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Review

Synergizing Machine Learning and the Aviation Sector in Lithium-Ion Battery Applications: A Review

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Abstract: Lithium-ion batteries, as a typical energy storage device, have broad application prospects. However, developing lithium-ion batteries with high energy density, high power density, long lifespan, and safety and reliability remains a huge challenge. Machine learning, as an emerging artificial intelligence technology, has successfully solved many problems in academic research on business, financial management, and high-dimensional complex problems. It has great potential for mining and revealing valuable information from experimental and theoretical datasets. Therefore, quantitative "structure function" correlations can be established to predict battery health status. Machine learning also shows significant advantages in strategy optimization such as energy optimization management strategy. For lithium-ion batteries, their performance and safety are closely related to the material structure, battery health, fault analysis, and diagnosis. This article reviews the application of machine learning in lithium-ion battery material research, battery health estimation, fault analysis, and diagnosis, and analyzes its application in aviation batteries in conjunction with the development of green aviation technology. By exploring the practical applications of machine learning algorithms and the advantages and disadvantages of different applications, this article summarizes and prospects the application of machine learning in lithium batteries, which is conducive to further understanding and development in this direction.

Keywords: machine learning; lithium-ion batteries; battery materials; estimation of SOH; fault diagnosis; aviation

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1. Introduction

In recent years, the energetic development of energy storage batteries has been driven by national policies to achieve the goal of "dual carbon". This has led to increased demand for higher-performance energy storage batteries. As a typical and high-prospect energy storage device, lithium-ion batteries (LIBs) have been widely used in mobile power, electric vehicles (EVs), home appliances, and even in the aviation area [1]. In order to further increase the percentage of renewable energy consumption, developing advanced batteries with high energy density, high power density, long life, and reliable safety is considered important and is the ultimate goal of the energy battery [2,3]. In addition to traditional LIBs, lithium-metal batteries (LMBs) including lithium-sulfur batteries (Li-S) and solid-state batteries (SSBs) has good research prospects because of the ultra-high energy density [4].

The energy density of LMBs has high expectations. However, its practical application still has great challenges. Reasonably preparing a safe and high-performance LMB and effectively surveying its working status remain huge challenges. The long-term cycling and rate capability in experimental testing has been widely used to evaluate the electrochemical performance of functional materials or formulations [5]. However, due to the plentiful material and spatial structure, it is almost impossible to improve the battery performance in a short period of time by trying and looking for the incorrect way. Various characterization techniques such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy are often used to monitor the morphological changes of chemical materials in solid-state LIBs during cycling [6,7]. In situ characterization at the atomic level of the LIBs is limited, which makes it extremely challenging for the discovery of structure–function relationships and the basic understanding of working mechanisms. Calculation methods in chemical materials, especially density functional theory (DFT) calculations and molecular dynamics (MD) simulations, are widely used in LIBs to predict the properties of the molecular structure, energy, reactivity, and so on. It combines the theory of quantum mechanics with molecular dynamics simulation methods to simulate and predict molecular systems at the atomic level. However, with the complexity of system structures and the accuracy of the experimental results that we need, it has been difficult for previous research methods to keep up. The gap between simplified theoretical models and reality largely hinders the application of computational simulations to describe complex interface problems in batteries. In the actual use of LIBs, LIBs will have different degrees of attenuation and aging, which will lead to a decrease in cruising range, shorten the service life, and also cause potential safety hazards. Therefore, accurately predicting the health status of LIBs is critical to improving their performance and safety. For the estimation of the health state of LIBs, there are several main methods: model-based methods, data-driven methods, hybrid methods, etc. [8–11]. We mainly describe the estimation of the health status of LIBs by the data-driven methods. For LIB applications, safety issues are paramount. Currently, battery management systems (BMS) are mainly used to monitor the performance and safety of battery systems. The BMS collects the current, voltage, and temperature data from the battery system and estimates the battery's state such as the state of charge (SOC) and state of health (SOH) [12]. The BMS also performs diagnostic functions based on measurements and estimates based on certain diagnostic methods and undertakes a series of corresponding measures to ensure the safety of the battery system. However, the failure problem is complex and diverse, so it needs to be further clarified as to which approach should be used to effectively respond to each situation.

In recent years, the development of green aviation technology has been valued, and many LIBs are used in the aviation field [5]. The aviation industry has shown that compared to construction, oil, and natural gas, digitalization has matured and can offer advantages in operational efficiency and cost reduction [13]. However, in the aviation industry, there is still space to gain more benefits from the subset of artificial intelligence. In green aviation technology, green means an environmentally friendly development model with the goal of energy conservation and environmental protection. The combination of green aviation and machine learning (ML) technology can optimize flight planning, save fuel, improve maintenance efficiency, optimize airport operation. and improve aviation safety, realize more efficient, safe and environmentally friendly air transport, and contribute to the sustainable development of the aviation industry.

ML, as a rapidly developing and powerful data analysis technology, can process and analyze a large amount of complex data and extract useful patterns and information from it. It can handle complex problems in various fields such as natural language processing, image recognition, recommendation systems, etc. ML algorithms can automatically learn and make decisions through training data without human intervention. This gives ML enormous advantages in real-time applications and large-scale data processing such as autonomous driving and financial risk assessment. ML algorithms can accurately predict and classify data by learning patterns [14]. It can discover hidden correlations in data, thereby improving the accuracy and precision of prediction. For LIBs, ML has the advantage of quickly capturing the complex relationships between the battery materials, structures, and performance, helping us study and improve the performance and safety of LIBs. For LIBs, its performance and safety are inseparable from the material structure, battery health, fault analysis, and diagnosis. The emerging interdisciplinary field of ML is still rapidly expanding and has been applied to many fields such as chemical materials, energy batteries, financial risk assessment, and even music education [6,15,16]. Although ML methods are helpful in various applications of LIBs, there are limited comprehensive and in-depth reviews on related topics. Therefore, this paper is an attempt to fill this gap. For the convenience of readers, Table 1 lists the existing review articles related to ML in the fields of battery materials, the estimation of SOH, fault diagnosis, and aviation batteries.

Table 1. Existing reviews related to ML in the fields of LIB materials, the estimation of SOH, fault diagnosis, and aviation batteries.

Topic	References	Focus
Battery materials	Chen et al. (2020) [17]	Reviewed the application of ML in energy materials, outlined different ML technologies and best practices.
Estimation of battery SOH	Sui et al. (2023) [18]	Reviewed the types of ML algorithms used for SOH estimation and analyzed their advantages and applicability.
Battery fault diagnosis	Samanta et al. (2021) [19]	Reviewed the most advanced ML based data-driven fault detection/diagnosis technology.
Aviation batteries	Raoofi et al. (2023) [13]	Reviewed the BMS strategy supported by intelligent algorithms in the propulsion system of electric aircraft; reviewed artificial intelligence security risk assessment and learning assurance.

The rest of this article is organized as follows. Section 2 introduces the concept of ML and several commonly used ML algorithms. Sections 3–5 introduce and discuss the application methods of ML in battery materials, the estimation of battery health, and battery fault diagnosis, respectively. Section 6 explores the application of ML in aviation batteries. Then, in Section 7, the application of ML methods in batteries is discussed. In Section 8, a summary is made and future directions are discussed.

2. Machine Learning Concepts, Algorithms, and Implementations

ML is an artificial intelligence technique that allows computers to automatically learn from data and provide accurate results based on the data.

ML involves the following concepts: features, which are variables that describe sample attributes such as height, weight, and age; training set, which is the dataset used to train the model; test set, which is the independent dataset for testing the model performance; model selection, which is the process of selecting the best algorithm or parameter configuration based on the performance evaluation [20].

ML algorithms can be divided into the following types: supervised learning, where a learning model is trained with a set of labeled data (data with known outputs), and then the trained model is used to make estimations on the unknown data; unsupervised learning, which solves various problems in pattern recognition based on training samples of the unknown class (not labeled); reinforcement learning, which is a ML method that improves behavior by simulating reward signals in the brain nerve cells. Self-adjusting through trial and error in the environment, in reinforcement learning, the algorithm receives feedback from its surroundings and makes the best decision based on the feedback.

ML implementations typically require the following steps. (a) Data cleansing and pre-processing: raw data are processed to ensure its quality and integrity. (b) Feature extraction and selection: identify a subset of features to use to train the model. (c) Model training and optimization: use the training set to fit the model and adjust the hyperparameters to achieve the best performance. (d) Model evaluation and testing: use test sets to evaluate the model performance and adjust the model or reselect features based on the results to improve performance. (e) Estimation and deployment: use trained models to make estimations or generate results.

In recent years, with the rapid development of data resources, ML has solved many problems in business, financial management, and academic research on high-dimensional and complex problems. In the following, we introduce several popular ML methods.

2.1. Linear Regression

Linear regression is a traditional supervised learning algorithm. Linear regression assumes a linear relationship between the input variable (X) and the single output variable (Y), as shown in Figure 1a.

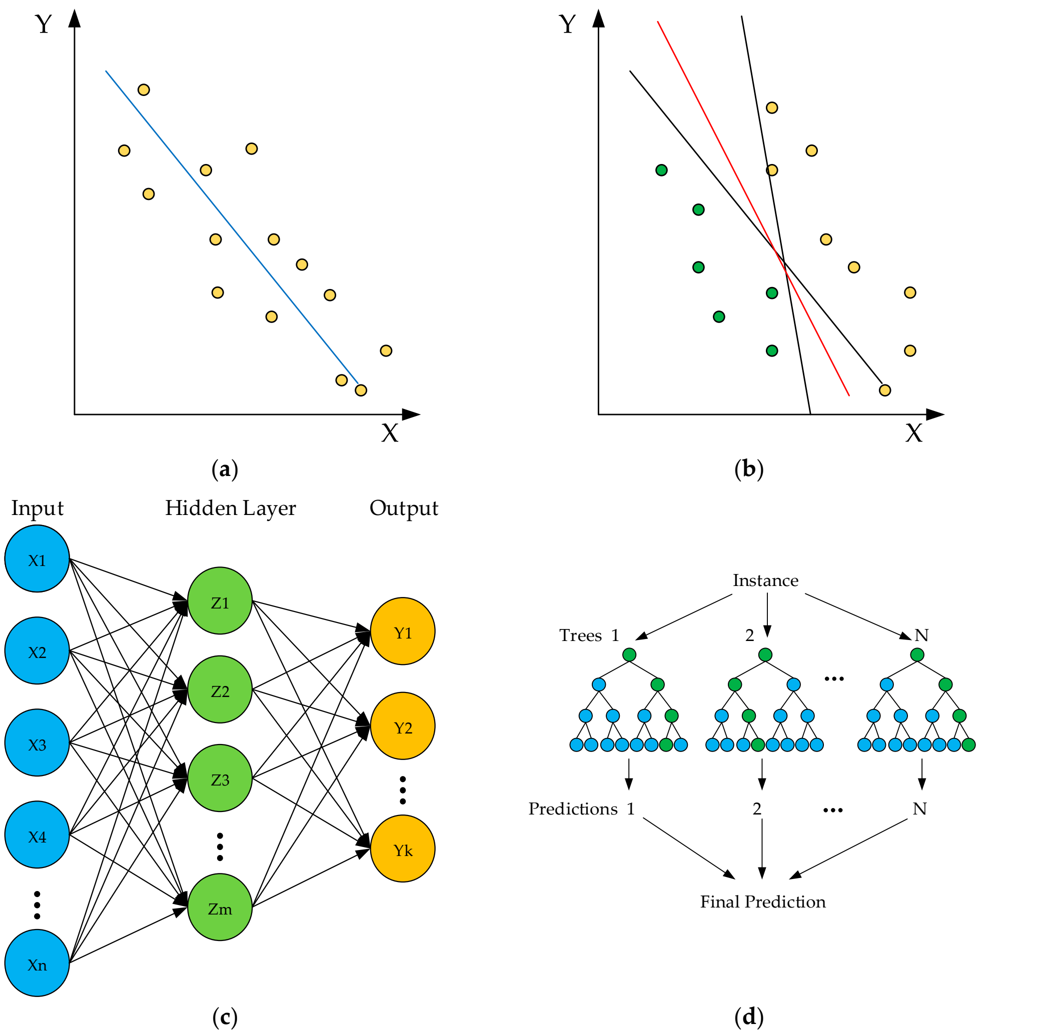

Figure 1. Several popular ML algorithms: (**a**) linear regression; (**b**) support vector machines; (**c**) artificial neural networks; (**d**) decision trees.

Mathematically, the linear function can be expressed as

$$Y = WX + b \tag{1}$$

where $X = (X_1, X_2, \ldots X_n)$ is the n-dimensional input variable, $W = (W_1, W_2, \ldots W_n)$ is the linear coefficient, and b is the bias term. The goal is to find the best estimate of the coefficient W so that the error of the predicted value Y is minimized. W and b are usually estimated using the least squares method, represented by minimizing the sum of squares of the difference between the Y value of the sample and the value predicted by (1). For simple problems, linear regression can provide fast, robust, and physically interpretable fitting results. However, for complex material problems, linear regression sometimes does not do a good job and may lead to some problems such as overfitting in the study of battery materials.

2.2. Support Vector Machines

Support vector machines (SVM) are a popular and widely discussed ML classification method and are linear classifiers. In two-dimensional space, a hyperplane can be treated as a straight line, assuming that all input points can be completely separated by the line, and the boundary between the two classes is determined by the hyperplane in Formula (2), as shown in Figure 1b.

$$g(x) = wx - b = 0 \tag{2}$$

where w is the normal vector and b is the threshold, based on the labeled data. The goal of the SVM is to find a set of segmentation coefficients w, b so that a hyperplane can optimally cut data x, that is, the two classes can be correctly separated with the largest class interval. In three-dimensional and above space, the plane that separates the data is called a hyperplane, which is the decision boundary for classification. It separates the existing training dataset and, for new data, determines which side of the hyperplane the data are located to obtain the classification of the new data. Therefore, the basic SVM algorithm is a binary classification algorithm, and for multi classification tasks, using SVM multiple times can solve the problem. SVM can solve high-dimensional problems, that is, large feature spaces; it can solve ML problems with small samples and handle feature interactions with strong generalization ability. However, when there are many observation samples, its efficient operation has certain challenges, and there are few universal solutions to nonlinear problems.

2.3. Gaussian Process Regression

Gaussian process regression (GPR) is a stochastic process (a collection of random variables indexed by time or space), and each finite set of these random variables is subject to multivariate normal distribution. GPR is a commonly used supervised learning method that can be used to solve regression and classification problems. The advantages of GPR model are mainly reflected in dealing with nonlinear and small data problems.

A Gaussian process is a set of random variables, and the joint probability distribution formed by each finite subset of this set of random variables is subject to multivariate Gaussian distribution, which is shown in Formula (3):

$$f \ \sim \ GP(\mu, k) \tag{3}$$

where $\mu(x)$ and $k(x, x')$ are the mean function and covariance function of the random variable x, respectively. Therefore, it can be seen that a Gaussian process is actually determined by the mean and covariance function of random variables.

In the traditional regression model, it is defined as $Y = f(x)$. In the GPR, let $f(x)$ obey the Gaussian distribution. Usually, assuming the mean is 0, which is Formula (4):

$$Y = f(x) \ \sim \ N(0, \textstyle\sum) \tag{4}$$

where Σ is the covariance function. Using the kernel technique, let $\sum ij = K(x_i, x_j)$, then the covariance function can be calculated by solving the kernel function K. Therefore, the covariance function Σ can be decomposed into $\begin{pmatrix} K, K_* \\ K_*^T, K_{**} \end{pmatrix}$, where K is the training kernel matrix, K_* is the training test kernel matrix, and K_*^T is the testing training kernel matrix. The conditional probability distribution of implicit function f can be expressed as Formula (5).

$$f_*\Big|(Y_1 = y_1, \ldots, Y_n = y_n, x_1, \ldots, x_n, x_t) \sim N(K_*^T K^{-1} y, K_{**} - K_*^T K^{-1} K_*) \tag{5}$$

2.4. Artificial Neural Networks

An artificial neural network (ANN) is a mathematical model based on the principles of biological neural networks. It can simulate the processing of information by the human brain and nervous system [21]. Neural networks simulate the brain through the following ways: neural networks gain knowledge by learning from external environments; synaptic weights of internal neuronal connections store acquired knowledge. Neurons are connected to each other in various patterns through links, which determines the strength of the effect of one neuron on another. Neural networks mimic biological axon–synapse–dendritic connections. A feedforward neural network ANN consists of an input layer X_i, hidden layers Z_i, and an output layer Y_i, as shown in Figure 1c. The output of neurons in the hidden layer can be calculated as the product of the input vector and the weight matrix of the neurons in the layer. After adding the bias term, it can be obtained through nonlinear transformation of the activation function. Mathematically, the output formula for neurons in the hidden layer is $Z_i = \sigma\left(w^T X_i + w_0\right)$, where σ is an activation function that defines whether the neuron can be activated by excitation. ANN is characterized by parallel distributed processing ability, high fault tolerance, intelligence, and self-learning ability. It combines information processing and storage together, and is actually a complex network composed of a large number of simple components connected to each other, with a high degree of nonlinearity, capable of performing complex logical operations and implementing nonlinear relationships.

Battery data typically contain complex nonlinear relationships. ANN, as a nonlinear model, can better fit and model nonlinear features in battery data. Battery data are usually multidimensional including multiple parameters such as voltage, current, and temperature. ANNs can process multidimensional data and learn and extract complex correlations between data through hidden layers. Due to the distributed computing nature of ANN, even if some neurons fail, the overall performance of the network can remain relatively stable.

2.5. Variational Autoencoder

Variational autoencoder (VAE) is a generative model, which combines the concepts of autoencoder and variational inference. Autoencoder is an unsupervised learning method that encodes the input data into a low dimensional representation and attempts to reconstruct the original input data from the low dimensional representation. The autoencoder consists of an encoder and a decoder. The encoder maps the input data to the low dimensional potential space, and the decoder maps the potential representation back to the reconstructed input data. VAE introduces the idea of variational inference on the basis of the autoencoder, which enables the model to learn the potential distribution of data. By introducing randomness into potential space, VAE enables the model to generate new samples and interpolate and operate in potential space. The training process of VAE involves maximizing the marginal likelihood of the observed data while minimizing the Kullback–Leibler (KL) divergence between the potential representation and the prior distribution. In this way, VAE can learn the potential structure of the data and generate new samples. VAE is widely used in the field of generative models including image generation, feature learning, and data compression. *KL* divergence is used to measure the degree of difference between these two distributions. Specifically, for each sample, we calculated the *KL* divergence between the potential variable distribution and the prior distribution, and summed the *KL* divergence of all samples as part of the loss function of VAE. Mathematically, for two probability distributions P and Q, the KL divergence between them is defined as Formula (6):

$$KL(P\|Q) = \sum_{i=1}^{n} P(x) \log \frac{P(x)}{Q(x)} \tag{6}$$

2.6. Decision Trees

Decision trees (DTs) are a commonly used classification and regression method, where each node represents a feature classification test and can only store one category or value, with each branch representing output or judgment conditions. Starting from the root node of the decision tree, select a branch of the tree and follow the selected branch all the way down to the leaves. The categories or values stored by the leaf nodes serve as the decision result. DT can be used for binary classification, multivariate classification, continuous variable prediction, and other problems, and are easy to explain and understand, as shown in Figure 1d.

3. Machine Learning Is Applied to Battery Materials

The research on battery materials involves multiple scale levels, from atomic to macroscopic levels. Common theoretical methods include DFT calculation, MD simulation, the phase field method (PFM), and finite element method (FEM) as well as experimental characterization techniques and electrochemical performance tests. These methods can help us understand the structure, properties, and behavior of battery materials, and provide guidance for designing more efficient batteries [6]. The research focus of battery materials includes performance prediction and the optimization of liquid and solid electrolyte materials. For liquid electrolyte materials, the main focus is on their conductivity, electronic conductivity, viscosity, and other properties; For solid electrolyte materials, the primary emphasis is on exploring their diffusion barrier, migration energy, and ion conductivity [22–24]. Factors such as temperature, molecular concentration, and component information are commonly used to describe electrolyte properties and can be used to predict the performance of battery materials [25,26]. These research results can help us design more efficient, stable, and safe battery materials.

ML plays an important role in many fields, not only in analyzing large datasets and establishing quantitative relationships to design materials or methods reasonably, but also by promoting the development of theoretical and experimental methods. For example, in chemistry, physics, and materials science, ML models have been widely used to predict the material properties and reaction kinetics including functional simulations and interatomic potential simulations. The application of ML in the fields of materials and chemistry has become one of the hot research fields. In addition to the above advantages, ML is also widely used in fields such as material structure prediction, catalyst design, and crystal discovery. The use of ML models can quickly screen out new materials with potential application value, optimize the process flow, and reduce production costs [27]. With the improvement of computing hardware performance and the increase in datasets, ML will play an increasingly important role in the future.

The simulation of Kohn–Sham (KS) equations based on decryption-degree functional theory has become an important part of modern materials and chemical science research and development portfolios. The research process is shown in Figure 2.

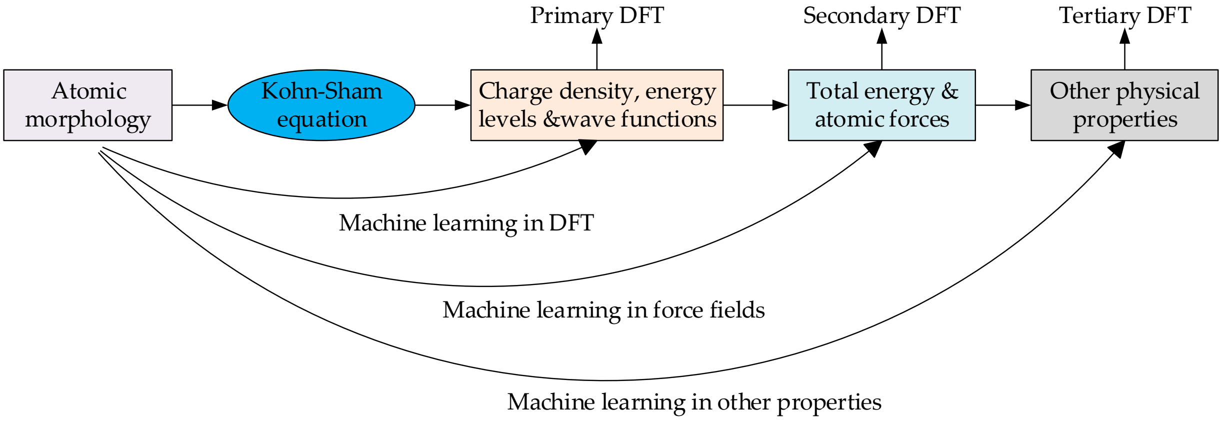

Figure 2. Simulation of Kohn–Sham (KS) equations based on decryption function theory (DFT).

Despite its versatility, conventional DFT calculations are typically limited to a few hundred atoms due to the computational bottleneck caused by the KS equation. In [28], the author introduced a method based on ML to predict the electronic structure of materials or molecules through a new rotational invariant representation, which avoids the use of the traditional KS equation. This method uses neural networks to generate reference DFT results on millions of grid points for training, which can achieve high fidelity simulation and is several orders of magnitude faster than traditional methods. For DFT density, in [29], the author used ML techniques to calculate the energy of coupling clusters from the DFT density for the geometric optimization and molecular dynamics of DFT density. This method could achieve a quantum chemistry accuracy lower than 1 kcal/mol and could obtain good results even in the strain geometry and conformational changes that do not perform well with the standard DFT method. This method can overcome the computational burden limitation of the advanced ab initio quantum chemistry method and improve its applicability. In [30], the author used supervised ML to develop a fast and accurate interatomic potential model through three emerging methods such as the moment tensor potential, message passing network, and symbolic regression. These models significantly improve the speed of atomic scale simulations and are changing the way molecular and material research is conducted with almost no loss of accuracy. In [31], the article proposed a machine-learning interatomic potential (MLIP) based method to accelerate the estimation of lattice thermal conductivity. This method used ML interatomic potentials trained on short ab initio molecular dynamics trajectories to evaluate inconsistent interatomic force constants and confirm its significant accuracy. This method can serve as a standard tool and can greatly accelerate and promote the estimation of lattice thermal conductivity compared to all commonly used DFT solutions. In [32], an E(3)-equivariant deep learning interatomic potential was introduced to accelerate molecular dynamics simulations. The method obtained state-of-the-art accuracy and could faithfully describe the dynamics of complex systems with remarkable sample efficiency. The work introduced neural equivariant interatomic potentials (NequIP), which is an E(3)-equivariant neural network approach for learning interatomic potentials from ab-initio calculations for molecular dynamics simulations. While most contemporary symmetric perceptual models use invariant convolution and act only on scalars, NequIP employs E(3)-equivariant convolutions for interactions of geometric tensors, resulting in richer and faithful representations of the atomic environment. The high data efficiency of this method allows for accurate potential construction using a high-order quantum chemistry theoretical level as a reference, with the ability to perform high-fidelity molecular dynamics simulations on long-time scales.

ML can be used as a new method for DFT calculations, MD simulations, and solving multi-scale physical equations. It can perform high-precision atomic simulations on large systems, making it possible to detect complex geometric shapes, charge distribution, thermal and dynamic stability as well as ion diffusion in interfaces or amorphous phases. This provides a deeper understanding of the working mechanism and material evolution schemes in electrochemical reactions, which helps to search for and design new materials and battery formulations. Using ML methods such as SVM, random forest (RF), neural networks, etc., a large number of candidate materials have been screened and optimized to find battery materials with excellent performance. This can greatly improve the efficiency of material research and reduce experimental costs. By training ML models, the performance of new materials can be predicted such as conductivity, energy density, cycle stability, etc. This helps researchers to have a general understanding of material properties before conducting experiments, thus enabling more targeted experimental design and optimization. ML methods such as graph neural network (GNN) and convolutional neural network (CNN) are used to model and optimize the crystal structure and nanostructure of materials [33]. This can help researchers discover new material structure design patterns and improve material performance. ML methods can be utilized to achieve material modeling and simulation at different scales. This helps researchers comprehensively understand the properties and behavior of materials, providing more information for material design.

4. Machine Learning Is Applied to Battery Health Estimation

The traditional research methods for battery health mainly rely on physical characteristics (such as open circuit voltage, internal resistance, etc.) and stoichiometry (such as coulomb counting) [34]. However, these methods have laboratory environmental limitations and require advanced data processing and analytical techniques. Therefore, modern battery health monitoring methods are based on advanced algorithms and models to achieve non-invasive monitoring and can be carried out in actual operating environments. These novel methods include the use of ML, artificial intelligence, and big data technologies to accurately predict battery life and performance [1,35–37]. The lifespan and performance of LIBs are influenced by aging stress factors such as the charging state, charging and discharging rate, number of cycles, and temperature [38]. Many studies have investigated the extension in the battery lifespan through derating methods, which are summarized in detail in [39]. ML methods offer advantages in data learning and processing as adaptive algorithms, and many businesses and academic organizations are collecting datasets to study a range of battery models used to predict battery degradation and fault diagnosis [40–43]. For example, in [44], the authors achieved case studies from the laboratory to the field by estimating the transmissible data transmission capacity of LIBs through deep learning. Data acquisition is the committed step of battery condition assessment and fault diagnosis. The voltage, current, temperature, capacity, and other parameters of the battery can be obtained through sensors, testing equipment, and other methods. At the same time, more comprehensive data information can also be obtained through recording the battery usage and inspecting the battery appearance [45,46]. Generally, in practice, it is not practical to collect all of the available data. Therefore, in practice, the amount of data available and the accuracy of the algorithm need to be weighed to find the best solution. At the same time, it is also necessary to pay attention to the quality and integrity of the data to avoid incorrect input, leading to incorrect results [47]. In order to ensure the accuracy and integrity of the data, data cleansing, data denoising, data alignment, etc. are usually used to ensure the quality of the data. Due to the fact that the data for battery status assessment and fault diagnosis are usually collected in real-time, there may be issues of data loss and poor-quality during data collection and processing. To address these issues, methods such as interpolation, extrapolation, and smoothing can be used to fill in missing data, or methods such as anomaly detection and data correction can be used to process poor quality data [48–50].

Despite the advantages of the high energy and power density of LIBs, maintaining the SOH of LIBs remains a challenge due to the effects of various environmental operating conditions such as temperature, humidity, charging and discharging rates, which can affect the cycle life of LIBs [51]. In addition, LIBs also age naturally during long-term storage, reducing their SOH. Therefore, appropriate measures need to be taken to extend the service life of LIBs and improve their reliability [21]. In [52], the authors proposed a battery capacity estimation method based on charging data and data-driven algorithms. They estimated the battery capacity by calculating variations in the ampere integral formula and used statistical values as the labeled capacity. The sequence-to-sequence (Seq2Seq) model is used to predict the future capacity change, and the estimation error is corrected by the residual model of GPR. Experiments have shown that this method can accurately predict the remaining capacity of batteries with an error of less than 1.6%. This study can effectively predict the battery capacity. When the electrode system is disturbed by a sinusoidal voltage (current) AC signal, a corresponding current (voltage) response signal is generated, from which the impedance or admittance of the electrode can be obtained. The impedance spectrum generated by a series of frequency sine wave signals is called electrochemical impedance spectroscopy (EIS) [53]. For the study of equivalent circuits and EIS, the EIS in the ultra-high frequency range can be described by inductor L. In particular, when the intersection of the EIS and the real axis corresponds to the conduction process, the EIS can be represented by a resistor R_0. As the frequency decreases, the EIS exhibits two arcs related to the SEI film (high-frequency part) and the charge transfer process (intermediate frequency part) of the battery. In the low-frequency section, the EIS appears as a straight line related to battery diffusion. In [54], the authors explored an approach that used a convolutional autoencoder (CAE) for overcomplete feature extraction from the EIS data. CAE-DNN is an end-to-end deep learning architecture that uses CAE to extract overcomplete features from EIS data. This architecture extracts useful features in an unsupervised manner and can be used for battery capacity maintenance and SOH estimation. Compared with other baseline estimation methods, CAE-DNN can more accurately estimate the SOH of LIBs. The proposed architecture based on end-to-end deep learning is called CAE-DNN. Compared with other baseline estimation methods, the proposed architecture extracts useful features in an unsupervised manner and estimates the SOH of LIBs more accurately. In [55], where they also used encoders, the virtual SOH experiment developed was based on incremental capacity measurement, using commonly recorded BMS signals to train digital battery cells. The first dataset was used for the proof-of-concept including the load distribution under the same old and new battery conditions. The second dataset was tested under more complex load distribution conditions and successfully estimated the SOH. Compared to continuous capacity testing, this framework does not impose restrictions on small currents and can be applied to actual driving cycles. It is entirely independent of the prevailing and unknown aging condition due to the application of battery models based on the novel encoder–decoder architecture and thus provides the cornerstone for a scalable and robust estimation of battery capacity on a pure data basis. In the research process, when the number of samples is too small, we can use transfer learning (TL), incremental learning, and semi-supervised learning combined with domain knowledge and experience and other methods. These methods can effectively use existing data and knowledge, improve the training efficiency and accuracy of the model, and provide more reliable support for battery status assessment and fault diagnosis.

BMS is mainly used to monitor the performance and safety of battery systems. It evaluates the health status of batteries by collecting data such as the current, voltage, and temperature [56]. At the same time, BMS can also perform diagnostic functions, use measurement data and specific diagnostic methods to determine the status of the battery, and take corresponding measures to ensure the safety of the battery system. In [57], the authors discussed digital twin technology and cloud collaboration for future battery management systems. They proposed a four-layer networked architecture based on cloud collaboration for battery management systems. The design of this architecture broke through the limitations of traditional battery management in terms of computing power and storage space, and achieved the application of high-performance algorithms. In addition, they established a digital twin model for batteries, which enabled refined management and safety control of the entire battery life cycle.

In [58], the authors used virtual experiments via transfer- and meta-learning to estimate the SOH of EV and improve the training efficiency for the remaining battery capacity based on pure data, while also emphasizing the robustness of the experiment. In [59], the authors used the battery early aging data to carry out DP identification and TL in the research, which effectively improved the accuracy of the SOH estimation. In addition, they also used the long short-term memory (LSTM) network to establish the SOH estimation model, and compared the performance with other ML algorithms. The experimental results indicate that LSTM performed best in estimation accuracy. In [60], the authors used a long short-term memory neural network model based on incremental capacity to estimate the SOH, which can predict the SOH of a single battery cycle for small sample data. Through TL, we can estimate the SOH under different load modes with high accuracy. In [61], the article proposed a health state estimation method based on collaborative feature selection and ML methods that was applied to actual EV data from over 1200 charging processes. After constraining the voltage range, they extracted and selected features from the capacity curve to describe the battery degradation process and estimate the SOH. Recursive feature elimination collaborates with linear regression models to prune unimportant features to find the relevant SOH estimation features. Therefore, the SOH estimation is based on the obtained features and the implementation of a low computational cost linear regression. In [62], the authors proposed a new SOH estimation method, which was divided into two stages. In the first stage, eight typical 300 s voltage distributions were used to describe the entire charging process and multiple aging features were extracted. Then, a stacked ensemble model with five basic models was introduced. In the second stage, the Shapley additive interpretation method was used to obtain the contribution of features and understand estimations, thereby reducing concerns about applying black box models. In summary, this new method achieved flexible, fast, and robust SOH estimation. The performance of the proposed model was verified using two different battery degradation datasets and the results showed that the accuracy of the proposed model was better than conventional ML models including light gradient boosting machine (GBM), eXtreme gradient boosting (XG Boost), RF, SVM, and GPR. The frame diagram of the algorithm is shown in Figure 3.

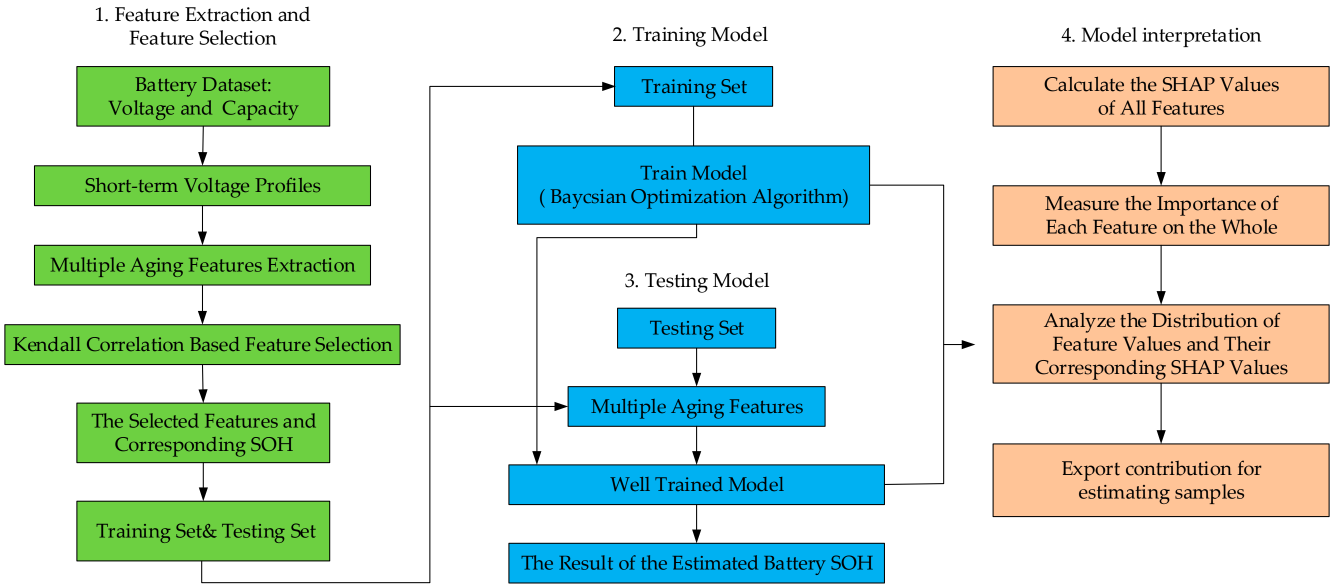

Figure 3. The framework of the battery SOH estimation based on the interpretable stacking ensemble model with the Bayesian optimization algorithm.

In the estimation of the LIB health status, ML methods such as CAE are used to extract and select features from the battery charging and discharging data, internal resistance data, temperature data, etc., in order to find key features related to the battery health status. This helps to improve the accuracy and robustness of the estimation model. A battery health estimation model can be established through ML algorithms such as SVM, RF, CNN, etc. [33]. This can help researchers monitor the health status of batteries in real-time and predict their remaining lifespan and failure time.

5. Machine Learning Is Applied to LIBs Fault Diagnosis

Potential failures in the LIB system may cause serious failure of the battery system and even induce serious safety accidents [63]. The faults of LIBs mainly include overcharging and discharging, increased internal resistance, battery short circuit, high temperature, and electrolyte leakage. These faults can lead to decreased battery performance and increased safety risks. Internal and external short circuits in battery systems are one of the main causes of thermal runaway of batteries, which may lead to serious consequences such as overheating, fire, or explosion. Therefore, monitoring and diagnosing the faults of LIBs is very important. In response to these issues, ML technology can utilize its powerful data processing and pattern recognition capabilities to improve the accuracy and efficiency of battery fault diagnosis through the real-time monitoring and analysis of batteries. For the condition with few experimental fault data samples, ML can use feature selection, data enhancement, TL, semi-supervised learning, and other methods to improve the accuracy and reliability of diagnosis [64–66]. In addition, ML can also optimize battery management strategies, thereby further improving the safety and reliability of battery systems. Therefore, ML technology has broad application prospects in the field of battery systems [67–69].

When conducting fault diagnosis for LIBs, we encounter insufficient data collection and too few samples, which can hinder the effectiveness of our prediction. Therefore, seeking suitable algorithms to solve this problem is a challenge. In [70], in response to the insufficient amount of collected internal short-circuit (ISC) fault data, the author proposed a multi-ML fusion method. This method uses voltage normalization to input the ISC faults into prediction, classifies fault warnings, trains simulation data through CNN, and then uses TL to build a multi-ML model. The migrated ML model greatly improves the prediction accuracy and can classify and warn of ISC faults at different levels.

In [71], the author used a symmetrical circuit topology structure to detect short circuit faults within a parallel series hybrid battery pack. This theory can accurately locate faults and provide necessary signals for detection and troubleshooting. By using an additional ammeter to detect an unbalanced current, it is possible to determine whether there is an internal short circuit. The recursive least squares algorithm is used to lock the faulty unit online, and the effectiveness of the algorithm at the grouping level is demonstrated through experimental verification by replacing the internal short circuits. This method can effectively and accurately detect the internal short circuit fault of the battery, and has great application potential in the fault diagnosis of battery packs in large-scale energy storage systems. In [72], a data-driven method was proposed for battery charging capacity diagnosis based on massive real-world EV operating data, as shown in Figure 4.

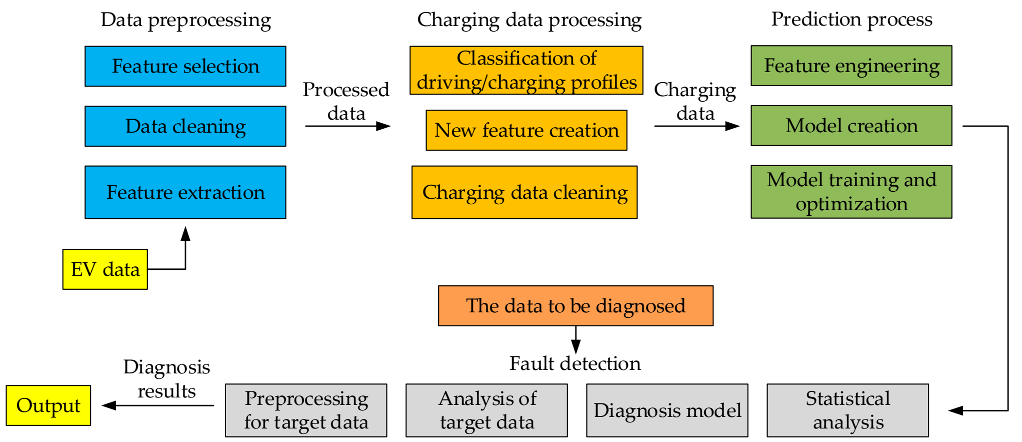

Figure 4. Framework of the proposed data-driven battery charging capacity diagnosis method.

Using the input of charging rate, temperature, charging state, and cumulative driving distance, a tree model and polynomial feature combination were used to predict the charging rate, temperature, charging state, and cumulative driving distance. Statistical methods were used to analyze the error distribution of large datasets to diagnose abnormal battery charging capacity. Compared with other state-of-the-art methods, the proposed tree model had the highest prediction accuracy. The overall diagnostic plan was validated using unknown data. In [12], the authors established a principal component analysis (PCA) model of the battery and used its contribution to detect abnormalities in the battery pack; after the fault was detected, parallel nuclear principal component analysis (KPCA) was used to reconstruct the fault waveform of the battery parameters including ohmic resistance, termination voltage, and open-circuit voltage. The combination of these parameters as fault indicators improved the reliability of the fault diagnosis. In [73], using neural networks and grey wolf optimization algorithms, the author proposed a charging safety warning model that adapted to the charging process of the EV. This model takes into account the polarization characteristics of LIBs and can dynamically monitor changes in battery charging voltage with good timeliness. In addition, the author improved the grey wolf optimization algorithm and adopted a search method based on clustering search results, which improved the diversity of grey wolves and avoided falling into local optimization problems.

In [74–76], the author used ML technology to diagnose and analyze battery faults, and proposed preventive measures. Considering the impact of inconsistent resistance and charge states on the correlation coefficient, voltage sensor faults, connection faults, and short circuit faults were detected and isolated by combining the correlation coefficient and voltage difference changes. For the fault diagnosis of signals, methods such as signal analysis, feature extraction, feature fusion, and dimensionality reduction were adopted to eliminate the impact of inconsistent states on the time series features, and abnormal signal features were identified through cluster based on anomaly detection. By supplementing the correction, the problem of determining the fusion feature threshold could be effectively solved, greatly reducing the number of false positives. In addition, the model-based system identification algorithm could also be integrated into the outlier detection algorithm to identify abnormal data more comprehensively and reduce the rate of missing reports. This method improved the accuracy and reliability of the anomaly detection algorithm from the perspective of the local outlier. Firstly, the identification model parameters are used to represent the dynamics of the battery and indicate the fault status of the battery. In this way, the fault detection problem can be transformed into abnormal parameters in the detection model parameter set. Next, local anomaly factors were used to describe the degree of parameter anomaly by evaluating the local bias of the observed data relative to the neighbors. Finally, the outlier filter based on the Grubbs criterion can use the calculated local outlier factor to detect the fault cell. The simulation and experimental results showed that the proposed method can accurately detect faults.

In [77], the author proposed an interactive multiple model (IMM) algorithm combined with an unscented Kalman filter (UKF) for the multi fault diagnosis of LIBs. This algorithm utilized a Markov transition probability matrix (TPM) to achieve the real-time interaction of the input information of various models and feeds back the updated probability information of each model to the input of the filter based on TPM, thereby reducing the impact of noise on the algorithm. In [78], the author proposed a real-time multi fault advanced diagnosis method based on sparse data observer (SDO) that could diagnose and predict battery faults including short circuit and open circuit faults. Among them, the outlier score was calculated to identify the fault, the fault flag was used to determine the fault battery and fault time, and the correction coefficient was introduced to detect the fault type. This method does not require an accurate battery model, but only uses the voltage data measured from the battery for diagnosis. Experimental results verified the feasibility and effectiveness of the proposed method, which had strong robustness and high sensitivity.

In LIB fault diagnosis, suitable ML algorithms such as SVM, NN, DT, etc. are selected for different fault diagnosis tasks to improve the accuracy and efficiency of fault diagnosis.

KPCA can be used to reconstruct the fault waveform of battery parameters including ohmic resistance, terminal voltage, and open circuit voltage. The combination of these parameters as fault indicators improves the reliability of fault diagnosis. The original data are preprocessed by data cleansing, feature extraction, feature selection, etc. to eliminate noise and redundant information and improve the generalization ability of the model. For example, considering the impact of inconsistent resistance and charge states on the correlation coefficients, fault diagnosis is performed on the signal. Methods such as signal analysis, feature extraction, feature fusion, and dimensionality reduction are used to eliminate the impact of inconsistent states on time series features. On the basis of anomaly detection, abnormal signal features are identified through clustering. When establishing a fault diagnosis model, consider the time series characteristics of the battery parameters and use recurrent neural network (RNN) and other algorithms for modeling to improve the accuracy of prediction.

6. Machine Learning in Aviation Sector

Aviation batteries such as lithium-ion batteries, lead-acid batteries, and nickel-cadmium batteries are widely used in many fields such as civil, military, and unmanned aerial vehicles, as shown in Figure 5. Aviation batteries are one of the key components of an aircraft, providing the necessary power to the aircraft [79]. However, due to the complexity and high safety requirements of aviation batteries, the requirements for their performance and reliability are very high. We can optimize the design and performance of aviation batteries through the application of ML technology, improving their reliability and safety. ML can predict the battery performance and lifespan by analyzing large amounts of the data in aviation battery including parameters such as the voltage, current, and temperature [5]. The data collected through sensors and other monitoring devices can train and optimize ML models, improve the battery prediction accuracy, monitoring and control capabilities, and optimize design and manufacturing processes. ML models can analyze the battery structure and materials to determine the optimal battery parameters; meanwhile, optimizing the charging and discharging processes can improve the battery efficiency and lifespan.

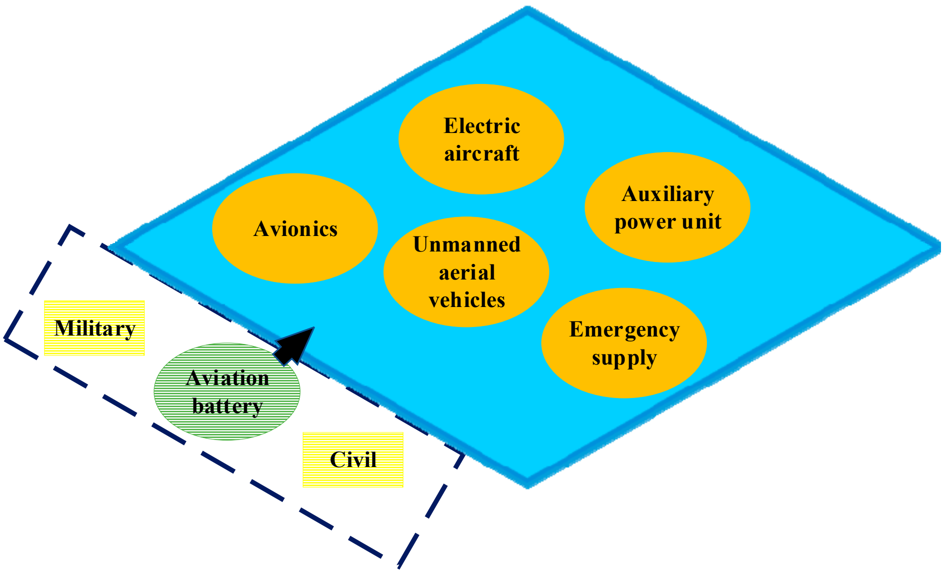

Figure 5. Application scenario of an aviation battery.

The luggage transportation system of unmanned EVs is an emerging research topic in civil aviation airports. However, the battery capacity of electric delivery vehicles limits the distance and load capacity during driving, thereby affecting the decision of vehicle scheduling. In [80], the authors studied a dynamic scheduling model for unmanned electric luggage carriers at airports that considered the load capacity and battery capacity constraints. In order to achieve real-time updates, they designed a dynamic scheduling algorithm based on the GCN-CNN-GRU neural network framework to determine the real-time driving status of vehicles. The performance of this method was verified through experiments in simulation scenarios. To improve the overall performance of fuel cell distributed electric propulsion unmanned aerial vehicles, in [81], the author proposed an energy optimization management strategy based on a combination of deep neural networks and model predictive control to address the issue of uncertain propulsion power requirements for unmanned aerial vehicles under different flight conditions affecting the performance of distributed electric propulsion systems. Digital simulation research was conducted using real-world drone flight experimental data to evaluate the performance of the proposed energy management system (EMS) and compare it with two benchmark schemes. Green aviation technology is receiving increasing attention, and more and more LIBs are being applied in the aviation field. In [82], in order to achieve the efficiency and long lifespan of hybrid power unit (HPU) vehicles under various working conditions, effective energy management is necessary. The author proposed an energy management strategy model predictive control (PMPC)—M-2 based on power prediction, which utilized data-driven methods to maintain the appropriate charging state of the battery and reduce the exhaust temperature of the turboshaft engine. This strategy is suitable for HPU vehicles equipped with turboshaft engines. Through verifying the simulation results, the effectiveness of the proposed vehicle EMS was confirmed, and the impact of different objective function weight coefficients on its performance can be further explored. ML methods can utilize a large amount of data to evaluate and analyze problems. Therefore, the use of ML methods can effectively optimize and improve vehicle energy management systems. In [83], the author recorded events related to the initial reliability challenge of the Boeing 787 Dreamliner, which was grounded due to safety problems related to a LIB fire. Its data can serve as input data for ML to predict and prevent faults, and provide advice and lessons for engineers and managers involved in future complex system development.

ML can help improve the performance and safety of LIBs, thereby promoting the development of aviation applications. On the one hand, ML can extract the characteristics and behavioral patterns of LIBs by analyzing a large amount of data. These modes can be used to predict the battery life, capacity degradation, and fault warning. Through real-time monitoring and prediction, airlines can better manage the use and maintenance of batteries, improving their reliability and safety [84]. On the other hand, ML can also help optimize the design and manufacturing process of LIBs. Through analysis and modeling, it is possible to understand the impact of different materials and structures on the battery performance, optimize key indicators such as energy density, charge discharge rate, and cycle life, and improve the fault diagnosis ability of aviation batteries [85]. This helps to develop high-performance batteries that meet the energy density and safety requirements of the aviation industry. In summary, ML has broad application prospects in LIB aviation applications. Through ML methods, the performance and safety of batteries can be improved, promoting technological progress in the aviation field.

7. Discussion

In the field of ML, the estimation and fault diagnosis of battery materials and battery health status is a hot research direction.

The first problem is that of feature selection. Although common methods include correlation coefficient analysis and principal component analysis, the impact of different features on the results may vary, so more detailed investigation and analysis are needed. Secondly, the model selection problem involves selecting ML algorithms suitable for the estimation of the battery SOH and fault diagnosis such as SVM, DT, NN, etc. However, each algorithm has its advantages and disadvantages, and different algorithms are suitable for different types of datasets and tasks. Therefore, several possible scenarios should be considered, compared, and evaluated when selecting a model, and the most suitable algorithm should be selected. Then there is the dataset problem. Dataset quality and quantity directly affect the accuracy and robustness of ML models. However, in the field of battery state of health estimation and fault diagnosis, obtaining high-quality large-scale datasets is a relatively difficult task. Therefore, it is worth exploring how to deal with the dataset and use limited data to improve the robustness of the model. Finally, issues related to practical applications also require attention. For example, in some scenarios, battery health estimation and fault diagnosis need to meet certain real-time requirements. Therefore, factors such as computational complexity and speed need to be considered when designing the model. In addition, different types of batteries may produce different types of failures, so different models and algorithms should be selected on a case-by-case basis.

For the contents discussed above, we can use hardware accelerators such as graphics processing unit (GPU), field programmable gate array (FPGA), tensor processing unit (TPU), etc., to carry out parallel computing and accelerate the model training and reasoning process. These accelerators can significantly improve the computing speed and meet the real-time requirements by selecting algorithms with lower computational complexity such as linear regression, SVM, etc. to reduce the computational costs. At the same time, the optimization speed can be improved through algorithm optimization techniques such as gradient descent, Newton's method, etc. Appropriate neural network architectures for different types of batteries can also be designed. For example, CNN can be used to process image data, RNN can be used to process time series data, and GNN can be used to process graph structure data. Through end-to-end ML, the steps of data preprocessing, feature extraction, model training, and inference are integrated into a unified framework, reducing the computational and communication costs of intermediate processes and improving the real-time performance. For example, unsupervised learning methods such as automatic encoder (AE) or VAE can be used to automatically extract features in an end-to-end framework. Using online learning methods, the model can be updated and optimized in real-time based on newly collected data. This helps to improve the accuracy and real-time performance of the model. The multi task learning method enables the model to simultaneously learn fault diagnosis tasks for multiple types of batteries during the learning process, thereby improving the model's generalization ability. By integrating multiple weak classifiers such as RF and gradient lifting tree, a more powerful classifier is constructed to improve the accuracy and robustness of the model. The advantages and disadvantages of different ML methods applied in different applications are shown in Table 2.

Table 2. Comparison of the ML methods applied in different applications.

ML Methods	Advantages	Disadvantages
SVM	It can handle high-dimensional data; has strong generalization ability; suitable for small sample data.	Improper parameter selection can lead to poor classification performance, requiring repeated experimentation and adjustment; its computational complexity is high and only applicable to binary classification problems.
GPR	It can adapt to different data distributions and nonlinear relationships; able to provide an estimate of the uncertainty of the predicted results; provides explanations and inferences about the data, which can help understand the distribution and relationships of the data.	High computational complexity; high memory consumption; difficulty in parameter selection.

Table 2. *Cont.*

ML Methods	Advantages	Disadvantages
ANN, CNN, RNN	ANN can learn nonlinear functions and has the ability to learn weights that map any input to output; CNN will automatically learn filters to help extract correct and relevant features from input data; RNN can capture sequence information from input data, share parameters at different time periods, reduce training parameters, and reduce computational costs.	ANN needs to determine the appropriate network structure and rely on hardware; CNN lacks the ability to keep the input data space unchanged and needs big data training; RNN has gradient vanishing and explosion problems.
DT	It can handle both nominal and data value problems simultaneously; it is suitable for handling samples with missing attributes.	It is easy to overfit and overlooks the correlation of attributes in the dataset.
RF	It can process big datasets, is not easy to overfit, and can also obtain good results for missing values.	For situations with high real-time requirements, the effect is poor.
KPCA	It can effectively capture and represent nonlinear structures and can be used for data denoising.	Consumes a lot of time and computing resources.
VAE	It is an unsupervised learning algorithm, learning potential variables in data, learning without labeling data, and processing continuous and discrete data	Its generation process is random and cannot guarantee the high quality of the sample.

In summary, ML has broad application prospects in the application field of LIBs. However, more in-depth discussion and analysis are needed to further advance related research.

8. Conclusions and Future Directions

With the acceleration in global energy consumption, research interest in energy storage batteries has surged around the world. For lithium-ion energy storage batteries, the development of advanced batteries with high energy density, high power density, long life, and reliable safety is considered critical. Therefore, it is necessary to accelerate the progress of LIB research and conduct research from three perspectives: the material characteristics and internal structure, battery health status, battery fault diagnosis and preventive measures. In addition, with the development of green aviation technology, the advancement of aviation battery research also relies on ML. Compared with traditional methods, ML methods have great advantages in data analysis and processing, and this article describes and discusses the above four aspects in combination with ML methods.

ML can accelerate the development of powerful theoretical tools in battery materials such as advanced function tools for DFT calculations and MD simulations as well as new methods for solving multi-scale physical equations. Through ML, high-precision atomic simulations of large-scale systems can be achieved, allowing for a deeper understanding of the working mechanisms and material evolution schemes in electrochemical reactions, providing assistance for the search and design of new materials and battery formulations. In the estimation of battery SOH, we can extract different features from the battery dataset and select appropriate algorithm models for prediction. Common features include the current, voltage, internal resistance, environmental temperature, and charge discharge ratio. In addition, magnetic testing equipment can be added to extract and predict the magnetic field strength of battery materials as new features. For battery fault diagnosis, ML algorithm models are used to predict the battery data. Usually, parameters such as the current, voltage, and resistance are selected as prediction results and compared with the ideal values to achieve an effective diagnosis. Fault diagnosis in different situations requires the selection of suitable diagnostic models.

For the field of ML itself, the future of ML will present a trend of intelligence, autonomy, and efficiency. Algorithms will become more intelligent and autonomous, with stronger learning and prediction capabilities, capable of handling complex real-world problems. At the same time, the ML model will more automatically select algorithms, models, and parameters, reduce human intervention, and improve efficiency and accuracy. In addition, future ML algorithms will also focus on interpretability and credibility. The current black box feature limits the use of ML in certain critical application areas as it is difficult to explain and understand its decision-making process. Therefore, future algorithms will strive to improve interpretability and credibility in order to better explain and understand the decision-making process of the model. In addition, data privacy and security are also the focus of future ML. With the widespread promotion of ML applications, people are increasingly concerned about the impact of ML on data privacy and security. Therefore, future ML algorithms will place greater emphasis on data privacy and security to better protect the data privacy and security of the users. In the future, the application of ML in LIBs can also develop toward more intelligent, autonomous, and efficient data analysis, prediction, and fault diagnosis. The research on the materials and internal chemical reaction mechanisms of LIBs can also rely on ML to better explain and develop in the future.

Although there has been extensive research on the application of ML algorithms in LIBs with the continuous development of ML algorithms, there are still many challenges.

- With the increasing complexity of ML algorithms and computational requirements, higher requirements have been placed on the performance and energy density of batteries. There is still a need to research and develop new LIB technologies to improve energy storage and release efficiency, extend the battery life, and reduce the charging time.
- The BMS in ML applications is critical to ensure the safety and performance of batteries. In order to further optimize the BMS, it will be necessary to develop an intelligent BMS to improve the efficiency and reliability of the battery through the real-time monitoring of battery status and the estimation of battery life.
- The application of ML in the aviation field is constantly expanding, and future research will explore more application scenarios. For example, utilizing the energy provided by LIBs to develop more intelligent flight control systems, thus improving the autonomy and safety of aircraft, and using ML algorithms to optimize the charging and discharging strategies of batteries and improve their efficiency in aircraft use.

Generally speaking, the ML method requires us to find an algorithm to solve the problem, and the choice of algorithm depends on the specific application.

- The data collection and annotation of LIBs are the foundation of ML applications, but there are still some challenges at present. Further research on effective data collection methods is still needed while developing more accurate and reliable annotation techniques to improve the data quality and availability.
- In the application of ML in LIBs, the selection of appropriate models and optimization algorithms is crucial for the accuracy and efficiency of the results. We need to consider comparing the performance of different models and algorithms, and propose more effective model selection and optimization strategies.
- In order to further improve the generalization ability of ML models, it is necessary to use different datasets for training and testing. Exploring how to build more comprehensive and diverse LIBs datasets and develop ML models that adapt to different environments and application scenarios is needed.
- In the aviation industry, the security of LIBs is crucial. We need to explore how to improve the security of LIBs through ML methods and develop interpretable models to better understand and interpret the decision-making process of the model. For example, using ML algorithms to analyze data in the aviation field and identify potential safety hazards and anomalies. In addition, interpretable models can be developed to better understand and explain the decision-making process of the model, improving the credibility and reliability of LIBs.

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