapter of this thesis contains four research questions. Based on the work achieved, the answers to the research questions are obtained.

Secondly, a literature review related to BDT technology is presented, with a focus on its integration into BESS. The review delineates the key components of BESS, the advantages and constraints of BDT, and current research trends in the field. It concludes with a summary of research gaps that the proposed study aims to address, setting a clear direction for the following research. This review serves as a reference point for understanding the role of BDT in enhancing battery management and provides context for the methodologies introduced later.

Following this, an innovative DT-driven framework for BESS is proposed to support real-time monitoring, predictive maintenance, and operational optimisation. The framework integrates multi-source data acquisition, advanced state estimation models, and decision support modules to improve battery management. The use of data-driven techniques combined with the hierarchical structure of the DT enhances the accuracy of state estimation and robustness of fault detection. This framework effectively addresses the nonlinearities and temporal dependencies in battery data, demonstrating its potential for comprehensive battery monitoring and management.

Subsequently, the research explores an advanced methodology for battery state estimation by utilising the hybrid TCN-LSTM model to predict SOC, SOH, and RUL under various operational conditions. Experimental results validate the hybrid model's effectiveness, showing significant improvements over traditional methods in prediction accuracy. Additionally, transfer learning is employed to dynamically update model parameters with real-time data, allowing the DT to adapt to new battery conditions with minimal computational overhead. This dynamic adaptation capability is critical for maintaining reliable performance over extended periods.

Additionally, the research continued to advance the DT framework to include situational awareness and multi-faceted monitoring properties by utilising the Transformer-CNN model to extract complex features from multi-source battery data. When these models are integrated, the DT framework is more sensitive to the behaviour of the BESS. It offers real-time insights into managing energy storage systems' operational complexities. To incorporate a self-evolving mechanism, the framework continuously improves its capabilities by adapting to new data inputs and improving the accuracy of its decision-making over time.

This research introduces an innovative decision support system to the DT framework, focusing on predictive maintenance and operational optimisation. RUL-based optimisation strategies are seamlessly integrated into the DT framework, while an LLM-based fault diagnosis system enhances decision support by providing AI-driven insights into battery faults. Together, these components improve failure predictions and optimise maintenance scheduling, reducing downtime and streamlining spare part ordering for cost-efficient operations.

The work presented in this thesis contributes to BESS management by proposing a framework that combines advanced modelling techniques for operational optimisation and predictive maintenance. This shows the promise of DT to change situational awareness and decision support, enabling more reliable, efficient, and cost-effective energy storage systems. The results demonstrate the importance of combining data-driven insights with intelligent decision-making to improve energy storage systems' operational and financial performance.

7.2 Future Works

Future research will focus on overcoming existing challenges to further enhance the capabilities of the HSE-DT framework for battery storage systems. The primary objective is to develop a more comprehensive DT model that effectively integrates both dynamic and static models, leveraging historical and real-time data to enrich situational awareness. This approach will involve creating a synergistic framework that combines past battery performance data with real-time operational information, providing a more holistic view of the battery system’s health and performance.

In addition, research efforts will be directed towards optimising the digital twin to reduce latency, enabling real-time synchronous updates and adaptive feedback control.

This improvement will empower the HSE-DT framework to respond swiftly to changes in battery conditions, increasing its accuracy and reliability in practical applications. Moreover, enhancing the interaction between the battery digital twin and external systems, such as Smart Local Energy Systems (SLES), will be a critical focus area. By integrating the digital twin with broader energy ecosystems, the research aims to expand its applicability and facilitate more effective energy management strategies.

Future work will also explore advanced data integration strategies and machine learning techniques to augment the digital twin's predictive capabilities. This includes refining the self-evolving mechanism within the HSE-DT framework to better handle data sparsity and variability, as well as incorporating new feature extraction methods to capture additional aspects of battery behaviour. Addressing these research dimensions will extend the functionality and robustness of the HSE-DT framework, paving the way for its widespread adoption and further development in diverse energy storage applications.

7.3 Conclusions

In conclusion, this study aimed to enhance the management and optimisation of BESS by developing a comprehensive DT-driven framework. The research systematically addressed the critical challenges in real-time monitoring, state estimation, and predictive maintenance of battery systems. Through the integration of advanced machine learning models, multi-source data fusion, and intelligent decision support mechanisms, the proposed framework offers a robust solution for the dynamic and complex nature of battery operations.

The study began by identifying the limitations of conventional battery management methods, particularly in accurately estimating key parameters such as SOC, SOH, and RUL. To address these limitations, a DT-supported framework was introduced, incorporating a hybrid TCN-LSTM model to improve the robustness and precision of battery state estimation. This framework effectively captures temporal dependencies and nonlinear behaviours in battery data, enabling accurate real-time monitoring and fault diagnosis.

Additionally, the research extended the DT framework to include situational awareness and multi-faceted monitoring capabilities, using advanced models such as Transformer and CNN to extract complex features from multi-source battery data. This approach significantly enhances the DT's ability to provide a comprehensive view of battery health, allowing for proactive decision-making and efficient fault management. Including a self-evolving mechanism further improves the adaptability of the framework, enabling continuous updates and refinements based on new data inputs.

Furthermore, the study proposed an innovative decision support system within the DT framework, focusing on predictive maintenance and operational decision-making. By utilising RUL-based strategies and incorporating an LLM-based fault diagnosis system, the research demonstrated a methodology for optimising maintenance schedules and reducing downtime. The experimental validation confirmed that integrating RUL predictions with LLM-enabled recommendations significantly improves the overall reliability and cost-effectiveness of BESS management.

Overall, this research provides a robust and scalable DT-driven solution for managing BESS, offering substantial improvements in state estimation accuracy, situational awareness, and maintenance decision support. The findings of this study lay a strong foundation for future research and development in energy storage systems and highlight the potential of DT technology to revolutionise the management of battery operations. The proposed methodologies and frameworks not only address current limitations but also open new avenues for the application of intelligent systems in energy storage management, paving the way for more sustainable and efficient battery solutions in real-world scenarios.

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Appendix A. Digital Twin Technology

Digital Twin (DT) technology refers to the virtual representation of a physical entity, system, or process, which is used to simulate, monitor, and optimise its performance. A digital twin leverages real-time data and advanced computational models to create a dynamic, continuously updated counterpart of the physical object, enabling predictive analysis, fault detection, and optimization strategies. The DT concept has become foundational to achieving the goals of Industry 4.0 by integrating cyber-physical systems (CPS) and enabling smart manufacturing (Tao et al., 2018).

According to Tao et al. (2018), the relationship between DT and CPS is both complementary and synergistic. While both concepts involve the integration of physical systems with computational models, their roles differ in focus and implementation. Cyber-Physical Systems are primarily concerned with the seamless integration of computation, networking, and physical processes, creating a feedback loop between the physical and cyber worlds. In contrast, Digital Twins provide a more comprehensive framework that not only captures the real-time state of physical entities but also incorporates historical data and predictive analytics.

The key differentiator between DT and CPS, as highlighted by Tao et al. (2018), lies in their capacity to handle different levels of system complexity and abstraction. CPS typically operates at the machine or production line level, where it monitors and controls operational processes in real-time. Digital Twins, on the other hand, operate at a higher level of abstraction, encompassing not only operational data but also simulating future scenarios and conducting "what-if" analyses for strategic decision-making.

Mathematically, a Digital Twin can be formulated using state-space representations. Let $S(t)$ represent the system's state at time t, which evolves according to a set of differential equations:

$$\frac{dS(t)}{dt} = f(S(t), U(t), D(t)) \tag{A1}$$

where $U(t)$ denotes the control inputs and $D(t)$ represents external disturbances. The function f defines the behavior of the physical system. A Digital Twin continually refines this function by incorporating real-time observations, historical data, and predictive models, making it capable of addressing both operational and strategic challenges.

Tao et al. (2018) also emphasise that the Digital Twin framework extends the functionality of CPS by integrating three core components: *physical models*, *virtual models*, and *connection mechanisms*. These components allow for comprehensive data acquisition, integration, and interaction between the physical and digital domains, facilitating advanced applications such as predictive maintenance, real-time performance optimization, and lifecycle management. The mathematical foundation of DT can be further enhanced through the inclusion of machine learning techniques, such as reinforcement learning, to optimise control strategies $U(t)$ or deep learning algorithms to enhance the predictive capabilities of the state function $S(t)$.

Appendix B. Advanced Data Analytics Technologies

B1 Machine Learning

Machine Learning (ML), a subfield of Artificial Intelligence (AI), is centered on developing algorithms and statistical models that enable computers to learn from data and make informed predictions or decisions. Unlike traditional programming, where explicit instructions are provided by human programmers, ML algorithms automatically identify patterns and relationships within the data, allowing systems to enhance their performance over time without being manually reprogrammed (Han et al., 2022). ML has been successfully applied in various domains, such as natural language processing, computer vision, and recommendation systems. The details of the benchmarking algorithms employed in this thesis are elaborated in the following sections.

- **LSTM**

LSTM networks, introduced by Hochreiter (1998), are a type of Recurrent Neural Network (RNN) designed to mitigate the vanishing gradient problem and effectively capture long-term dependencies in sequential data. Unlike standard RNN, LSTM feature a more sophisticated cell structure comprising memory cells and three distinct gates: input, forget, and output gates. These gates regulate the flow of information into, out of, and within the memory cell, enabling the network to selectively retain or discard information over extended sequences. The memory cell retains the long-term state of the network, while the hidden state represents the output of the LSTM cell at each time step.

The input gate regulates the extent to which new information is incorporated into the memory cell:

$$f_t = \sigma(W_{xf}x_t + W_{hf}h_{t-1} + b_f) \tag{B1}$$

where σ is the Sigmoid activation function, which outputs values between 0 and 1. W_{xf} is weight matrix for the input-to-forget gate connection, x_t is the input vector at time step t, W_{hf} is weight matrix for the hidden-to-forget gate connection, h_{t-1} is hidden state from the previous time step, and b_i is the bias term for the input gate. The output gate controls how much of the memory cell state is output as the hidden state:

$$o_t = \sigma(W_{xo}x_t + W_{ho}h_{t-1} + b_o) \tag{B2}$$

where σ is the Sigmoid activation function, which outputs values between 0 and 1. W_{xo} is weight matrix for the input-to-output gate connection, x_t is the input vector at time step t, W_{ho} is weight matrix for the hidden-to-output gate connection, h_{t-1} is hidden state from the previous time step, and b_i is the bias term for the input gate. By using these gates, LSTMs can effectively manage the flow of information over time, allowing them to capture long-term dependencies and mitigate the vanishing gradient problem. It makes LSTMs particularly effective for tasks involving sequential data, such as natural language processing, speech recognition, and time series forecasting.

- **RNN**

Recurrent Neural Networks (RNNs) are a class of deep learning algorithms specifically designed to process sequential data. Unlike CNN, RNN leverages feedback connections to incorporate information from previous states into the current state of hidden units. In this thesis, RNN models are applied to predict strip breakage during the cold rolling process.

This architecture deviates from conventional network structures by accepting input sequences of variable lengths rather than a fixed number of vectors. By utilizing all available input data up to the current moment, RNNs effectively capture temporal dependencies. Moreover, the depth of RNNs can be adjusted to reflect real-world conditions, thereby enhancing their ability to learn complex patterns over time. Therefore, the final output depends not only on the current input but also on the cumulative influence of previous hidden states.

The mathematical formulation of the RNN process is presented as follows:

$$t_i = \boldsymbol{W}_{hx}x_i + \boldsymbol{W}_{hh}x_{i-1} + \boldsymbol{b}_h \tag{B3}$$

$$h_i = \sigma(t_i) \tag{B4}$$

$$s_i = \boldsymbol{W}_{oh}h_i + \boldsymbol{b}_y \tag{B5}$$

$$\hat{o} = g(s_i) \tag{B6}$$

where x_i indicates the input variables, $\boldsymbol{W}_{hx}$, $\boldsymbol{W}_{hh}$ and $\boldsymbol{W}_{ox}$ are weight matrices, $\boldsymbol{b}_h$ and $\boldsymbol{b}_y$ are bias vectors, σ and g are sigmoid functions, t_i, h_i and s_i are the temporary variables, and $\hat{o}$ is the expected output. The cost function is defined as follows:

$$f = \sum_i \left(\frac{\|\hat{o}_i - o_i\|}{2}\right) \tag{B7}$$

where o_i is the actual output. As such, the output at $t + 1$ is the joint function of the input at $t+1$ and the historical data. The RNN simulates the correlation in sequential data, and the depth of the network is the time span.

- **RF**

RFs are a widely used and effective ML algorithm categorized under ensemble learning methods. RFs consist of multiple decision trees and leverage the collective output of these trees to improve prediction accuracy and mitigate overfitting. To increase diversity and reduce variance, RFs introduce randomness by selecting data subsets and features randomly when constructing each decision tree. Each decision tree in RFs is constructed using a subset of the training data, typically selected through bootstrapping (sampling with replacement).

Decisions at each node are based on a subset of features and determined by metrics such as Gini impurity or information gain for classification, and variance reduction for regression. For classification tasks, Gini impurity is calculated as:

$$mg(\mathbf{X}, Y) = av_k \boldsymbol{I}(h_k(\mathbf{X}) = Y) - \max_{j \neq Y} av_k \boldsymbol{I}(h_k(\mathbf{X}) = j) \tag{B8}$$

where $\boldsymbol{I}(\cdot)$ is the indicator function. The margin measures the extent to which the average number of votes at $\mathbf{X}, Y$ for the right class exceeds the average vote for any other class. The larger the margin, the more confidence in the classification. The generalization error is given below:

$$PE^* = P_{\mathbf{X},Y}(mg(\mathbf{X}, Y) < 0) \tag{B9}$$

where the subscript $\mathbf{X}, Y$ demonstrates that the probability is over the $\mathbf{X}, Y$ space. Eqs. (B10) indicates that $\{h(X, \Theta_k) | \mathrm{k} = 1, 2, \dots, N\}$ follow the rule of large numbers as the value of N is large enough for the model, and the classifier has enough trees. Meanwhile, it has been proved that the upper limit of generalization error is convergent as the almost everywhere convergence of random vectors $\theta, \dots, PE^*$. It is given as follows:

$$P_{\mathbf{X},Y}(P_{\Theta}(h(\mathbf{X},\Theta) = Y) - \max_{j \neq Y} P_{\Theta}(h(\mathbf{X},\Theta) = j) < 0) \tag{B10}$$

$$\bar{\varepsilon} \leq \frac{\bar{\rho}(1-s^2)}{s^2} \tag{B11}$$

where $\bar{\varepsilon}$ indicates the upper limit of the generalization error, and $\bar{\rho}$ means the average correlation coefficient between trees, and s represents the average classification performance of the decision trees. Eqs. (A8) illustrates that the larger the average correlation coefficient is, the larger the upper limit of generalisation error will be. Likewise, the larger the average classification is, the larger the upper limit of generalisation error will be. Essentially, the classification performance is affected by two factors, one is the overall performance of trees, and the other is the diversity between trees.

Appendix C: Large Language Models (LLM)

Large Language Models (LLMs) are advanced artificial intelligence systems designed to understand and generate human-like text, making them pivotal in numerous Natural Language Processing (NLP) applications. These models are typically built on the transformer architecture and consist of neural networks with billions of parameters trained on extensive datasets of text from diverse sources. The primary goal of LLMs is to learn the statistical patterns and structures of language, which enables them to perform a broad range of NLP tasks, such as text generation, translation, summarization, and question-answering. Their remarkable effectiveness stems from their ability to capture long-range dependencies and contextual information, facilitated by self-attention mechanisms and multi-layered architectures (Vaswani et al., 2017).

The core of most LLMs is the transformer architecture, introduced by Vaswani et al. (2017). Transformers leverage self-attention mechanisms to weigh the importance of different words in a sentence, allowing the model to focus on relevant parts of the input. This architecture is particularly beneficial for understanding context and generating coherent text. The training process involves unsupervised learning on large text corpora, where the model learns to predict the next word in a sequence or to fill in missing words, thereby capturing the underlying structure of language.

The transformer model can be mathematically expressed using a self-attention mechanism, where the relationship between input tokens is represented as:

$$Attention(Q, K, V) = softmax(\frac{QK^T}{\sqrt{d_k}})V \tag{C1}$$

where $Q, K\ and\ V$ are matrices representing the query, key, and value, respectively, and d_k is the dimension of the key vectors. This mechanism allows the model to consider the influence of all other tokens when computing the representation of a particular token, capturing complex dependencies in the input text.

LLMs have become transformative tools in NLP, driving significant advancements across various domains, from content creation and customer support to scientific research and software development. However, the ongoing development of LLMs poses challenges such as ethical considerations, data privacy, and model interpretability. Research is being directed toward improving model transparency and fairness, ensuring that these models are aligned with human values and can be safely deployed in real-world scenarios (Bender et al., 2021).

Future research should also focus on enhancing the efficiency and scalability of LLMs. Techniques such as model pruning, knowledge distillation, and quantization are being explored to reduce the computational resources required for training and deployment. Additionally, hybrid models that integrate symbolic reasoning with neural networks are being investigated to improve the generalization and problem-solving capabilities of LLMs (Marcus, 2020).

In conclusion, LLMs such as ChatGPT, Claude 2.0, LLaMA 2, and Mistral 7B represent the state-of-the-art in NLP, each with unique features and strengths. Their continued development and integration with emerging technologies will further expand their impact on various industries and research fields.