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Review

Specialized deep neural networks for battery health prognostics: Opportunities and challenges

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ABSTRACT

Lithium-ion batteries are key drivers of the renewable energy revolution, bolstered by progress in battery design, modelling, and management. Yet, achieving high-performance battery health prognostics is a significant challenge. With the availability of open data and software, coupled with automated simulations, deep learning has become an integral component of battery health prognostics. We offer a comprehensive overview of potential deep learning techniques specifically designed for modeling and forecasting the dynamics of multiphysics and multiscale battery systems. Following this, we provide a concise summary of publicly available lithium-ion battery test and cycle datasets. By providing illustrative examples, we emphasize the efficacy of five techniques capable of enhancing deep learning for accurate battery state prediction and health-focused management. Each of these techniques offers unique benefits. (1) Transformer models address challenges using self-attention mechanisms and positional encoding methods. (2) Transfer learning improves learning tasks within a target domain by leveraging knowledge from a source domain. (3) Physics-informed learning uses prior knowledge to enhance learning algorithms. (4) Generative adversarial networks (GANs) earn praise for their ability to generate diverse and high-quality outputs, exhibiting outstanding performance with complex datasets. (5) Deep reinforcement learning enables an agent to make optimal decisions through continuous interactions with its environment, thus maximizing cumulative rewards. In this Review, we highlight examples that employ these techniques for battery health prognostics, summarizing both their challenges and opportunities. These methodologies offer promising prospects for researchers and industry professionals, enabling the creation of specialized network architectures that autonomously extract features, especially for long-range spatial-temporal connections across extended timescales. The outcomes could include improved accuracy, faster training, and enhanced generalization.

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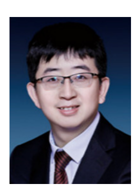

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1. Introduction

The transformational impact of lithium-ion batteries on global technology, driven by countless research endeavors and substantial funding for battery innovation, is unquestionable [1]. These powerhouses have given life to revolutionary devices [2] like mobile phones, portable computers, and green transportation alternatives like hybrid and electric cars [3]. In order to stimulate a broader acceptance of these batteries in large-scale applications, it is imperative that the technology further evolves. Key areas for advancement include energy density, storage capacity, durability, charging efficiency, safety, and affordability. Strides in these areas will not only enhance performance but also improve practicality and accessibility, making these powerful energy storage solutions more viable for an array of applications. In the context of field applications, the role of battery health prognostics is indispensable. These methods contribute substantially towards preserving the longevity and reliability of batteries throughout the duration of the system's operational lifetime [4,5]. By precisely forecasting battery state of health (SOH) and remaining useful lifetime (RUL), these techniques guarantee optimal performance and avert unforeseen failures. This significantly boosts the efficiency and reliability of energy-dependent systems, thereby enhancing their overall effectiveness.

A battery is an intricate amalgamation of materials whose performance depends on numerous variables, including ion and charge transport across interfaces and phases, reversible and irreversible chemical interactions, and a variety of material-specific attributes. Though we have made strides in physics-driven electrochemical modeling of batteries from the atomic level to macro systems, the lack of uniform predictive models has slowed advancement. Software accessibility and the capability for high-throughput optimization, combined with efficient automation in battery modeling, have paved the way for the inclusion of machine learning. The emerging field of data-driven machine learning-based battery research seeks to overcome these obstacles [6], bolstering technology transition from academic settings to commercial applications [7] for in several aspects, including state of charge (SOC) estimation [8–10], SOH prediction [11–14], safety monitoring and failure prediction [15,16]. A number of nice reviews have succinctly summarized that machine learning has emerged as a promising and viable alternative in battery prognostic and preventive health management [17–19]. The characteristics of common methods used for battery health prognostics are summarized in Table 1, which clearly illustrates the advantages of each technique in various application scenarios and for different application purposes.

An illustrative example is the use of early-cycle discharge voltage curves to predict battery lifespan using data-driven methods, prior to observable degradation in capacity [20]. This study involves a wide-ranging dataset of 124 commercial lithium iron phosphate/graphite cells subjected to quick charging and demonstrating varied cycle lives. Machine learning tools are applied to predict and categorize cells based on their cycle life.

Advancing beyond traditional machine learning methods, representation learning emerges as a powerful approach that enables machines to autonomously extract and refine the necessary features from raw data for tasks such as detection or classification or regression. In this paradigm, deep learning stands as a potent tool, capable of crafting multi-layered computational models that learn data representations with increasing levels of abstraction.

Table 1
The characteristics of some common techniques for battery health prognostics.

Method	Advantages	Shortcomings
Physics-based models	Based on fundamental principles.	Require deep knowledge of battery chemistry.
	Predictive even in untested conditions.	Complex and computationally intensive.
	Provide insights into degradation mechanisms.	Need accurate parameters which may not always be available.
Equivalent circuit models	Simplifies complex battery behavior into circuits.	Can miss finer details of battery behavior.
	Suitable for real-time applications due to reduced computation.	Need to be calibrated for each specific battery type.
	Relatively easy to understand and interpret.	May not be precise for all battery conditions.
Empirical models (e.g., arrhenius, Peukert equation and so on)	Based on observed data rather than theories.	Only valid for conditions under which they were derived.
	Typically, simpler and computationally efficient.	Don't provide insight into the underlying physical or chemical processes.
	Easy to integrate into control systems.	Need frequent recalibration with new data.
Traditional machine learning (e.g., SVM, decision trees and so on)	Can handle large datasets.	Require labeled training data.
	Capable of identifying complex patterns and relationships.	May not generalize well to new battery chemistries.
	Wide variety of algorithms available for different use cases.	Interpretability can be challenging.
Deep learning (e.g., transformer, generative model and so on)	Excellent for detecting patterns in large datasets.	Require vast amounts of data for training.
	Suitable for sequential data (e.g., time-series battery data).	Computationally intensive.
	Continuously improve with more data.	Often considered a "black-box" - hard to interpret.

Deep learning harnesses the power of the backpropagation algorithm to iteratively adjust the internal parameters within each layer, basing these alterations on the learnings acquired in preceding layers. This method has demonstrated exceptional effectiveness in unraveling complex structures embedded in vast datasets, thereby solving challenges that have historically perplexed the AI community [21]. Notably, deep learning's proficiency in identifying complex patterns in high-dimensional data renders it especially pertinent to fields such as battery and materials science. Here, it can help unlock insights that can drive advancements in these critical areas.

A recent example that reflects this new learning philosophy is the real-time, personalized health status forecast for lithium-ion batteries achieved through deep transfer learning [22]. The undertaking faces challenges due to diverse user preferences, dynamic operating patterns, and scarce historical data. The research team compiled an extensive dataset encompassing 77 commercial cells with over 140,000 charge-discharge cycles— reportedly the most substantial dataset of its kind. They also devised a transfer learning framework to facilitate real-time health status predictions for unobserved battery discharge protocols at any charge-discharge cycle. These studies underscore the benefits of uniting targeted data generation with data-centric modeling for forecasting complex dynamic system behavior.

Up to now (2023), numerous online resources offer data on battery testing and cycling [23–30]. These openly available resources offer valuable opportunities to refine battery design, modeling, and management through strategic data exploitation. Within this context, deep learning may provide robust tools to decode intricate patterns within vast datasets, predominantly by employing the backpropagation algorithm. This algorithm aids the machine in adjusting its internal parameters, which are used to calculate the representation in each layer based on the preceding layer's output. This Perspective aims to introduce a curated selection of promising techniques for advancing deep learning. These techniques have showcased remarkable effectiveness in producing accurate predictions for multiphysics battery systems. In total, we outline five specialized techniques that can enhance deep learning-based battery health prognostics.

(i) Transformer learning emerges as a key concept within the arena of equivariant transformer networks, a collection of differentiable mappings designed to enhance model durability by recognizing specific continuous transformation groups. These networks skillfully adapt to a myriad of symmetries and transformations, cultivating models that are more robust and dependable across a diverse array of scenarios.

(ii) Transfer learning surfaces as a potent tool to reinforce supervised online learning tasks in a particular domain by leveraging knowledge from a separate domain. Despite the lack of an assumption of identical data distributions across the two domains, transfer learning exemplifies its adaptability and versatility. Specifically, within the context of lithium-ion batteries, the marriage of data-driven and transfer learning techniques reveals substantial potential in boosting battery state estimation and forecasting.

(iii) Physics-informed machine learning stands as a crucial pillar in modern data-driven learning. It effectively employs existing data from observational, empirical, physical, or mathematical studies to enhance the proficiency of a learning algorithm. By taking advantage of this vast reservoir of knowledge, physics-informed learning paves the way for algorithms to achieve exceptional accuracy and broad applicability, thus producing models that are both reliable and resilient.

(iv) Generative adversarial networks, also known as GANs, constitute a specialized category of artificial intelligence algorithms tailored to address generative modeling tasks. Their primary objective is to scrutinize a set of training examples, with the goal of discerning the underlying probability distribution that produced them. Once this distribution is understood, GANs are capable of generating new instances that conform to the same pattern, thus spawning additional examples that are reflective of the identified probability distribution.

(v) Reinforcement learning provides a systematic approach to a unique learning problem, drawing inspiration from the principles of behavioral psychology. The underlying premise is that an artificial agent can evolve through its interactions with the environment, emulating the learning mechanism of biological organisms. Reinforcement learning solves the challenges an agent encounters when it needs to develop its behavior through trial-and-error within a dynamic environment. In essence, reinforcement learning navigates agents in devising action sequences within a specific environment, aiming to maximize cumulative rewards.

This perspective delves into how modern data-driven machine learning methodologies, especially deep learning, can catalyze lasting innovation in the battery industry. It begins with a succinct exploration of five popular deep learning techniques, scrutinizing their strengths and limitations for time-series prediction tasks (Section 2). In the fast-paced field of AI research, democratizing this knowledge for the wider battery community becomes a pressing necessity. Before venturing into the specifics of each deep learning technique through practical examples, an overview of openly shared data related to lithium batteries under varied test and cycling conditions is provided (Section 3). Research utilizing these openly accessible datasets manifests the promising potential and indispensable contributions of shared data resources. An in-depth analysis of various instances where machine learning has been integrated with relevant datasets is presented, highlighting the remarkable effectiveness of AI and deep learning techniques across diverse aspects (Section 4). In Section 5, a comprehensive guide to commonly used software and hardware for deep learning training is introduced. Finally, in Section 6, a forward-looking perspective that considers existing limitations and challenges is offered. By bridging the divide between AI and battery sciences, and by encouraging collaboration and open data sharing, new avenues for innovation can be unlocked. This paves the way for the development of advanced, efficient, and sustainable energy storage solutions, aligning with broader goals of energy sustainability and technological advancement.

2. Five promising techniques for advancing deep learning

Deep learning, a subclass of machine learning methodologies, has deeply integrated into various facets of our contemporary world and has been gaining significant attention in recent times [31]. Traditional machine learning methods encountered hurdles when dealing with raw data. The construction of a pattern-recognition or deep learning system required substantial domain knowledge and painstaking engineering to craft feature extractors that converted raw data into a suitable internal representation. In a stark contrast, representation learning enables deeps to autonomously uncover the necessary representations for recognition or classification from raw data. In the ensuing section, we will provide a brief overview of a few notable deep learning methodologies, with a particular focus on neural networks. This is aimed to assist novices in the electrochemical energy storage field, and

Table 2
Techniques for enhancing deep learning-based prediction tasks.

Technique	Advantages	Cautions/Limitations
Transformer	Excellent at capturing long-range dependencies in data. Highly parallelizable, leading to faster training. Scalable with respect to input length.	Requires large datasets for training to avoid overfitting. Can be computationally intensive, especially for longer sequences.
Transfer learning	Accelerates training by leveraging pre-trained models. Requires less labeled data. Often results in better performance and generalization.	Domain mismatch between source and target data can hinder performance. Fine-tuning might be needed, which requires domain expertise.
Physics-informed machine learning	Incorporates physical laws and constraints, enhancing model interpretability. Can perform well with smaller datasets.	Needs careful integration of physical information. May require domain expertise to define relevant physical laws.
Generative adversarial models	Capable of generating new data samples. Useful in data augmentation, anomaly detection, and imputation of missing values.	Can be difficult to train. Generated data may not always be realistic or may lack diversity.
Reinforcement learning	Enables learning through interaction with the environment. Can optimize complex decision-making and control problems.	Often requires a large amount of data. Sensitive to hyperparameters and exploration strategy. May struggle with real-world scenarios where data is costly or hard to obtain.

other scientists and engineers who may be unacquainted with deep learning jargon. The merits and drawbacks are summarized in Table 2.

2.1. Self-attention transformer

Transformers, as depicted in Fig. 1, have garnered considerable attention due to their effectiveness in tackling a wide range of complex problems ever since their inception in 2017 by Vaswani and his team of researchers [32]. Their applications span diverse domains, including but not limited to, language understanding, image recognition, and audio classification. Their design, heavily reliant on attention mechanisms, allows for superior handling of long-range dependencies in data and parallel computing, effectively overcoming the limitations of their recurrent and convolutional counterparts. The Transformer's unique structure has also set the stage for various derivative models such as bidirectional encoder representations from transformers (BERT) [33], generative pre-trained transformer (GPT) [34], and text-to-text transfer transformer (T5) [35], which continue to push the boundaries of what's possible in the realm of artificial intelligence. The emergence of Transformer networks represents a paradigm-shifting breakthrough. Due to their impressive achievements in various tasks, Transformer models have drawn significant attention from the time series analysis community [36,37]. By utilizing self-attention mechanisms and positional encoding strategies, Transformers excel at capturing both short-term and long-term correlations within sequences. This proficiency makes them especially potent for time series modeling and forecasting.

In the practical implementation of the Transformer model, we execute the attention mechanism on a batch of queries, collectively assembled into a matrix represented as Q. Similarly, one can systematize the keys and values into corresponding matrices, denoted as K and V, respectively. These matrices, Q, K, and V, each play a crucial role in determining the attention scores and subsequently the contextual embeddings

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V \tag{1}$$

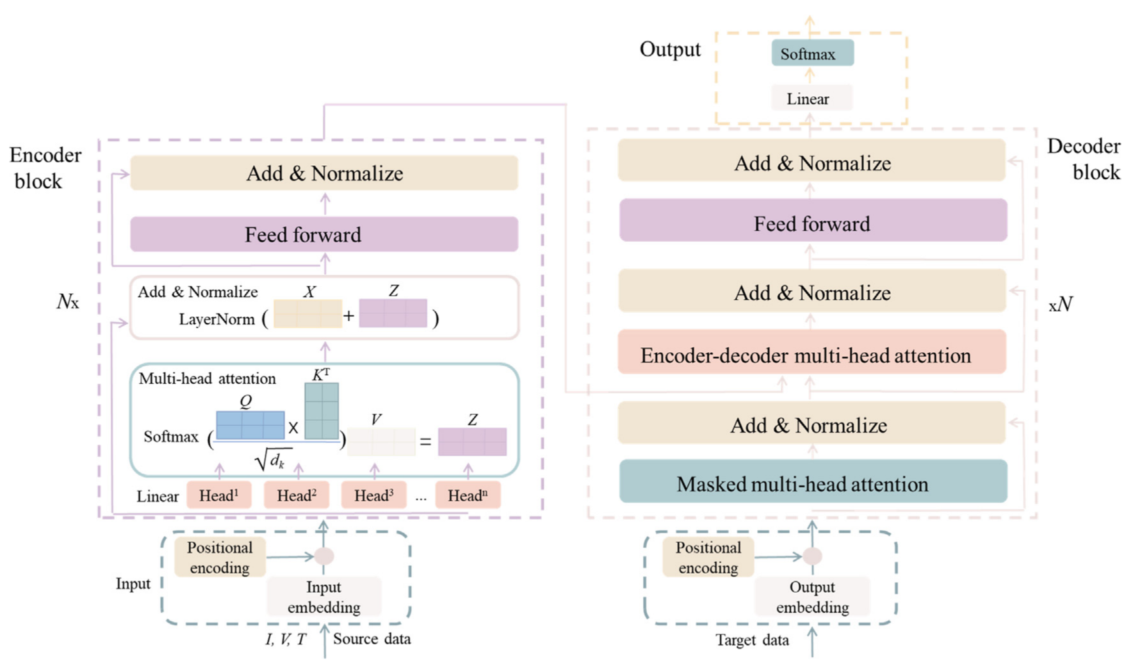

Fig. 1. Multi-head self-attention Transformer architecture for battery health prognostics.

The attention function operates by aligning the queries with keys, thereby determining the importance of each key to a given query. The resulting scores are then used to compute a weighted sum of the values. This attention score computation and weighted sum generation are carried out in parallel across all queries and keys using matrix multiplication for efficient processing. With the employment of the softmax function, the attention scores are normalized, ensuring they are proportionate and sum up to one. This process allows the model to focus more on certain words (values) while paying less attention to others during encoding and decoding stages, hence the term "attention." Through the computation of the output matrix, one can obtain the result, which is a weighted sum of the values. The output matrix signifies the model's aggregated knowledge of the input at each position, having taken into account not just the individual word, but its wider context within the sequence. This attention-driven representation of the input sequence becomes the foundation for subsequent processing layers.

By incorporating multi-head attention, the model gains the ability to simultaneously focus on various representation subspaces at different positions. Unlike a single attention head, which limits the model's capacity to do so by averaging the information.

$$\mathrm{MultiHead}(Q,K,V) = \mathrm{Concat}(\mathrm{head}_1,\ldots,\mathrm{head}_h)W^O \tag{2}$$

$$\text{where } \mathrm{head}_i = \mathrm{Attention}(QW_i^Q, KW_i^K, VW_i^V) \tag{3}$$

The model lacks recurrence and convolution, which makes it necessary to incorporate information about the relative or absolute positions of tokens within a sequence to take account of the sequence's order. Consequently, "positional encodings" is utilized to the input embeddings at the base of the encoder and decoder stacks. The dimensional parity between positional encodings and the embeddings (both having a dimension $d_{mod\ el}$) facilitates their addition.

$$\mathrm{PE}_{(pos,i)} = \left\{ \begin{array}{l} \sin\left(\dfrac{pos}{10000^{i/d_{\mathrm{model}}}}\right), \text{ if } i \text{ is even} \\ \cos\left(\dfrac{pos}{10000^{(i-1)/d_{\mathrm{model}}}}\right), \text{ if } i \text{ is odd} \end{array} \right\} \tag{4}$$

The positional encoding leverages two variables: '*pos*' and '*i*'. Here, '*pos*' designates the position of a token within the input sequence, and '*i*' denotes the dimension of the positional encoding. In essence, the positional encoding in the Transformer model is a crucial element that boosts the model's capability to interpret sequential data, establishing it as a fundamental component for advanced language comprehension and generation tasks.

In recent years, the Transformer model has demonstrated tremendous power in time-series analysis [38]. By utilizing sequences of current, voltage, and temperature data as inputs, the specialized Transformer models have been widely put to use to forecast intricate electrochemical dynamics within batteries [8,10,39] Capitalizing on self-attention and positional encoding techniques, Transformers are adept at detecting both long and short-range interactions within sequences, making them an enticing choice for time series modeling and forecasting. Transformer models offer several advantages for multivariable time series prediction.

(a) Handling long-term dependencies: Transformers are equipped with attention mechanisms that allow them to focus on different parts of the input sequence, no matter how far apart they are. This feature is particularly advantageous for handling long-term dependencies in multivariable time series data.
(b) Parallel processing: Unlike recurrent architectures such as long short-term memory (LSTM) and gated recurrent unit (GRU), Transformer models can process data in parallel. This significantly reduces the time needed for training and makes them more efficient when dealing with large datasets.
(c) Interpreting complex relationships: The self-attention mechanism in Transformers helps in capturing complex relationships among multiple variables over time. This is particularly useful in multivariable time series where the interactions between different variables can be highly complex and nonlinear.
(d) Capturing seasonal and cyclical patterns: Transformers are capable of recognizing and learning seasonal and cyclical patterns in time series data, which is essential for accurate forecasting in many applications such as finance, weather, and energy consumption.
(e) Scalability: Transformer models are highly scalable and can be trained on large datasets with a high number of variables. This makes them well-suited for applications where there are many related time series to consider.
(f) Customization of attention mechanisms: Transformers allow for the customization of attention mechanisms, making it possible to design models that focus on particular aspects of the time series data, such as high-frequency changes or long-term trends.
(g) Noise reduction: By weighing the importance of different parts of the input sequence, Transformer models can often effectively filter out noise and focus on the significant underlying patterns in the data.
(h) Robustness to missing data: Through attention mechanisms and positional encodings, Transformer models can often handle missing data more robustly than some other models, as they can infer information from other parts of the sequence.

Table 3
Hyperparameters of the Transformer model.

Aspect	Description	Typical values
Number of layers	Controls the depth of the neural network. Increasing the number of layers captures more complex patterns, but can lead to overfitting.	6–12
Number of heads	Controls the perspectives in multi-head attention. More heads allow for a nuanced understanding, but increase computational cost.	8–16
Dimensionality of the model	Determines the size of input and output layers. Higher dimensionality captures more detailed representations, but increases computational cost.	128–512
Feed-forward network dimensionality	Dimensionality of the feed-forward network inside each Transformer block. Higher dimensionality captures complex relationships between inputs and outputs.	256–1024
Positional encoding	Gives the model a sense of relative positions in the input sequence. The choice of encoding impacts its utilization.	Sinusoidal encoding
Learning rate	Controls the step size during gradient descent optimization. Higher rates speed up training, but can hinder convergence if excessively high.	0.0001–0.001
Dropout rate	Probability of dropping out neurons during training. Helps prevent overfitting by encouraging diverse learned representations.	0.1–0.5

Meticulous setting of hyperparameters (Table 3), encompassing input-output units, encoder-decoder dimensions/architecture, sliding window length, batch size, and training epochs, is paramount for generalized application in field situations, where battery packs may consist of hundreds or thousands of cells, each containing multi-variate long sequences of time-series data. Moreover, it is important to consider the computational resources needed for training large Transformer models, and the need for large datasets to fully leverage their capabilities. Additionally, care should be taken in tuning hyperparameters and designing the architecture to avoid overfitting, especially in cases where the amount of training data is limited.

2.2. Transfer learning

Transfer learning offers practical solutions for managing few-shot learning tasks [40]. In these circumstances, transfer learning is utilized to acquire and transfer knowledge between task domains using a proficient transfer mechanism, which can ease the burdensome data labeling process by only needing a few target training samples based on fine-tuning pre-existing models [41].

For the context of inductive transfer learning, supervised feature construction methods, akin to those used in multi-task learning, are commonly employed. The essential concept is to cultivate a shared, low-dimensional representation across correlated tasks. This newly established representation not only aids in reducing errors in classification or regression models but also bolsters the performance on each distinct task. In this scenario, common features can be ascertained by solving an optimization problem, delineated as follows

$$\underset{W}{\text{minimize}} \sum_{i=1}^{n} L_i(W) + \lambda \| W \|_F^2 \tag{5}$$

where W is the shared low-dimensional representation (feature matrix). $L_i(W)$ is the loss function for the i-th task, which measures the model's performance on that specific task using the shared representation. λ is a regularization hyperparameter that balances the task losses and the complexity of the parameters. $\| W \|_F^2$ denotes the Frobenius norm, used to regularize the parameters W to prevent overfitting. By minimizing the above optimization problem, a shared low-dimensional representation W can be learned, which performs well on each correlated task, enabling beneficial information transfer across tasks and improving the overall generalization and performance of the model.

Beyond supervised feature construction techniques, unsupervised methods become crucial when handling extensive volumes of unlabeled data in transfer learning scenarios. These methods aim to learn higher-order features to maximize transferability. The essential paradigm of this approach unfolds in two stages. The initial stage involves extracting higher-level basis vectors, symbolized as $b = \{b_1, b_2, ..., b_s\}$, from the data of the source domain. This is realized by resolving the optimization problem (2), which can be articulated as follows

$$\underset{Z}{\text{maximize}}\, F(Z) + \lambda R(Z) \tag{6}$$

where, Z signifies the superior basis vectors, symbolizing the unsupervised feature representations. $F(Z)$ is the representation learning's objective function, which aims to heighten transferability. λ stands for a regularization hyperparameter that is used to maintain a balance between the objective function and the regularization term. $R(Z)$ represents the regularization term, which might be L1 regularization, L2 regularization, or others. This term is utilized to limit the complexity of the higher-level basis vectors, thus preventing overfitting. The resulting Z from this phase can then be deployed for the subsequent target task, such as target domain classification or regression tasks. By utilizing the learned feature representations extracted from the source domain data, the transfer learning model enhances its performance on the target task, even in the absence of labeled data in the target domain. This strategy enables the acquisition of universal feature representations from vast volumes of unlabeled data, which ultimately leads to improved generalization of the model on the target task.

The framework of using transfer learning (Fig. 2) for battery health prognostics is a powerful approach in the diagnosis and prognosis of battery states. Transfer learning leverages the knowledge gained from pre-trained models on related tasks and adapts it to the battery health domain. This process offers several advantages, including.

(a) The employment of a transfer learning framework for battery health prognostics proves a robust method in the diagnosis and prognosis of various battery states. Transfer learning capitalizes on insights gained from pre-existing models pertinent to similar tasks and tailors these to the battery health sphere. This approach offers a plethora of advantages:
(b) Enhanced accuracy: Through the application of insights gathered from previously undertaken tasks, transfer learning has the capacity to elevate the precision of health assessments and prognostics for a multitude of batteries.
(c) Efficient convergence: Typically, transfer learning expedites convergence during training as the model is initially furnished with pre-existing information. This attribute proves invaluable when dealing with scarce data.
(d) Improved generalization: The generalization capabilities of the model can be enhanced through transfer learning as it utilizes information derived from a wide array of battery types and their operating conditions. This aspect is especially crucial since batteries exhibit diverse aging patterns under varying conditions.
(e) Data efficiency: This approach proves advantageous in scenarios where gathering ample training data for each specific battery type and condition is unfeasible. Transfer learning optimizes the use of limited data by incorporating pertinent information from other realms.
(f) Feature reusability: Features such as standard deviation, Shannon entropy, and principal components, once extracted from one battery dataset, can be repurposed for other related battery datasets. This enhances pattern recognition and facilitates more accurate SOH estimations.

Transfer learning in battery prognostics holds promise in enhancing estimation accuracy by leveraging knowledge across domains, but faces challenges such as the necessity for real-world data for model retraining, discrepancies between source and target domains, and the complexity in adapting base models to new tasks. Emerging strategies like employing semi-supervised learning to reduce data requirements offer potential solutions, though ensuring the reliability and avoiding biases in the process remain concerns.

2.3. Physics-informed learning

Physics-informed learning is a promising field that offers new possibilities for solving complex physical systems in both forward and inverse problems [42]. Although it does not specifically address few-shot problems, it provides an alternative approach to training networks with improved generalization in small data regimes by embedding informative priors in the form of theoretical constraints, such as physical laws and domain knowledge. These kernel-based or neural network-based methods help predict the

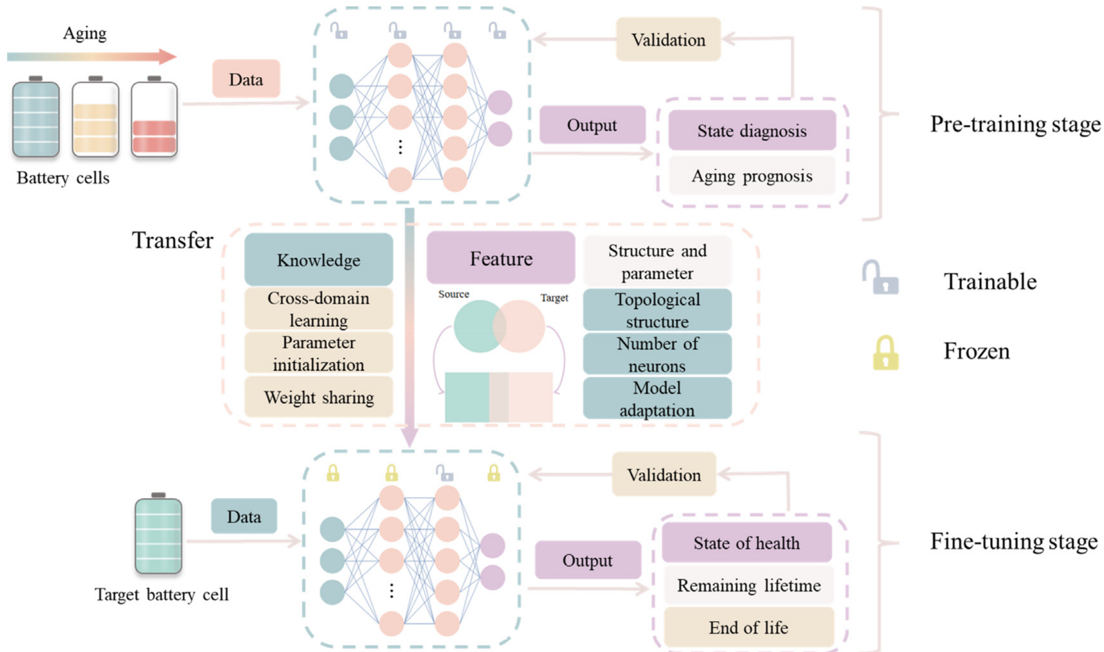

Fig. 2. Transfer learning architecture for battery health prognostics.

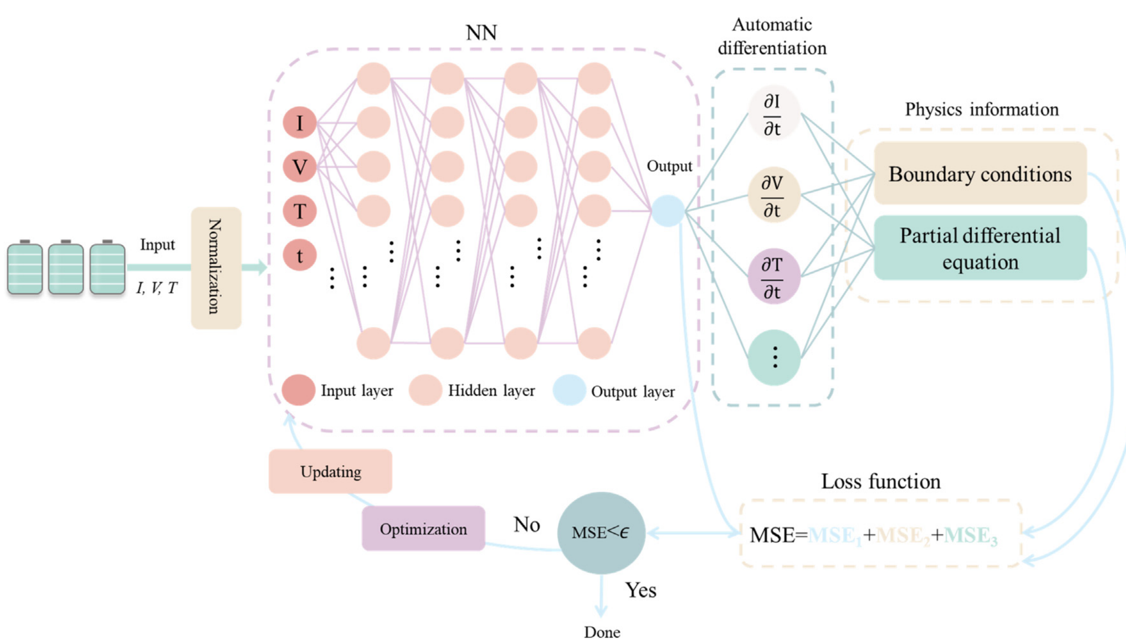

Fig. 3. Physics-informed learning architecture for battery health prognostics.

evolution of multiphysics systems by introducing appropriate observational, inductive, or learning biases. Prior knowledge from mathematical, physical, and engineering sciences plays a critical role in prediction accuracy and generalization.

Physics-Informed Neural Networks (PINNs), as shown in Fig. 3, can seamlessly achieve the amalgamation of measurement data and partial differential equations (PDEs) by incorporating these PDEs directly into the neural network architecture. This method demonstrates remarkable versatility, proficiently managing a broad spectrum of PDE types, from integer-order PDEs and fractional PDEs to stochastic PDEs.

To demonstrate its efficacy, the PINN model can be effectively used to resolve forward problems using the viscous Burgers' equation, which can be articulated as follows.

$$\frac{\partial u}{\partial t} + \mu\frac{\partial u}{\partial x} = v\frac{\partial^2 u}{\partial x^2} \tag{7}$$

where, u is the unknown function of x and t which we aim to find.v is the variable, a positive constant.x is the spatial variable.

Physics-uninformed networks act as proxies for the solution of the PDE, represented as $u(x,t)$, while physics-informed networks encapsulate the residual of the PDE. The loss function comprises both supervised and unsupervised elements. The supervised loss includes data measurements of u obtained from the initial and boundary conditions. Concurrently, the unsupervised loss addresses the variance within the PDE.

$$L(\theta)\ominus = L_{\text{boundary}}(\theta) + L_{\text{initial}}(\theta) + L_{\text{PDE}}(\theta) \tag{8}$$

where, the $L_{\text{boundary}}(\theta)\ominus$ boundary condition loss can be computed over the spatial boundary points x_{boundary}, t, and u_{boundary} represents the corresponding known boundary values, while the initial condition loss $L_{\text{initial}}(\theta)\ominus$ can be computed over the points at the initial time x, t_{initial}, and u_{initial} represents the corresponding known initial values

$$L_{\text{boundary}}(\theta)\ominus = \sum\ _i (u(x_{\text{boundary}}, t; \theta) - u_{\text{boundary}})^2 \tag{9}$$

$$L_{\text{initial}}(\theta)\ominus = \sum\ _i (u(x, t_{\text{initial}}; \theta) - u_{\text{initial}})^2 \tag{10}$$

The PDE loss $L_{\text{PDE}}(\theta)$ corresponds to the residuals of the PDE, and is given by

$$L_{\text{PDE}}(\theta)\ominus = \sum\ _i f(x_i, t_i; \theta)^2 \tag{11}$$

The neural network undergoes training using gradient-based optimizers like Adam, with the aim of reducing the loss until it dips beneath a predefined threshold ε. For a detailed exploration and introduction to PINNs, one can refer to an exhaustive review [42]. PINNs offer several advantages in modeling and predictions.

(a) Synergistic incorporation of theory and data: PINNs adeptly marry theoretical physics with observational data by assimilating mathematical equations alongside data inputs, ensuring a synthesis that adheres to established physical principles.
(b) Resilience to data deficiencies: The utilization of inherent physical laws renders PINNs more resilient to shortcomings in the data, such as noise or incomplete datasets, as they draw upon these laws to bolster their predictions.
(c) Increased transparency: Where traditional neural networks are often criticized for their opacity, PINNs open the ‘black box’ by bringing in physical laws, thus offering more insight into how conclusions are derived.
(d) Robust predictions beyond data range: PINNs are adept at making predictions that not only are accurate but also maintain physical consistency, even when venturing beyond the bounds of the data used in training.
(e) Tailored physical constraints integration: PINNs allow for the introduction of customized biases reflecting observational, inductive, or learning preferences, guiding the learning process in a physically coherent direction.
(f) Versatile inclusion of physical principles: Through adaptable loss functions and constraints, PINNs can incorporate a wide spectrum of physics-oriented biases, including those expressed through various mathematical equations.
(g) Potential for multi-faceted integration: The diverse methods for integrating physical insights in PINNs can be amalgamated, giving rise to an extensive range of multifaceted methodologies for crafting physics-informed learning algorithms.
(h) Efficacy in handling complex systems: With their ability to seamlessly blend data and abstract mathematical operators, PINNs excel in modeling nonlinear systems encompassing multiple scales, something that conventional tools find daunting due to inherent challenges and uncertainties.

PINNs have garnered attention for their innovative approach in combining physical laws with machine learning. However, they are not without challenges and limitations: PINNs face difficulty in effectively modeling systems where physical, chemical, and biological processes interact across a vast range of spatiotemporal scales. Earth’s system, for example, is an incredibly complex multiscale system, and accurately predicting its nonlinear dynamics through PINNs still poses challenges. Moreover, PINNs attempt to address the difficulties in solving nonlinear multiscale systems with classical computational tools. However, their implementation can incur significant computational costs and introduce various sources of uncertainty, especially when the system involves inhomogeneous cascades of scales. In addition, the absence of universally acceptable models for various physical systems and the diversity in available data calls for an adaptable approach, which is challenging to achieve in practice.

2.4. Generative models

Modeling high-dimensional probability distributions for multiscale and multivariate systems, especially in scenarios with sparse data, continues to be a scientific challenge. Generative Adversarial Networks (GANs), one of the promising techniques in generative deep learning first developed by Goodfellow in 2014, offer a potential solution [43]. GANs have demonstrated remarkable capabilities in learning data distributions in an unsupervised or semi-supervised fashion [44]. The GAN structure (Fig. 4) includes a generator model that produces samples for a domain specific to a task, and a discriminator model that distinguishes between real data and fabricated ones from the generator. During the training phase, the generator strives to convince the discriminator that the samples it produces are real, based on a reward-punishment mechanism. As the GAN model optimizes itself, seeking a Nash equilibrium between the adversarial networks, the ’virtual representations’ produced by the generator increasingly resemble real data.

In GAN models, the training cost is assessed through a value function that relies on both the generator and discriminator models, effectively solving

$$\max_D \min_G V(G, D) \tag{12}$$

where

$$V(G, D) = E[\log(D(x))] + E[\log(1 - D(G(z)))] \tag{13}$$

$E[\log(D(x))]$ represents the expected value of the logarithm of the discriminator’s output when given real data samples x. The output $D(x)$ represents the discriminator’s probability of classifying real data samples as authentic. The discriminator seeks to maximize this term as its goal is to correctly identify real samples as real, which is reflected by a higher probability value. $E[\log(1 - D(G(z)))]$ stands for the expected value of the logarithm of one minus the discriminator’s output when provided with fake data samples, which the generator G produces from random noise z (hence $G(z)$). $D(G(z))$ is the discriminator’s probability of classifying these generated samples as authentic. The generator seeks to minimize this term because its objective is to produce samples that the discriminator classifies as fake with a low probability. During this process, one model’s parameters are optimized while the others are kept constant. Given a fixed generator, there exists a distinct optimal discriminator defined as

$$D^*(x) = p_{\text{data}}(x) / (p_{\text{data}}(x) + p_g(x)) \tag{14}$$

They further demonstrated that the generator G reaches its optimum when the generated data distribution, $p_g(x)$, aligns with the real data distribution, $p_{\text{data}}(x)$. This equation essentially states that the optimal discriminator classifies samples based on the likelihood ratio of a sample coming from the real data distribution versus the generator’s distribution. If a sample is more likely to come

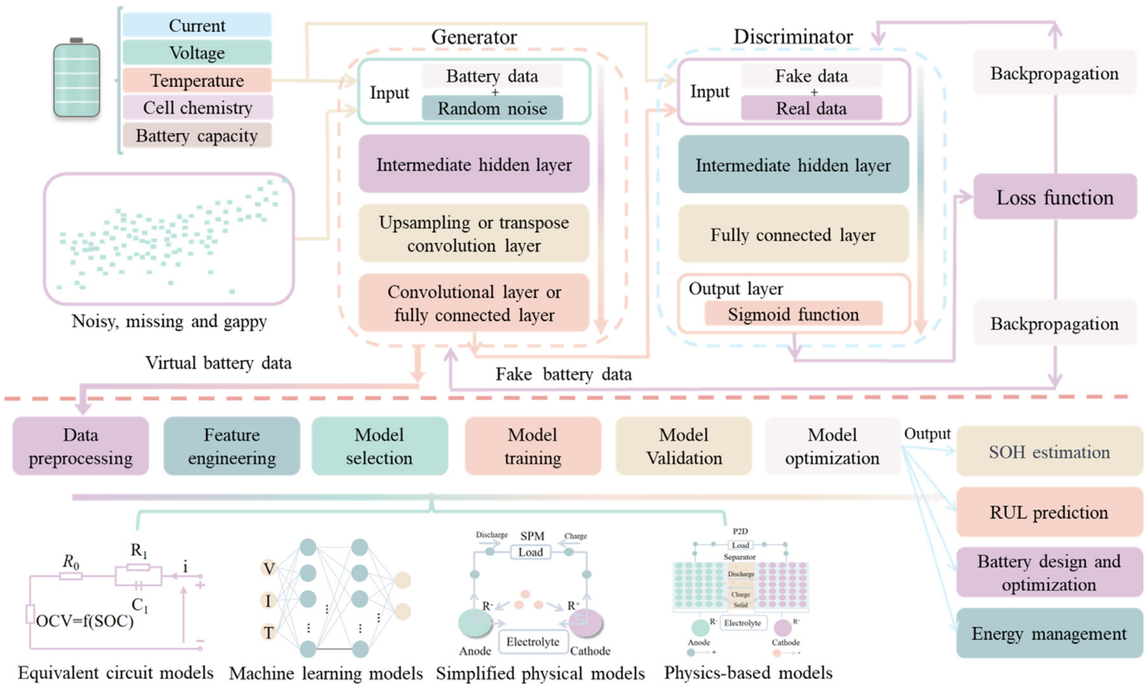

Fig. 4. Generative adversarial networks architecture for battery health prognostics.

from the real data distribution, the discriminator should classify it as real; otherwise, it should classify it as fake. The training process of GANs necessitates the concurrent optimization of two interconnected networks: a generator and a discriminator. This process involves the use of authentic data from a dataset and fabricated data produced by the generator during training. The discriminator, akin to traditional deep neural network classifiers, aims to distinguish between authentic and fabricated data.

In essence, GAN training is an intricate dance between the generator and the discriminator, with the former striving to generate more realistic outputs and the latter aiming to better distinguish real from fake. This iterative process refines both networks over time, enhancing the synthetic data generation capabilities. Here, we elucidate some of the salient benefits of employing GANs in this niche area.

(a) Data augmentation: Batteries, given the myriad of conditions under which they operate, often present with non-uniform data distributions. GANs, being generative models, can produce synthetic battery data that mimics real-world scenarios. This capability is invaluable for augmenting datasets, especially when specific conditions are underrepresented.
(b) Unsupervised feature learning: GANs can autonomously learn intricate features from battery data without requiring labeled instances. This becomes crucial when deriving insights from vast amounts of unlabeled battery operation and performance data.
(c) Modeling complex distributions: Battery health can be influenced by multifaceted and nonlinear factors. GANs excel in capturing complex data distributions, which is pivotal in accurately modeling the intricate relationships influencing battery health.
(d) Noise reduction: Given their adversarial framework, GANs can be trained to distinguish genuine battery data patterns from noise. This is particularly beneficial when dealing with raw battery data, which might be corrupted by noise or other anomalies.
(e) Predictive capacity enhancement: When integrated with other deep learning architectures, GANs can enhance the predictive accuracy for state-of-charge (SoC) and state-of-health (SoH) estimations by providing refined, high-quality data inputs.
(f) Real-time prognostics: GANs, once trained, can generate predictions swiftly, which is essential for real-time battery health monitoring and timely intervention.

In practical applications, GANs predominantly focus on the parameter space of the generator function, creating a discernible gap between theoretical models and their real-world implementations. Such disparities prompt questions about the relevance and utility of theoretical frameworks when it comes to tangible GAN deployments. Additionally, the realm of GANs is a hotbed of active research, evolving at a breakneck pace. This swift progression stems from continuous refinements in GAN algorithms, advancements in the foundational deep learning methodologies, and upgrades in both software and hardware platforms. Given this rapid evolution, sustaining a cutting-edge GAN implementation poses challenges, as the benchmark for 'best practices' is incessantly shifting.

2.5. Reinforcement learning

Reinforcement learning, a framework that allows agents to optimize their actions in an environment based on received rewards, offers a strategic way to integrate machine learning models with neuroscientific methodologies. A notable application of reinforcement learning is its use in the development of AlphaGo [45]. Deep reinforcement learning merges the capabilities of deep learning and reinforcement learning to address challenges in developing models that can autonomously learn and adapt. By taking advantage of the robust representation learning properties inherent in deep learning, it provides a mechanism for an agent to understand and interact with its environment more effectively [46–48]. As the agent acts, the environment responds, transitioning states based on established reward functions, enabling the agent to iteratively

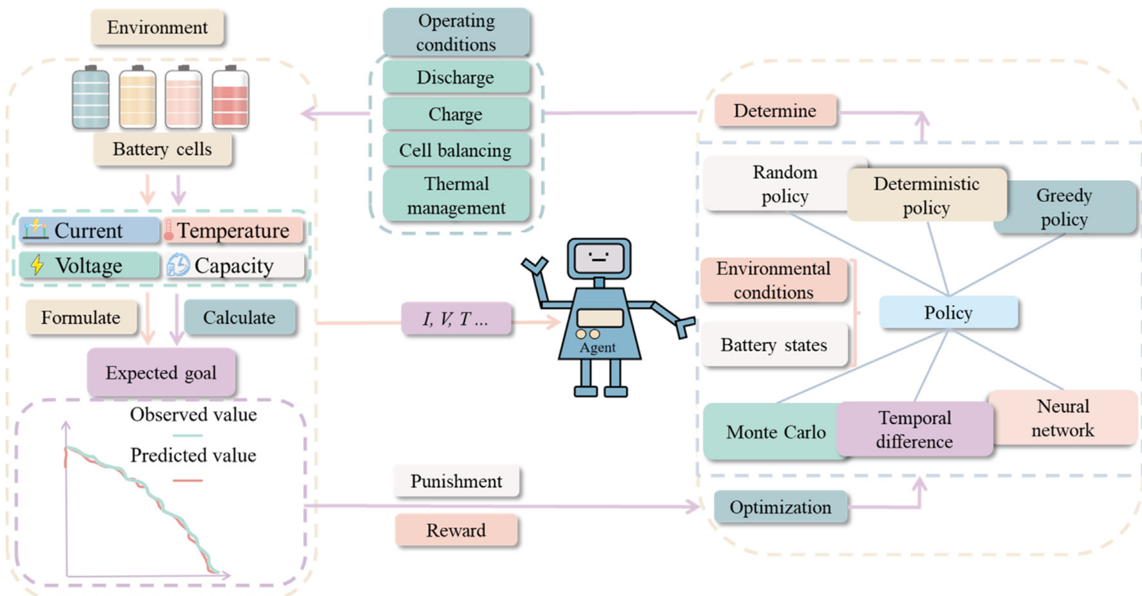

Fig. 5. Reinforcement learning architecture for battery health prognostics.

Table 4
Key components of reinforcement learning.

Term	Definition
Agent	An entity that takes actions and makes decisions to achieve certain goals within an environment.
Environment	The setting or context in which the agent operates. It responds to the agent's actions by changing its state and providing rewards.
State	The set of variables that describe the current condition or status of the environment. It is the context in which the agent makes decisions.
Action	The set of options or moves that the agent can execute. Actions are the means by which the agent influences the environment.
Policy	A decision-making strategy or mapping that tells the agent what action to take under what circumstances or states.
Reward	A numerical feedback signal that the agent receives as a consequence of its actions. It indicates how well the action aligns with the agent's objectives.
Return	The sum of rewards accumulated over a sequence of steps or an episode, possibly with a discount factor applied to future rewards.
Action-value function	A function estimating the expected long-term returns from taking a particular action in a specific state, reflecting the desirability of that action in that state.
Discount factor	A scalar between 0 and 1, representing the preference of the agent for immediate rewards over future rewards. The closer it is to 0, the more short-sighted the agent is.
Model-free	A strategy where the agent learns how to act by directly estimating value functions or policies, without attempting to model the environment.
Model-based	A strategy where the agent attempts to learn a model of the environment's dynamics, and uses this model for decision-making and planning.
Bellman equation	A central equation in reinforcement learning which expresses the relationship between the value of a state and the values of its successors. It forms the basis for various reinforcement learning algorithms.
Deep reinforcement learning	Combines deep learning and reinforcement learning, using neural networks to represent complex functions for high-dimensional state or action spaces.

learn optimal strategies. When combined with deep neural networks (DNN), this methodology excels at discerning actions that will lead to the highest cumulative rewards in the future, even when starting from a point of minimal domain knowledge [49].

Within the realm of reinforcement learning (Fig. 5), an autonomous agent, empowered by deep learning algorithms, continuously monitors the state of its environment. The agent interacts with its environment by executing an action. This interaction catalyzes a transition to a subsequent state, contingent on the prevailing state and the selected action. Here, the state embodies an all-encompassing snapshot of the environment, encompassing all requisite information, including sensor readings and actuator statuses, essential for the agent's decision-making. Table 4 provides an overview of the fundamental components in reinforcement learning.

By integrating reinforcement learning with deep neural networks (DNN), one can achieve exceptional performance on a range of challenging tasks by selecting actions to maximize future rewards, even with limited prior knowledge. Below, we outline the key benefits of harnessing deep reinforcement learning for modeling and predictions in battery health.

(a) Adaptive decision-making: Batteries operate under a plethora of conditions, which constantly vary based on usage, environment, and age. Deep reinforcement learning models, by their nature, can adapt to new information, enabling them to make optimal decisions regarding battery usage and maintenance, even as conditions change.
(b) State estimation: Deep reinforcement learning is inherently designed to estimate and act upon states in an environment. This makes it uniquely positioned to provide accurate estimations of a battery SOC and SOH, pivotal metrics in battery health monitoring.
(c) Long-term optimization: Reinforcement learning's focus on cumulative rewards allows deep reinforcement learning models to strategize for long-term battery health. Instead

of short-term gains, such as immediate charge speed, deep reinforcement learning can optimize for actions that enhance overall battery lifespan.
(d) Real-world simulation and training: Deep reinforcement learning can be integrated with battery simulators, allowing the models to be trained in varied, realistic scenarios without risking actual equipment. This aids in preparing the model for a wide range of real-world conditions.
(e) Data efficiency: It can often make effective decisions based on fewer data points, reducing the need for vast amounts of training data. This is especially useful when high-fidelity battery data is scarce or expensive to procure.
(f) Continuous learning: As battery technologies and usage patterns evolve, deep reinforcement learning models can continue to learn and adapt, ensuring their predictions and decisions remain relevant over time.

Deep reinforcement learning has been impressively successful in solving autonomous control problems across diverse fields, including video games, nuclear fusion reactions, and stratospheric balloon navigation. However, practical implementations of reinforcement learning often reveal some inherent challenges and limitations. (a) Dependence on Pre-Programmed Knowledge: It's been observed that to make reinforcement learning work effectively in real-world applications, it is often necessary to supplement the fundamental algorithm with additional knowledge that is pre-programmed into the system. This means that rather than learning solely from the environment, some prior human knowledge and insights need to be injected into the system to achieve practical performance. (b) Reduced Autonomy and Increased Human Effort: The necessity for incorporating pre-programmed knowledge makes the reinforcement learning system less autonomous as it relies on human-designed components. Moreover, it increases the required human effort and insight which can be expensive and time-consuming. (c) Computational Demands and Real-time Constraints: Different reinforcement learning applications have varying computational demands and real-time constraints. For example, a juggling robot needs to make very fast decisions in a short time but has more time between trials for computations. On the other hand, a mobile robot that is supposed to operate for hours requires a different computation regime. Adapting reinforcement learning algorithms to these varying computational demands and real-time constraints is challenging.

3. Deep learning techniques in battery health prognostics

Deep learning, a subclass of machine learning, offers multi-level representation learning by capturing data abstractions through several layers. These hierarchical representations are built by composing simple, nonlinear modules that transform raw data into progressively more abstract forms. As one progresses through these layers, they allow the model to focus on the crucial features of the data, deemphasizing any noise or irrelevant variations [21]. Unlike traditional approaches where features are handcrafted, deep learning models autonomously learn them directly from the data. Deep learning's strength in discerning intricate patterns within high-dimensional data makes it a formidable tool in battery health prognostics. Its application goes beyond general machine learning tasks, providing nuanced insights into battery health and performance 6. In this section, we explore seminal works that harness deep learning for battery health management, positioning it as an invaluable tool in an era characterized by big data and the Internet of Things (IoT). Our discussion pivots on the opportunities and challenges deep learning presents within battery health management, as illustrated in Table 5. We delve into the merits and demerits of various deep learning techniques in the context of battery technologies, promoting a nuanced understanding of their practical applications and potential enhancements. Harnessing the power of deep learning can revolutionize battery health prognostics, setting the stage for innovations in battery technology.

3.1. Transformers for long-sequence battery prediction

In the domain of machine learning, the emergence of Transformer networks [32] represents a paradigm-shifting breakthrough. Due to their impressive achievements in various tasks, Transformer models have drawn significant attention from the time series analysis community [36,37]. By utilizing self-attention mechanisms and positional encoding strategies, Transformers excel at capturing both short-term and long-term correlations within sequences. This proficiency makes them especially potent for time series modeling and forecasting.

Recently, the application of Transformer-based models, celebrated for their superior efficacy across diverse machine learning endeavors, has expanded to the study of the complex electrochemical dynamics inside batteries. Equipped with self-attention mech-

Table 5
Five techniques for enhancing deep learning-based battery health prognostics discussed in this study.

Method	Applications	Advantages	Considerations
Transformer	Predicting battery state-of-charge Estimating state-of-health Predicting remaining useful life	Capable of capturing long-term dependencies Efficient in handling large datasets High accuracy	Computationally expensive Requires large datasets for training Complex to interpret
Transfer learning	Accelerating model training by reusing pre-trained models Improving performance in data-scarce environments	Reduces training time- Requires fewer data samples Can leverage knowledge from similar tasks	Requires relevant pre-trained models Fine-tuning can be tricky
Physics-informed learning	Modeling of degradation mechanisms Thermal and electrochemical state estimations Safety monitoring	Incorporates physical laws for more reliable predictions Can perform well with less data	Requires domain expertise Can be computationally expensive
Generative adversarial networks	Data augmentation for small datasets Synthetic generation of battery operational profiles for testing and simulation	Can generate realistic data samples Useful for improving model performance with limited data	Training can be unstable Mode collapse issues Hard to tune
Deep reinforcement learning	Optimizing battery charging and discharging schedules Battery maintenance policy optimization	Can optimize decisions over time Able to adapt to changing environments	Sensitive to reward function design Requires significant training data Can be computationally expensive

anisms and a multi-layered architecture, these models are uniquely positioned to capture long-term dependencies and nuanced patterns. This makes them adept at analyzing the multi-faceted interactions and underlying processes characterizing battery systems. For instance, through a small fragment of voltage versus current data, Transformer-based deep learning was capable of forecasting the entire voltage discharge curve under a broad spectrum of operational conditions [50]. The encoder-decoder neural network design was proficient at distinguishing between different aging states; the encoder gleans physics-oriented information from observations, and the decoder forecasts the end-of-discharge point. The study discovered a robust correlation between the latent representation (drawn out by the encoder from the observations) and degradation parameters (like lithium inventory loss and resistance increase), which was backed by empirical evidence, physical comprehension, and mathematical validation of the learning algorithm. The innovative network designs—referred to as Dynaformer—act as adaptable tools for understanding complex battery dynamics under widely fluctuating operating conditions. They need only a minimal volume of real or field data to calibrate the model.

To address the complexities associated with data processing, one study designed a robust prognostic model package [51] from NASA's Ames Research Center. This package can generate a significant amount of simulated charge-discharge data, founded on an electrochemistry-centric battery aging model. Crucially, this model prioritizes physics and electrochemistry when forecasting the battery's end-of-discharge, incorporating factors such as equilibrium potential and various overpotentials. Furthermore, the study expedited the training process and optimized the methodology to adapt to real-world battery data, which was generated under stringent test conditions by NASA Ames. This adaptation was accomplished through the integration of a pre-trained model using synthetic data and the application of transfer learning.

Looking towards the future and drawing inspiration from recent advancements in AI research, particularly in the realm of language models and Transformer architectures, a potentially fruitful direction emerges in the field of battery health prognostics. The central idea envisioned involves pre-training a Transformer model by harnessing extensive open data sets, leveraging its robust capabilities, such as managing large-scale data and capturing long-range dependencies, to build a baseline model. Subsequently, efficient few-shot learning strategies are proposed to fine-tune the baseline model for specific battery health tasks. The usage of few-shot learning techniques could allow the model to swiftly adapt to new data with limited labeled samples—a pivotal factor when obtaining comprehensive labeled data is challenging or costly. The broader objective of this envisioned research is to achieve a more refined understanding of battery health prognostics, potentially leading to improved predictions and enhanced management of battery lifetimes. This could catalyze advancements in energy storage technology by extending operational lifespans and enhancing overall battery performance. However, potential challenges must be anticipated, particularly in terms of data quality, model interpretability, and the model's generalization capabilities across diverse battery chemistries and usage patterns. Developing strategies to address these challenges will significantly influence the ultimate impact of this research and pave the way for meaningful progress in the field of battery health prognostics.

The study also substantiated that Transformer networks are well equipped for predicting the RUL of batteries [52]. However, real-world model performance can be greatly affected by the uncertainties arising from noise in sensor data. To counter this issue, a denoising auto-encoder was incorporated into the prediction networks. This addition enhanced the system's robustness in learning representations from somewhat tainted inputs by reconstructing the loss function [53]. The system, which merges the denoising auto-encoder with single encoder-based Transformer networks, offers greater flexibility in addressing real-world physical problems with noisy data, due to its comparatively simple sequential implementation.

The self-attention mechanism emerges as an indispensable tool, predominantly attributed to its adeptness in extracting crucial holistic information from massive volumes of data. The spatio-temporal transformer model (Fig. 6), harbors inherent advantages 8. Notably, its integration of incremental (temporal) alongside multi-dimensional (spatial) data presents potent instruments for adeptly learning the intricacies of nonlinear systems that are characterized by multiple scales and physical interactions, and display diverse degradation trajectories. This markedly amplifies the model's competence in predicting cell states across a spectrum of aging processes and operational environments, thereby expanding the horizons of what can be achieved in this arena. To harness the capabilities of Transformer models, an abundance of unlabeled battery data can be incessantly generated through operational procedures and stored in cloud repositories, eliminating the necessity for laborious manual annotations by engineers for self-supervised inferences. Confronted with vast, unlabeled datasets, self-supervised learning has the potential to instigate ground-breaking innovations, tackling the intricacies of protracted monitoring and diagnostics in multi-scale and multi-physics battery systems in previously uncharted ways. To triumph over these barriers, continued investigations are paramount for the adept extraction of knowledge from historical data, enabling seamless self-learning, and handling the issue of catastrophic forgetting in scenarios involving continuous observations with fluctuating data distributions. This approach significantly lessens the need for supervised training and fine-tuning, making it ideal for analyzing long sequences of time-series sensor data. However, applying self-supervised learning to vast, unlabeled, and complex data sets inherently presents challenges, such as ensuring efficient training, handling non-IID data, and maintaining continuous learning without memory loss [54]. These issues are widespread in deep learning and are particularly salient in lifelong learning contexts [55]. Overcoming these requires persistent research and strategies to mitigate catastrophic forgetting, particularly with non-stationary data in continuous monitoring. Moreover, it's essential to effectively extract insights from historical data, fostering a cycle of self-improvement in continuous learning via self-supervised methods [56].

Transformer has the distinct advantage of reducing reliance on additional supervised training and fine-tuning, which excels particularly in analyzing lengthy sequences of time-series sensor data. Employing Transformer models for battery health prognostics opens up a myriad of opportunities:

While the Transformer model has the marked advantage of lessening dependency on extensive supervised training and fine-tuning, it particularly excels in analyzing extended sequences of time-series sensor data. Applying Transformer models for battery health prognostics brings forth a plethora of opportunities.

(a) Data-driven insights: The ability to extract valuable knowledge from historical data can foster a cycle of self-improvement in continuous learning, particularly when utilizing a self-supervised methodology.
(b) Harnessing open datasets: The vast availability of open datasets can facilitate pre-training the model, thereby reducing the necessity for intensive fine-tuning.
(c) Few-shot learning: Utilizing few-shot learning strategies enables the model to swiftly adapt to new data, even when there's a limited supply of labeled samples.

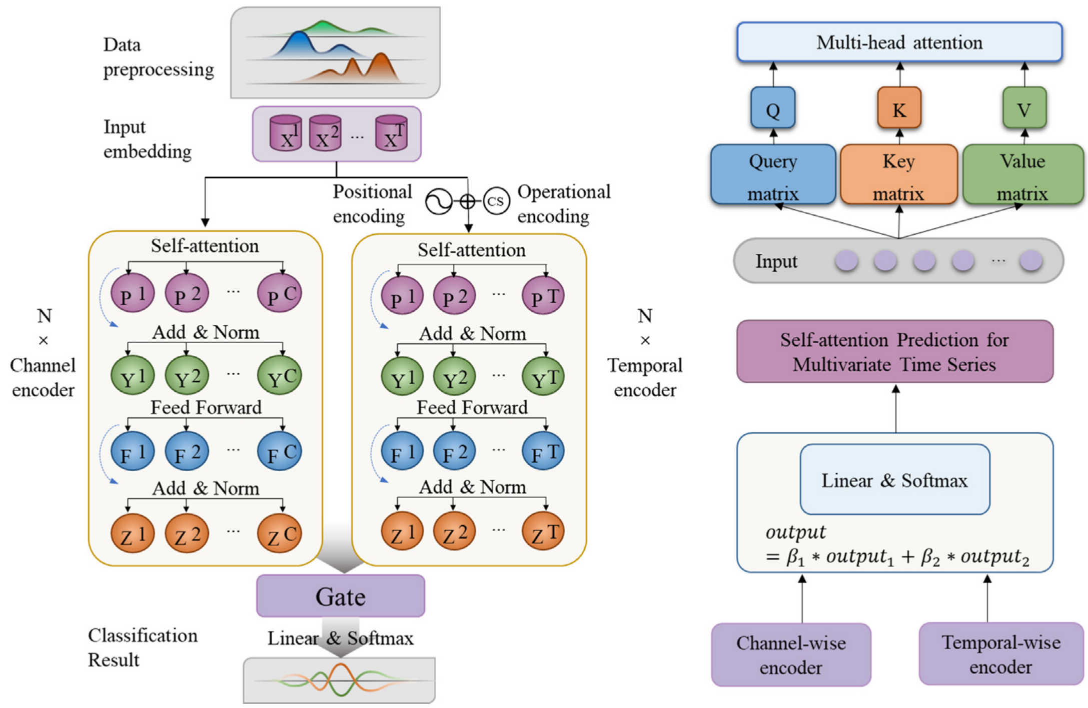

Fig. 6. Spatial-temporal self-attention transformer model. Copyright 2023, MDPI [8].

(d) Improved battery health management: Ultimately, employing Transformer models can lead to more accurate predictions for battery health, which can enhance management practices and extend operational lifetimes.

Nevertheless, implementing this innovative approach presents its own set of challenges, particularly when applied to extensive, complex, unlabeled datasets:

(i) Efficient training: Streamlining the training process, especially when dealing with large and intricate data sets, is a considerable challenge.
(ii) Handling non-IID data: Constructing a resilient model that can handle non-Identically and Independently Distributed (non-IID) data—a frequent occurrence in real-world scenarios—is a significant hurdle.
(iii) Sustaining learning without memory loss: In the context of a self-supervised framework, it is crucial to maintain consistent learning without compromising previously acquired knowledge—this issue is particularly pronounced in ongoing lifelong learning scenarios.

These challenges, ubiquitous across various deep learning domains, necessitate dedicated research initiatives and focused strategies to mitigate the effect of catastrophic forgetting, especially when dealing with non-stationary data distributions in continuous monitoring scenarios.

3.2. Neural networks-based transfer learning for predicting battery health

In the domain of battery health prognostics, transfer learning stands out as a vital tool, particularly for tasks requiring few-shot learning. It seamlessly facilitates the knowledge transfer between diverse task domains. Incorporated within a deep learning framework, transfer learning notably diminishes the demand for exhaustive data labeling specific to batteries. By leveraging and fine-tuning pre-trained models with a carefully chosen subset of battery-related training samples, this technique ensures more effective and efficient prognostics with less reliance on extensive datasets. A recent manifestation of this learning principle is personalized battery health status forecasting employing a transfer learning framework (Fig. 7), composed of an offline pre-training model and an online transfer model [22]. An exhaustive dataset of 77 commercial lithium-ion batteries, featuring over 140,000 diverse cycles, was compiled for the purpose of training and assessing the performance of transfer learning. The deep transfer learning technique, incorporating a convolutional module, a recurrent module, and a pair of fully connected modules, successfully grasped the hidden connection between charge curves and health status for LFP/graphite cells offline. The online model enables real-time prediction of SOH (Ah capacity) and RUL (cycle lives) at any given cycle for varying discharge protocols. This is accomplished by dynamically fine-tuning specific recurrent network layers while maintaining the other modules unchanged. Additionally, a pair of open datasets from Sandia National Laboratory (SNL) [30] and Toyota Research Institute (TRI) [23] were employed to investigate personalized health condition forecasting under different operating conditions and battery chemistries (NMC//graphite).

Fully supervised models frequently encounter difficulties in delivering high-quality performance and generalization without substantial labeled data in the training dataset. Conversely, entirely unsupervised models are usually confined to numerical outlier identification. In the realm of battery diagnosis and prognosis, the existence of noise and the deficiency of labels obscure the demarcation between supervised and unsupervised learning. Hence, the integration of the beneficial attributes from both learning methods into semi-supervised machine learning opens new doors in application fields abundant in unlabeled data. Semi-supervised learning amalgamates the merits of its constituent elements while attenuating their associated shortcomings. Employing semi-supervised learning enables the effective deployment of a vast quantity of unlabeled data, reducing dependence on labor-intensive and extensive labeling efforts.

For instance, the researchers utilized kernel ridge regression and transfer component analysis to establish a semi-supervised transfer learning method for projecting battery health status using historical data [57]. They partitioned the publicly accessible battery dataset from NASA Ames Prognostics Center of Excellence (PCoE) [25] into training and testing sets, choosing labeled cycles from 20 to 60 and cycles from 61 to the end, respectively. The semi-supervised model stands as a potent instrument for prediction when handling limited labeled source data (historical cycles) and large amounts of unlabeled target data (future cycles). Transfer component analysis, a component of a multi-model fusion approach, facilitates domain adaptation in a reproducing kernel Hilbert space employing maximum mean discrepancy [58]. This becomes particularly beneficial when battery degradation behavior alters as the count of charging-discharging cycles escalates. Transfer component analysis adeptly handles noisy data by denoising and discerning latent space to synchronize marginal distributions across source and target domains.

The wealth of publicly available datasets for the health prognostics of lithium-ion batteries holds immense potential. Nevertheless, despite encouraging computational outcomes underscoring the effectiveness of transfer learning for knowledge transmission without exhaustive manual labeling, applying this approach to more intricate operational conditions for battery health prediction remains a formidable task. This difficulty is particularly significant when dealing with datasets exhibiting differences in capacities, chemistries, and cell assemblies.

(a) Adaptability and versatility: The strides in transfer learning have amplified its capability to adapt across a range of unprecedented usage protocols and cell chemistries.
(b) Exploring intrinsic variables: Exploring intrinsic variables can lead to robust models that perform well even under diverse operating conditions.
(c) Capitalizing on sparse data: Sparse data, when leveraged correctly, can be used to generate comprehensive representations.
(d) Innovative frameworks and mathematical methodologies: The development of these can help amalgamate crucial insights, concepts, and discoveries from various domains, including physical mechanisms, domain knowledge, and machine learning, enhancing battery health prognostics.

However, as with any innovative approach, it's not without its challenges, particularly when applied to broad, unlabeled data sets that encompass complex and overlapping scales. The hurdles include.

(i) Limited transfer to "Unhealthy" batteries: The majority of knowledge transfers have primarily focused on "healthy" batteries, leaving a gap when it comes to faulty or problematic cells that commonly encounter dynamic, stochastic loading patterns in real-world scenarios.
(ii) Noisy data and dynamic operating conditions: Transferring knowledge about the progression of dangerous battery failure risks often proves challenging due to noisy data and dynamic operating conditions.
(iii) Diverse aging mechanisms: The vast differences in aging and degradation mechanisms across individual cells pose significant challenges in knowledge transfer.
(iv) Cell-to-Cell variations: The significant discrepancies among individual cells further complicate the process, requiring a comprehensive examination of aging mechanisms and meticulous formulations.

Addressing these challenges will significantly improve the effectiveness of transfer learning in the field of battery health prognostics, advancing our capabilities in managing battery health.

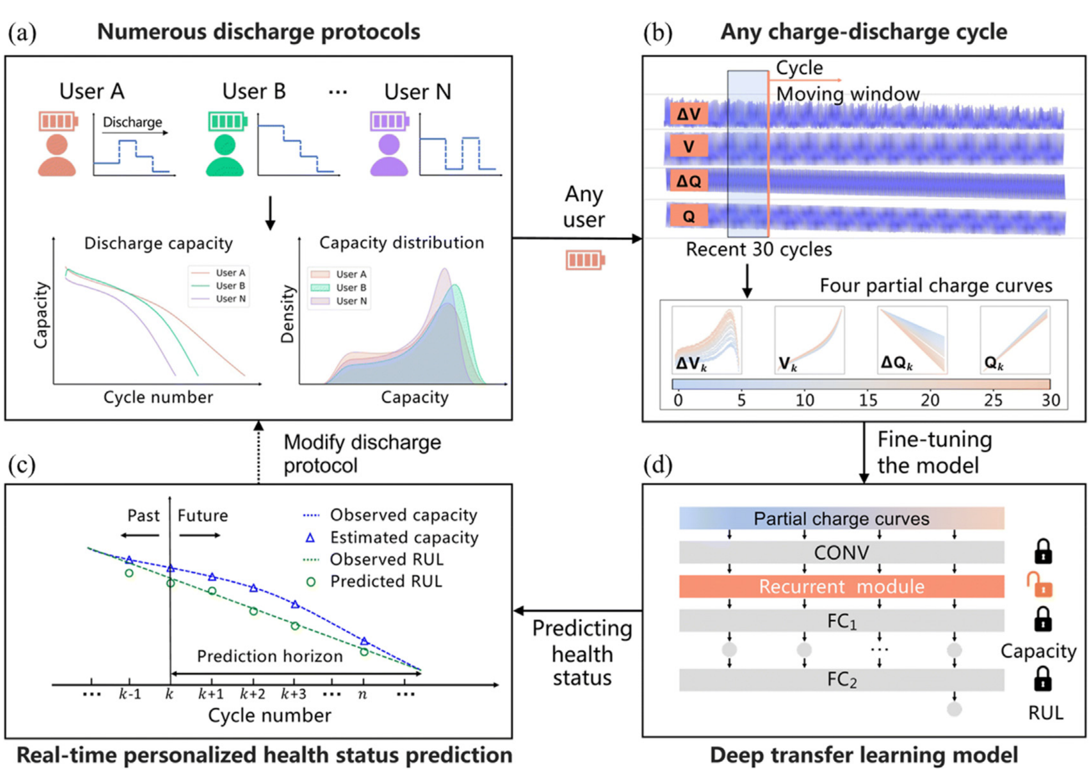

Fig. 7. A transferable deep learning network for forecasting lithium-ion battery health status. Reproduced with permission from ref. [22]. Copyright 2022, Royal Society of Chemistry.

3.3. Physics-informed neural networks by enforcing the physical laws

In the ever-evolving domain of battery health prognostics, the fusion of physics-based insights with computational models stands out as a pioneering approach. Recent strides in physics-integrated learning for battery applications emphasize its remarkable adaptability and its innate capability to merge theoretical constructs with real-world challenges. This synergy between physics and machine learning paves the way for a comprehensive, insightful, and forward-looking framework that can pinpoint and anticipate issues in battery systems. For example, a symbiotic approach that employs PINNs has been introduced for battery modeling and prognostics [59], as shown in Fig. 8. Through the application of order reduction methodologies to the battery model representation and the incorporation of electrochemical constraints within the PINN, scientists at NASA's Ames Research Center have successfully produced precise and physically coherent predictions of voltage discharge curves and battery end-of-discharge (DOD). This model, which synergizes data and physics into Recurrent Neural Networks (RNNs), is competent in one-step-ahead prediction of the discrete state-space representation of ordinary differential equations (ODEs). In this scenario, the Nernst and Butler-Volmer equations were employed to calculate the concentration overpotential and the surface overpotential, respectively. To assimilate historical data, a multilayer perceptron model was integrated into the hybrid network structure, operating under the presumption that the physics and theoretical groundwork are partially known. The flexibility of soft penalty constraints, such as the Redlich-Kister expansion [60], facilitates accommodating missing physics and learning battery dynamics (e.g., non-ideal voltage behaviors influenced by internal resistance and the quantity of accessible Li-ions) that are not apprehended by the physical model.

More recently, one study presents an innovative framework for the health prognosis of lithium-ion batteries, built on an adaptive evolution enhanced PINN [61]. The objective is to seamlessly incorporate physical information into the prognostic model and allow for its adaptive updating. The physical data, derived from both real-time monitoring and multiphysics simulations, informs the training of an LSTM Neural Network-based prognosis model. This integration ensures a more precise health prognosis without compromising efficiency. We introduce a new dynamic sliding window LSTM approach, termed KL-DSW LSTM NN. This method employs the KL (Kullback-Leibler) divergence measure to quantify and assimilate the physical information. Additionally, we've designed an adaptive model evolution technique that strikes a balance: it addresses the long-term overarching trends while also capturing short-term, immediate fluctuations. In another study, the researchers initially lay the groundwork through the SPMT model, adeptly suited for assimilating the physical attributes tied to HGR. Following this foundational step, a marriage between these physical characteristics and a Bidirectional Long Short-Term Memory (BiLSTM) network manifests a robust PINN blueprint dedicated to HGR estimation. To bolster the efficacy of BiLSTM, the Bayesian Optimization Algorithm (BOA) is employed, specifically to pinpoint its optimal hyperparameters. The resultant PINN exhibits a noteworthy proficiency in gauging battery HGR, particularly under the rigorous paradigms of Dynamic Stress Test (DST) and Worldwide Harmonized Light Vehicles Test Procedures (WLTP).

Recent advancements in physics-informed learning have shown promising results in tackling real-world physical challenges, including applications in battery modeling and prediction. One such advancement is the introduction of a hybrid PINN approach. This method combines order reduction techniques on battery model representation and incorporates electrochemical constraints within the PINN. Consequently, this approach can offer precise and physically consistent forecasts of battery voltage discharge curves and end-of-discharge (DOD), as well as one-step-ahead predictions of the discrete state-space representation of ordinary differential equations (ODE).

Another application features physics-informed learning integrated with a multi-fidelity model created for battery SOH prognostics. Here, the degradation mechanism is linked to Solid Electrolyte Interface (SEI) growth on anode particle surfaces. This approach merges mechanical laws into neural networks under Neumann (traction) and Dirichlet (displacement) boundary conditions. This integration allows the automatic update of parameters describing the geometry of voids/inclusions in a differentiable and trainable manner.

Physics-informed learning is a novel approach that seamlessly integrates (noisy) data and mathematical models, employing neu-

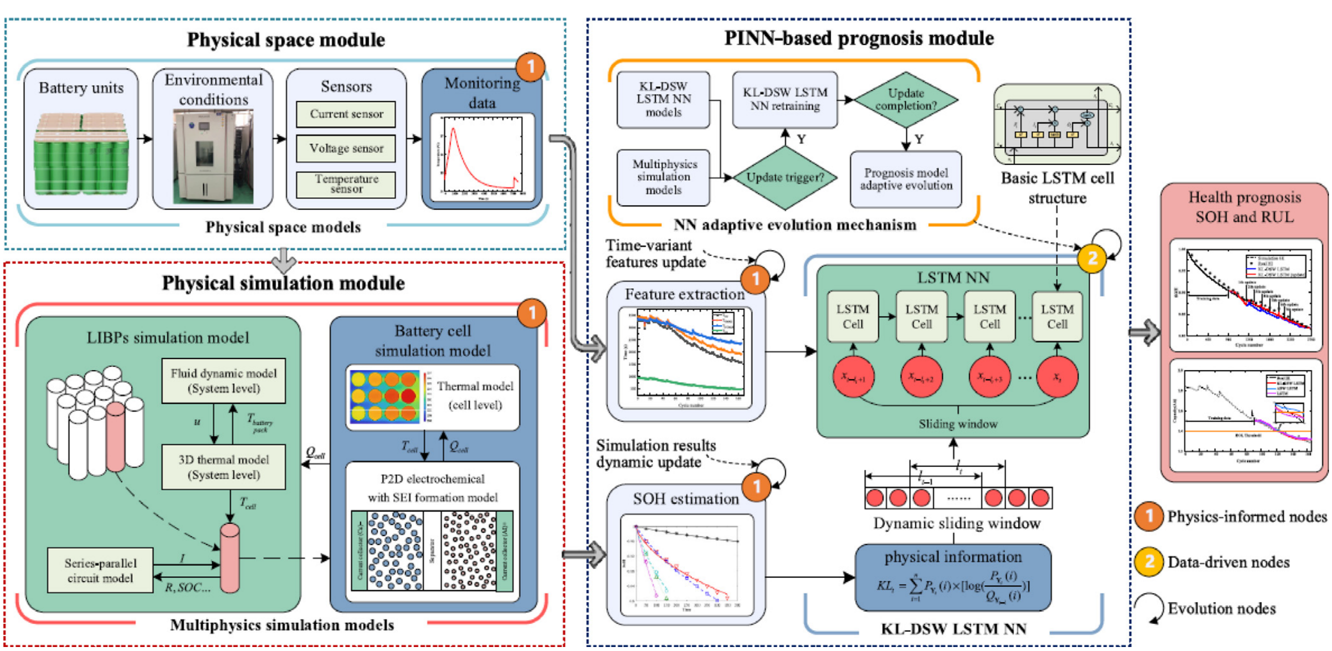

Fig. 8. PINN-based time-variant health prognosis framework. Reproduced with permission from ref. [61]. Copyright 2023, Elsevier.

ral networks or other kernel-based regression networks as its implementation framework. This powerful technique holds great promise as it opens up new possibilities for achieving superior performance in various applications. It offers exciting opportunities for advancing scientific understanding, solving complex battery real-life problems, and achieving remarkable results in diverse aspects of model performance.

(a) Enhanced accuracy: Physics-informed learning can harness empirical, physical, and statistical understanding of a specific predictive task, such as battery health and safety, to boost accuracy.
(b) Improved generalizability: The integration of physics knowledge can help improve the generalizability of models by providing additional, fundamental constraints on model behaviors, which can be especially helpful when the data is scarce or noisy.
(c) Insights into underlying mechanisms: Incorporating physical laws into machine learning can provide valuable insights into the underlying mechanisms of complex systems, offering opportunities to discover new phenomena and drive advancements in the field.

While physics-informed machine learning offers exciting opportunities for battery health condition analysis, it demands a well-thought-out approach to leverage both physics-based knowledge and machine learning capabilities effectively. By addressing these challenges with precision, we can unlock the full potential of this approach for enhancing battery diagnostics and prognostics in practical applications.

(i) Subpar generalization performance: Improper application of physics into machine learning models may lead to subpar generalization, limiting the model's utility across different scenarios.
(ii) Obscure underlying mechanisms: In real-world scenarios like battery failure, the underlying mechanisms, physical principles, and boundary conditions may be difficult to decipher in the continuous space-time domain.
(iii) Integration complexity: The integration of physical knowledge into machine learning models can add a layer of complexity, requiring more sophisticated model architectures and training strategies.

3.4. Generative adversarial networks for data enhancement and prediction

In the dynamic landscape of battery health prognostics, GAN-based models are rising as a paradigm of innovation. Particularly for cell-level battery diagnostics, GANs exhibit unmatched expertise. With their dual-network design that champions both generation and discrimination, GANs adeptly discern subtle patterns and emulate authentic battery behaviors. Paired with their proficiency in producing synthetic data, they provide a robust framework, paving the way for in-depth insights and precise predictions on battery health trajectories. Taking cues from interpretable representation learning facilitated by information maximizing generative adversarial networks (infoGAN) [62], a convolutional recurrent generative adversarial network was engineered for data-driven RUL) forecasting [63]. The generator, a two-channel fusion model, encapsulates the progress of a multivariate time-series system across spatial and temporal dimension s by amalgamating CNN and LSTM. CNN strata capture spatial features of the sequence, whereas LSTM strata understand temporal correlations between past and future cycling data. The discriminator assesses these time-series data by juxtaposing them with authentic battery data from NASA Prognostics Center of Excellence (PCoE) [25]. Through continuous interplay between the generator and the discriminator, the GAN model engenders lifelike temporal sequences. Crucially, incorporating the generated data into the RUL estimation model yields predictions with greater accuracy than models trained exclusively on scarce real battery data, leading to considerable savings in generating end-of-life cycling data.

In a parallel study, one research endeavor used a synergistic algorithm that married GAN-Conditional Latent Space (CLS) with BiLSTM to augment the prediction efficiency of lithium-ion rechargeable battery states [64]. In this scheme, the GAN-CLS algorithm is used to create images from input label descriptions, while the LSTM element facilitates sequence predictions with a higher degree of accuracy than traditional Recurrent Neural Networks (RNNs). The amalgamation of these two methods resulted in notable time efficiency and improved prediction accuracy, underscoring the potency of this approach for battery state prediction. In another research, a GAN-based approach was proposed for the purpose of data augmentation, with the intent to broaden sparse datasets and thus enhance the learning capabilities of Neural Networks used for SOC/SOH estimation [65]. The efficacy of this method was tested on two publicly accessible battery datasets, yielding a high degree of diversity in the battery profile data. Establishing an accurate SOH estimation through data-driven methods is fraught with challenges, primarily due to the difficulties encountered in real-world measurements, as well as the potential for noise or sensor failure. To counter these hurdles, a research study proposed an innovative regression GAN to create a general model for batteries of the same specifications [66]. This model utilizes a generator to develop auxiliary training samples that mirror real samples but exhibit distinct distributions. Concurrently, the discriminator component learns the distribution of real samples to identify anomalous aging indicators. This novel approach outperformed other models in prediction performance.

The utilization of GANs for battery health prognostics presents both intriguing opportunities and substantial challenges. Their potential in this realm is primarily derived from their ability to generate battery cycling data based on estimated probability distributions, which could be instrumental in predicting battery health under both standard and extreme operating conditions.

Opportunities:

(a) Microstructural data generation: GANs have been used effectively to generate representative microstructural data for battery electrodes, which can contribute significantly to understanding battery health and potential failures.
(b) Predictive modelling: The ability of GANs to learn generative models of complex data distributions could enable them to predict calendar aging of batteries accurately.
(c) Defect detection: The application of GANs extends to the detection of cracks and other structural defects in batteries, which can extend battery life.
(d) Estimating remaining useful life (RUL): GANs have demonstrated potential in estimating the RUL of batteries, an important aspect of battery health management.
(e) Data augmentation: GANs can overcome the limitations of data-driven battery safety assessment by generating statistically realistic samples, expediting the discovery and understanding of battery health.

Challenges:

(i) Model evaluation: Evaluating the effectiveness of generative models, including GANs, can be challenging due to the lack of specific target guidance in their output generation.

(ii) Arbitrary predictions: When GANs are applied to samples outside of the training set, the experiential learning-based decision-making can result in arbitrary or inaccurate predictions due to a lack of suitable evaluation metrics.
(iii) Need for algorithmic tools: For GANs to be trusted in this field, the development of algorithmic tools is needed to process training examples and extract relevant high-dimensional features effectively.
(iv) Training difficulties: Training GANs involves challenges such as averting mode collapse, enhancing model robustness, and developing effective model assessment measures.
(v) Unverified forecasting ability: The capability of these models to predict battery health under varying operational conditions using generated data remains largely untested, which is a critical gap in their application.

In conclusion, while the adoption of GANs in battery health prognostics is at a nascent stage, their potential for further development and application is considerable. Overcoming the inherent challenges in the implementation of GANs could significantly enhance their ability to predict and manage battery health effectively.

3.5. Intelligent battery management through deep reinforcement learning

Deep reinforcement learning, with its demonstrated capabilities, holds significant promise in the realm of battery health management. This approach can be adeptly used to fine-tune charging and discharging protocols, implement adaptive thermal management, and provide precise state-of-health estimations. Such optimizations ensure both extended battery longevity and optimized health-conscious management. Embracing deep reinforcement learning in the domain of batteries can lead to more sophisticated and autonomous battery management system (BMS), adapting in real-time to varying conditions and user demands.

Within the deep reinforcement learning framework, the environment and the agent are two key components. In the context of battery health prognostics—specifically in optimizing fast-charging protocols—the BMS is the agent, making decisions based on the rewards of potential actions by interacting with the environment, i.e., the battery [67]. A pseudo-two-dimensional electrochemical model, the Doyle-Fuller-Newman model [68], predicts the evolution of multiphysics battery systems, capturing macroscopic physics such as lithium concentration in the solid and electrolyte, solid electric potential, and more. Deep Deterministic Policy Gradient (DDPG)-based reinforcement learning has shown effectiveness in managing continuous state and action spaces, thereby improving safety under fast-charging protocols. Derived from DDPG, a recent study addresses energy management in hybrid electric buses using a twin delayed deep deterministic policy gradient (TD3)-based strategy, tailored to minimize energy consumption and prolong the energy storage system's life by considering battery health [69] (Fig. 9). A key feature is the construction of a precise driving cycle through a data-driven approach, simulating a specific bus route for accurate operational cost assessment. The TD3-based strategy seeks an equilibrium between fuel consumption and battery degradation to reduce overall expenses. Comparisons with other advanced strategies, such as DDPG and Double Deep Q-learning, were conducted, demonstrating the TD3-based approach's effectiveness in realistically simulating traffic conditions and efficiently reducing operational costs while extending battery life.

The inevitable structural degradation and performance decline of batteries over their operational life necessitate an exploration of how data-driven techniques can support health-conscious battery energy management. Recent research points towards the potential of deep reinforcement learning in this area, utilizing merely time-series data from the BMS such as voltage, current, and temperature. For instance, deep reinforcement learning has demonstrated potential in forecasting the progression of nonlinear battery systems grounded in electrochemical model parameter calibration [70]. This calibration of parameters is approached as a tracking problem, modeled through a Markov decision process [71]. The electrochemistry-centric model established by NASA's Ames Research Center [72] is crucial to the triumph of reinforcement learning in this domain, as it accurately captures electrochemical procedures and aging impacts. Lyapunov-based maximum entropy deep reinforcement learning presents tools for instructing an agent to learn intricate electrochemical behavior through trial-and-error interactions with a dynamic environment. Comparative research has demonstrated that this framework yields superior accuracy relative to Kalman-based filter approaches and presents stronger generalization capacities than supervised learning methods, all without depending on ground truth information.

Despite the commendable advancements achieved by deep reinforcement learning in real-world scenarios, there exist substantial challenges and limitations, particularly when applied to physical problems that involve uncertain or missing parameters. When applied to batteries and materials, these challenges underscore the necessity for an integrated approach that combines reinforcement learning with neural networks, facilitated by knowledge from robust physical models. Nonetheless, reinforcement learning also offers significant opportunities, particularly in battery health prognostic scenarios.

(a) Robust decision-making: In battery health management, reinforcement learning frameworks can play a pivotal role in decision-making, such as optimizing fast-charging protocols where an agent like the BMS interacts with the battery environment.
(b) Improved simulation models: The use of reinforcement learning has proven effective in developing improved simulation models, such as the pseudo-two-dimensional electrochemical model known as the Doyle-Fuller-Newman, which models the evolution of multiphysics battery systems.
(c) Effective use of continuous state and action spaces: The deep deterministic policy gradient (DDPG), a variant of reinforcement learning, demonstrates potential in managing continuous state and action spaces, updating control policies, and minimizing safety hazards during fast-charging.
(d) Potential for transfer learning: Reinforcement learning could utilize transfer learning, leveraging knowledge from one context and applying it to another. This strategy could alleviate the exploration-exploitation conundrum and foster the development of more potent reinforcement learning systems.

In conclusion, while the application of deep reinforcement learning in battery health prognostics presents notable challenges, its potential advantages make it a worthwhile area for continued research and development. To maximize the benefits of reinforcement learning in this field, efforts should be directed toward developing innovative strategies to mitigate its limitations, as following.

(i) Uncertain or missing parameters: Reinforcement learning applications can struggle when dealing with physical problems that are characterized by uncertain or missing parameters. This issue necessitates a learning system capable of understanding objects and conducting systematic reasoning across large spatial and temporal scales.

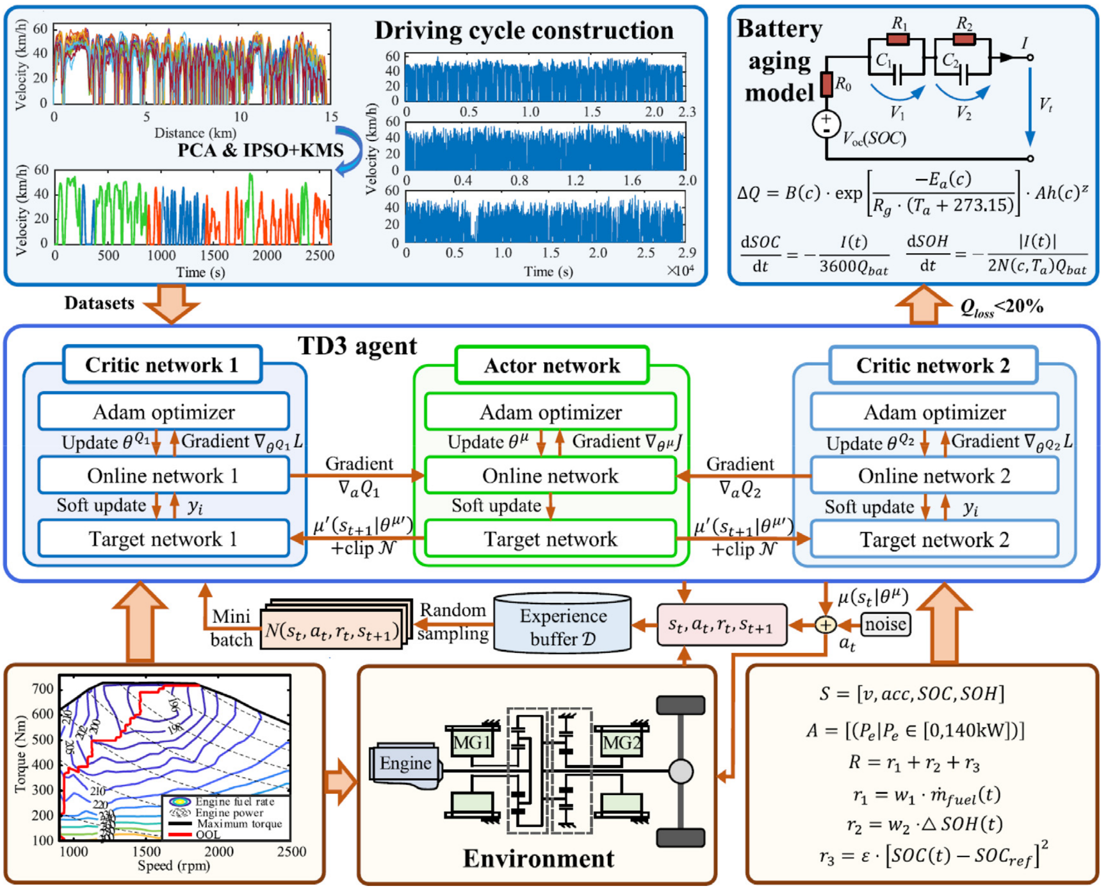

Fig. 9. The framework of the battery health-aware and naturalistic data-driven energy management by leveraging the TD3 deep reinforcement learning algorithm. Reproduced with permission from ref. [69]. Copyright 2022, Elsevier.

(ii) High data demands: Reinforcement learning typically requires a large amount of data, requiring numerous interactions for efficacious learning. This requirement might pose a challenge when data collection is resource-intensive or logistically difficult.

(iii) Exploration-exploitation trade-off: Reinforcement learning faces the challenge of balancing between utilizing known information (exploitation) and seeking new knowledge (exploration).

(iv) Integration with systematic reasoning: A significant limitation is the difficulty of integrating systematic reasoning across large spatial and temporal scales, a requirement for addressing complex real-world issues.

(v) Seamless integration with neural networks: While the combination of reinforcement learning with neural networks is essential, achieving this integration is a challenging task that necessitates the equipping of AI agents with foundational knowledge derived from physical model formulations.

4. Openly shared battery cycling dataset

The convergence of open data accessibility, simplified automation of materials simulations, and machine learning has effectively ushered computational materials science into a new era. Examples of successful data sharing initiatives in various scientific sectors serve as benchmarks and shape our vision for an open scientific discourse and data exchange within the battery field. A more open science environment and enhanced data exchange will add further value to all facets of battery research.

Currently, a substantial portion of the data derived from battery research is inaccessible to the broader scientific and technical communities. Often, battery solutions recommended to customers are based on skewed and significantly incomplete information. These deficiencies usually come to light in the technical and research community when safety issues surface with regards to battery technology or other energy storage mechanisms. Previous instances of battery health prognositcs have underscored the importance of public access to exhaustive battery research data for a thorough comprehension of battery safety and performance.

Sharing of battery research data is not only crucial for product safety but also for scientific progression. As science thrives on collective knowledge, constantly building on shared ideas, it's critical in the digital age to improve collaboration methods as open access to data becomes standard practice in most scientific disciplines. In recent years, some research organizations and universities have openly shared their test and cycling data (Table 6), which can be freely downloaded online through their official or designated websites [23–30]. In examining aging profiles, most datasets primarily deploy the CC-CV (constant current-constant voltage) charging and CC (constant current) discharging methods. By promoting open access to battery research data, we spur innovation through the harnessing of varied expertise and the encouragement of collaborative endeavors. This transparency not only optimizes the return on investments but also champions independent validation, reinforcing the integrity of the scientific method. Moreover, by equipping educational establishments with tangible, real-world data, we bolster public confidence in scientific research, laying the foundation for a self-sustaining cycle of perpetual progress.

Table 6
Open battery lab test and cycling data.

Institution	Battery chemistry	Amount	Cells capacity	Available online
Toyota/Standard/MIT	Cylindrical LFP	124 192	1.1 A h	https://data.matr.io/1/
NASA	Cylindrical LCO	28	2.1 A h	https://ti.arc.nasa.gov/tech/dash/groups/pcoe/prognostic-data-repository/
Oxford	Pouch NCA	8	740 mA h	https://howey.eng.ox.ac.uk/data-and-code/
University of Cambridge	Coin cells	88	35 mA h	https://zenodo.org/record/6645536#.Y5YKgXbMJD8
University of Maryland-CALCE	Pouch and prismatic LCO	43	2 A h & 1.1 A h &1.35 A h	https://calce.umd.edu/battery-data
Huazhong University of Science and Technology	Cylindrical LFP	77	1.1 A h	https://data.mendeley.com/datasets/nsc7hnsg4s/2
Sandia National Laboratory	NCA, NMC, and LFP	86	1.35 A h & 2.8 A h & 0.74	https://www.batteryarchive.org/snl_study.html

5. Software and hardware for training deep learning techniques

To effectively harness the power of deep learning techniques—including Transformer models, transfer learning, physics-informed machine learning, generative models, and reinforcement learning—one should judiciously leverage the strengths of established machine learning libraries. TensorFlow [73] and PyTorch [74] emerge as prime contenders, given their extensive functionality and widespread adoption among researchers and practitioners. Moreover, the landscape of deep learning has been enriched by an array of specialized software libraries specifically engineered to streamline the training process, which, in turn, has been instrumental in the field's meteoric progression (Table 7). However, the efficacy of deep learning algorithms is not solely dependent on the choice of software; the selection of suitable hardware is equally vital. Deep learning models often involve intricate computations and demand substantial processing power for training. State-of-the-art hardware can vastly reduce training times and facilitate more complex models and experimentation. Table 8 delineates a selection of hardware options commonly employed for training deep learning models, each with its distinct set of attributes that cater to different requirements and use cases.

When making a choice of hardware, it is important to consider factors such as processing power, memory capacity, and parallel processing capabilities. Additionally, given the dynamic nature of deep learning research, it is advisable to stay abreast of new developments in both hardware and software domains to make informed choices that maximize performance and efficiency in training deep learning models.

6. Outlook

The future of battery health prognosis holds tremendous potential, with substantial advancements made in recent years. However, current research is still in its infancy, primarily focusing on RUL prediction under predefined conditions. Four critical directions (Fig. 10) are ready for more in-depth exploration and growth. (a) Explainable machine learning: Progress in this field can lead to the development of models that offer understandable insights into their decision-making mechanisms, enhancing transparency and building trust in RUL predictions. (b) Robustness and generalization: The creation of models that excel across a wide variety of conditions and battery types can form a more robust and adaptable predictive framework. (c) Data and model fusion: Merging diverse datasets and incorporating multiple prognostic models can bolster predictive accuracy and provide more exhaustive insights (d) Cooperation between academia and industry: Reinforcing the bonds between academic research and industrial applications can speed up the transition of groundbreaking predictive technologies into practical engineering applications.

Table 7
Software specifically designed for deep learning-based battery health prognostics.

Technique	Software options	Advantages in battery health prognostics	Considerations and challenges
Transformer model	TensorFlow PyTorch OpenNMT Keras	Excellent at capturing sequential relationships in battery data. Efficiently handles large datasets to uncover intricate patterns.	Necessitates ample training data to excel. Computationally intensive, which might not be ideal for time-sensitive applications.
Transfer learning	TensorFlow PyTorch Keras Fast.ai	Expedited model training through the utilization of pre-existing models. Particularly advantageous where labeled battery data is scarce.	Adaptation and calibration may be imperative for specialized battery scenarios. Domain discrepancies can impinge upon model efficacy.
Physics-informed Machine learning	TensorFlow PyTorch Julia	Enriched model fidelity through the incorporation of underlying physical principles. Possible minimization of data requisites by employing physical insights.	Physic-based integration can be arduous and intricate. Mandates proficiency in battery physics.
Generative models	TensorFlow PyTorch Keras GANLab	Facilitates data enrichment in cases of limited battery datasets. Viable for anomaly detection pertinent to battery health.	Model training may prove to be obstinate. The authenticity and diversity of synthesized data may be inconsistent.
Reinforcement learning	TensorFlow PyTorch OpenAI Gym RLlib	Optimal for devising and fine-tuning policies for battery management. Exhibits adaptive behavior concerning changes in battery characteristics.	Extensive training datasets are essential. Sensitive to hyperparameters and necessitates judicious exploration strategies. Complexity of real-world deployment.

Table 8
The hardware tailored for deep learning-based battery prognostics and health management.

Hardware type	Introduction	Examples	Deep learning applications
GPUs (Graphics Processing Units)	Known for parallel computations, ideal for matrix and vector operations in deep learning.	NVIDIA Tesla V100, Titan RTX, GeForce RTX 3090, AMD Radeon Instinct	Suitable for training various deep learning models including transformers, GANs, transfer learning, physics-informed machine learning, and reinforcement learning.
TPUs (Tensor Processing Units)	Custom-developed for neural network machine learning, excelling in tensor operations.	Google Cloud TPU, TPU v2, TPU v3	Favored for training large-scale transformer models such as BERT and GPT. Also applicable for other deep learning models.
FPGAs (Field-Programmable Gate Arrays)	Configurable post-manufacturing, prized for adaptability and efficiency in low-latency scenarios.	Xilinx Alveo series, Intel Arria, Stratix	Best for physics-informed machine learning with real-time inference and reinforcement learning requiring low-latency decision-making.
CPUs (Central Processing Units)	General-purpose processors, slower compared to GPUs and TPUs for deep learning.	Intel Xeon series, AMD Ryzen series	Used for small-scale model training or prototyping, especially when parallel processing is not essential.
ASICs (Application-Specific Integrated Circuits)	Custom-built chips optimized for performance and efficiency in specific tasks.	Google's TPU	Used in specialized scenarios requiring optimized performance and efficiency.

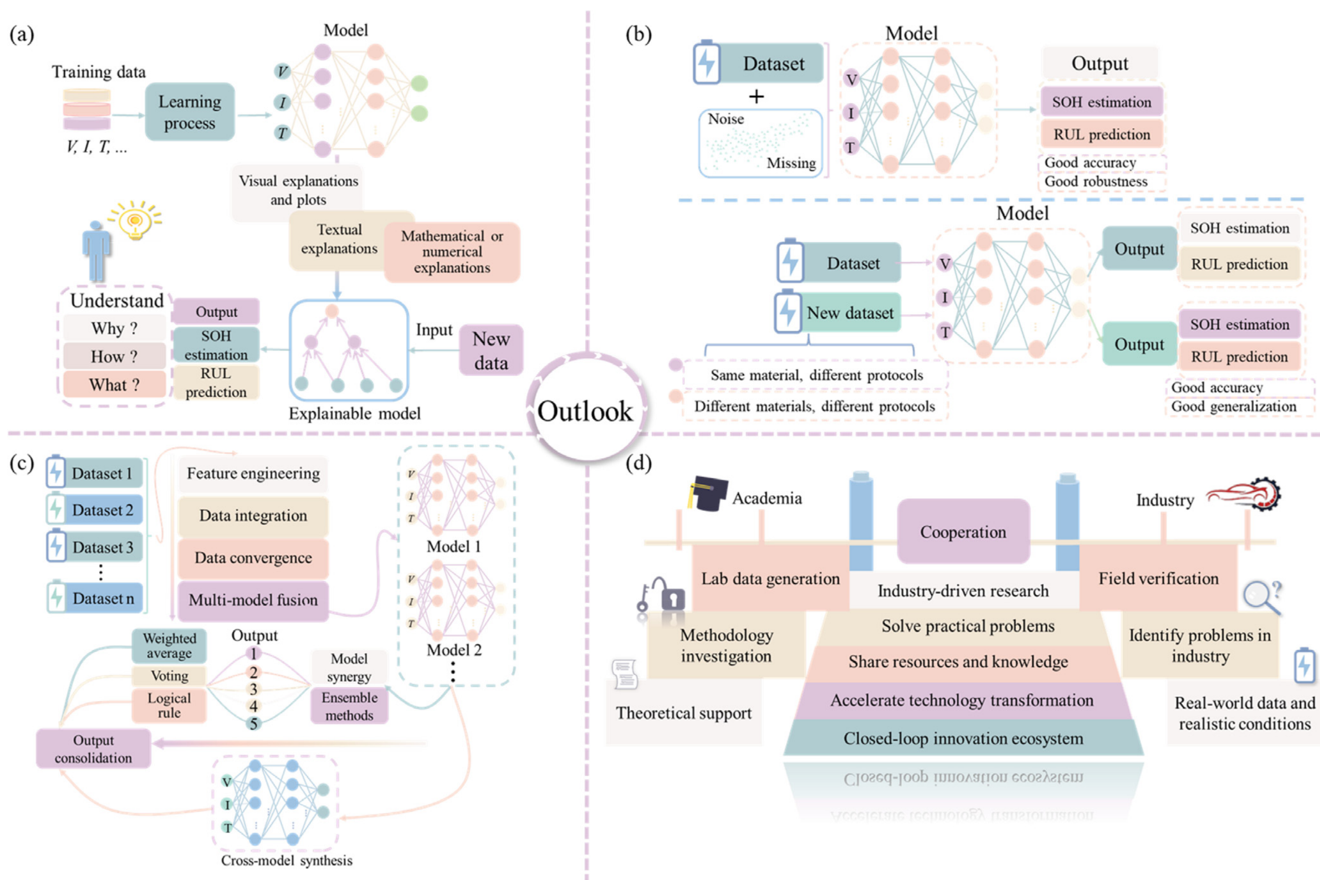

Fig. 10. Promising directions for battery health prognostics. (a) Explainable machine learning. (b) Robustness and generalization. (c) Data and model fusion. (d) Academia-industry cooperation.

6.1. Explainable machine learning

Physics-informed learning has demonstrated its potential across a multitude of fields, yet in order to confront the intricate web of multiscale and multiphysics problems, we must aim for continued evolution. One of the hurdles intrinsic to densely connected neural networks (NNs) is their notable difficulty in grasping high-frequency functions, a phenomenon often termed the "F-principle" or "spectral bias." High-frequency characteristics in the target solution induce steep gradients, which complicate the task for PINN models in effectively penalizing PDE residuals. To surmount this obstacle, innovative methodologies like domain decomposition, Fourier features, and multiscale DNNs are required for enhanced network learning. Moreover, given the computational burdens associated with learning multiphysics concurrently, explorations into alternative strategies such as individual physics learning followed by a collaborative union are underway.

The amalgamation of artificial intelligence (AI) and machine learning with battery research has seen remarkable strides, fueled by the progression in computational capabilities, voluminous datasets, and access to open-source software. The emerging philosophy of explainable AI (XAI) is designed to augment comprehension, trust, and the governance of AI systems [75]. Nevertheless, the restricted explainability of deep learning methodologies acts as a deterrent to their broader acceptance, especially in scientific explorations where the ability to observe, select, and explain are essential for constructing causal inferences, domain insights, and verifiable hypotheses. XAI techniques can provide assistance in decoding the inherent physics in materials science, navigating scientific conjectures, and bolstering faith in learning models. Challenges confronting XAI include the lack of accessible or well-established ground-truth labels, calling for the integration of domain-specific expertise into the modeling and decision-making processes. Live data demonstrations and interdisciplinary dialogues can aid in striking the right chord between precision and explainability.

The paradigm of continual or lifelong machine learning [55], aiming for AI systems to achieve human-like proficiency in assimilating new knowledge and learning new concepts, presents substantial benefits. Lifelong learning's hallmarks encompass ceaseless learning, knowledge accumulation and recall, and knowledge transfer across numerous tasks and domains. Overcoming the phenomenon of catastrophic forgetting and safeguarding the integrity of previously acquired knowledge are paramount. The combination of representation learning with intricate reasoning can lead to considerable advancements in lifelong learning AI systems.

While the realm of lifelong learning is still nascent, it has an ambitious aim. By delving into biological mechanisms, one can engineer highly effective lifelong learning machines. Achievement can be realized through ceaseless learning, gathering, and generalizing, employing novel frameworks and merging physical models and machine learning in a lifelong learning context. Continuous learning can be utilized to ensure the safety of battery systems by identifying manufacturing defects and prognosticating states throughout operational lifetimes [76], utilizing comprehension of multiphysics and multiscale issues across spatial and temporal scales at material, cell, pack, and system levels.

In sum, it's crucial to tackle the challenges in physics-informed learning, XAI, and lifelong machine learning to push the boundaries of battery research. By pioneering new techniques, encouraging interdisciplinary exchanges, and integrating domain-specific know-how, one can construct AI systems that are not only high-performing but also uphold transparency and trust. These advancements will invariably lead to safer and more effective battery systems, proving beneficial for an array of industries and applications.

6.2. Robustness and generalization

The escalating demand for scalable, resilient, and rigorous next-generation physics-embedded learning machines necessitate pioneering frameworks, uniform benchmarks, and advanced mathematical strategies. The aim is to utilize pre-existing knowledge and constraints to craft machine learning methods that offer interpretability while handling imperfect data, such as missing or noisy values and anomalies. These methods should guarantee precise and physically consistent forecasts, even in extrapolation or generalization tasks.

Equivariant transformer networks present differentiable mappings that boost model robustness for predefined transformation groups. Yet, their applicability is currently limited to simpler physics or symmetry groups, often demanding expert knowledge and complex implementations. Expanding these methods to more intricate tasks is a challenge, given the poorly comprehended or hard-to-encode invariances or conservation laws that govern many physical systems.

Physics-embedded machine learning machines could potentially revolutionize battery prognostic technologies. However, robustness issues associated with PINNs emerge, particularly when high signal-to-noise ratios in sensor measurements and complicated charging-discharging patterns are present. Large-scale neural networks with complex loss functions present highly non-convex optimization issues, which can lead to potential instability and a lack of assurance of convergence to the global minimum. To surmount this hurdle, the creation of more robust neural network architectures and training algorithms across various applications is necessary.

A harmonious collaboration between deep learning, optimization, numerical analysis, and PDE theory is crucial to scrutinize physics-informed machine learning models anchored in rigorous theory. This partnership will foster more resilient and effective training algorithms and lay the groundwork for this emerging generation of computational methodologies. While machine learning approaches demonstrate potential, many struggle to extract interpretable information from sizable datasets. Purely data-driven models may adequately fit observations, yet their predictions may suffer from a lack of physical consistency or credibility due to extrapolation or observational biases, leading to subpar generalization performance.

The incorporation of fundamental physical laws and domain expertise into machine learning models is pivotal, informing them about prevailing physical rules and offering "informative priors" or sturdy theoretical constraints and inductive biases. Physics-informed learning has numerous benefits, particularly when procuring vast amounts of high-precision data proves challenging. By imposing or embedding physics, deep learning models are effectively limited to a lower-dimensional manifold, enabling training with fewer datasets. Physics-informed learning also facilitates extrapolation, not just interpolation, rendering it apt for spatial extrapolation in boundary-value problems.

In the end, testing the generalization boundaries of these transformations is essential, determining the extent of observations for which machine learning models can be mapped to another machine learning model or physical model, and pinpointing the threshold at which these mappings become unattainable. By tackling these challenges and further integrating physics into machine learning models, one can hasten training, bolster generalization, and devise more resilient and effective algorithms for a broad array of applications.

6.3. Data and model fusion

As the convergence of machine learning and physics-centered modeling deepens, researchers might encounter instances where unique data-driven models emerge for the same event, even when trained on identical or equivalent datasets. Such scenarios could give rise to varied neural networks with disparate latent spaces and operators, despite their predictions being almost alike on the training set. Given the often absent unique physical interpretation of observed phenomena, it is vital to establish authenticated, one-to-one machine learning-based transformations between predictive models, models of differing fidelities, and theories. Researchers are finding such transformations in a data-centric manner, thus facilitating the systematic integration of data and models. By forging transformations between machine learning latent space characteristics and physically interpretable observations, or between machine learning-learned operators and defined equations, one can enhance the interpretability of machine learning models [77].

Equally important, however, is the need to test the broad applicability of these transformations. This involves defining the extent of observations for which an machine learning model can be mapped to another machine learning model or a physical model, and pinpointing the generalization threshold beyond which these models cannot be transformed or calibrated to one another. Concentrating on devising and understanding transformations will aid in crafting more interpretable, resilient, and dependable machine learning models within the scope of physics-centric research. Through this process, one can augment the capacity to distil valuable information from vast datasets and infuse physical laws and domain knowledge into machine learning models, thereby resulting in more precise and reliable forecasts for a diverse array of applications.

6.4. Academia-industry cooperation

Deep learning, a formidable subset of machine learning, is spearheading groundbreaking transformations across a plethora of scientific and technological arenas. With its extraordinary capacity to decode complex patterns within vast and structured datasets, deep learning stands as a cornerstone for extracting sophisticated insights from colossal volumes of data. While its initial forays were largely centered around perceptual tasks such as image processing and voice recognition, deep learning's ambit has burgeoned to encompass a rich tapestry of domains, including physics, chemistry, electrochemistry, and materials science, underlining its sheer versatility. Specifically, within the ambit of battery research, deep learning serves as a catalyst for innovative problem-solving tactics. It offers avenues for delving into the intricacies of electrochemical interactions, and bolsters the efficacy of physics-oriented simulations and models. Through the judicious deployment of machine learning algorithms, cutting-edge multiscale strategies can be conceptualized, galvanizing the development of energy storage technologies that are both high-performing and ecologically benign.

Nonetheless, to harness the full spectrum of deep learning's capabilities, it is essential to cultivate resilient cross-disciplinary partnerships, especially between AI mavens and cognoscenti in electrochemistry, bridging the worlds of academia and industry. The confluence of these distinct realms offers a reservoir of insights and competencies that can collaboratively surmount prevalent obstacles such as data standardization and model optimization, propelling the wheels of invention and progress at an expedited pace. Such a collaborative ethos is not only a sine qua non for the forward march of battery technologies but also an impetus for a more encompassing migration toward sustainability in energy, championing the cause of electric vehicles and renewable energy paradigms.

Moreover, the fusion of cloud-based data aggregation from real-world deployments heralds an exciting new frontier in deep learning's applicability within battery research. Cloud technology facilitates the capture and scrutiny of data in real-time from batteries employed across diverse settings. Such data is invaluable for garnering insights on battery efficacy, attrition rates, and functional dynamics under assorted operational regimes.

In this context, the emergence of cloud-driven AI-centric BMS is poised to ascend as a pivotal development in the coming decade [78]. By intertwining AI with cloud-based BMS, it is possible to evoke a suite of capabilities including real-time analytics, predictive upkeep, and strategic optimization of operations. These, in turn, foster enhanced battery longevity and performance. Additionally, cloud computing's inherent scalability and accessibility pave the way for unimpeded cooperation and data interchange among scientists and professionals across the globe.

To sum up, the synergistic integration of deep learning, cloud computing, and interdisciplinary alliances promises to be a game-changer for the battery research domain under industry 4.0 [79]. This trinity not only fuels innovation but also serves as a lynchpin for the larger crusade toward an energy-sustainable future, playing a pivotal role in the electrification initiatives spanning transportation and energy systems.

7. Conclusions

As we navigate the era of renewable energy, the development of lithium-ion batteries takes on a central role, with effective data utilization being of paramount importance. Open-access lithium-ion battery cycling datasets serve as invaluable data resources, encompassing comprehensive information on experimental test protocols, variables, and outcomes. This paper diligently reviews seven such openly shared datasets and their associated test conditions, offering potent resources for researchers to freely utilize in their research and development endeavors. The potential of these datasets can be amplified by employing machine learning techniques and architectures that leverage pre-existing knowledge to devise models that are both robust and adaptable.

For a more nuanced understanding of battery system science problems, and to enhance the predictive capability of seasonal forecasting and modeling of long-range spatial connections across multiple timescales, five deep learning techniques emerge as particularly promising for battery health prognostics, each offering unique strengths: (a) Transformer Learning: Transformers excel at handling complex dependencies in data due to their attention mechanisms. This trait makes them ideal for modeling intricate relationships in battery data, resulting in superior accuracy, faster training, and improved generalization. (b) Transfer Learning: By drawing upon pre-existing models and knowledge from related tasks, transfer learning can substantially enhance battery state assessments and predictions. This can lead to improvements in battery performance and management, thereby accelerating the transition towards green energy. (c) Physics-Informed Learning: This approach utilizes the laws of physics as a priori to enhance model training and performance. It assists in understanding and predicting battery states and behaviors, thereby facilitating the optimization of battery management and promoting the adoption of green energy. (d) Generative Models: These models can generate new data instances that closely resemble the training data. In the context of batteries, they can simulate realistic operating scenarios, providing a comprehensive understanding of battery behavior under diverse conditions. (e) Reinforcement Learning: Reinforcement learning employs a system of rewards and penalties to train models. Within the domain of battery health prognostics, it can optimize battery control strategies, thereby enhancing battery lifespan and performance. Additionally, this paper scrutinizes the challenges associated with each specialized deep learning technique in the context of battery health prognostic scenarios, following an extensive review of examples that employ each technique. The integration of specialized deep learning, effective data utilization, and the exploration of advanced deep learning techniques are instrumental to the future advancement of lithium-ion batteries, propelling us ever closer to a sustainable future.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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