ENERGY STORAGE SYSTEM AND ARTIFICIAL INTELLIGENCE

Producer: Ali Zeinodiny

Move towards the future of advanced rechargeable batteries (Blue Advance Battery)

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Volume I

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Preface

This book has been written with the aim of examining modern technologies such as artificial intelligence and machine learning in order to design and develop energy storage devices such as batteries. In the first volume of this book, an attempt has been made to get acquainted with the concepts of artificial intelligence and machine learning and then its methods in designing rechargeable batteries and energy storage sources are explained.

Efforts are being made to identify new solutions in the field of batteries, and these solutions will be available to those interested so that new windows can be provided to researchers. Therefore, all our efforts will be in the development of high-capacity batteries in the future. Machine learning will be the only tool to reduce running costs, which can be an efficient roadmap for improving energy storage (batteries, super capacitors, fuel cells, conversions cells, etc.). What the reader and researcher needs is to try to learn the basics of using this emerging technology.

To examine all the present aspects, various articles, books and various sites have been reviewed in order to find a different and useful solution in using artificial intelligence in designing battery components such as cathode, anode and electrolyte, etc., and body storage resources. Payment energy. We hope that the contents of this book will be considered and can be a roadmap for the development of next generation batteries. Dear reader, in case of any mistake or shortcoming in this book, please send the information to the author's e-mail so that it can be corrected in the next volumes and more up-to-date versions and a comprehensive book will be provided to the researchers.

Author: Ali Zeinodiny

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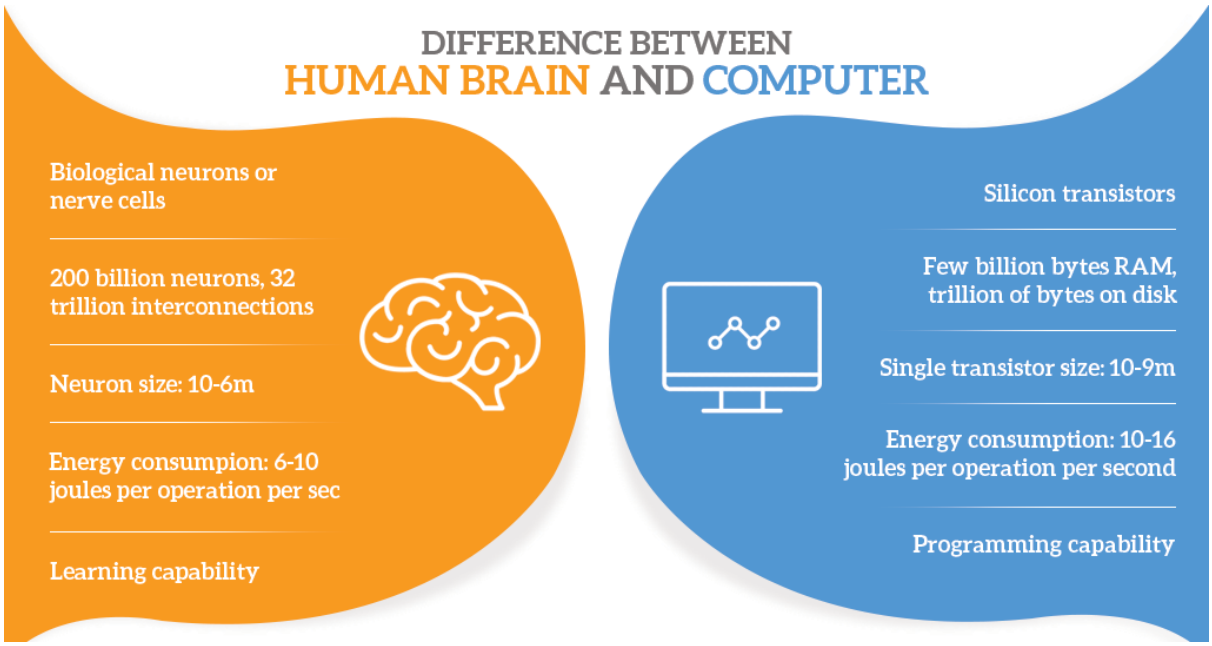
Introduction and History

Lithium batteries have been in great demand due to their widespread use in portable electronics, electric vehicles, and smart grids. Therefore, the cost of materials and spending a lot of time to find these materials and methods is always an unsolvable challenge. Due to the spread of computer science in all fields, today computer science in the field of energy storage, including rechargeable batteries and among them Lithium batteries have arrived. Machine learning, or ML for short, can effectively accelerate material discovery and predict their performance for lithium batteries, which significantly increases the development of these batteries. There have been many successful uses of artificial intelligence and machine learning. In this study, the basic methods and methods of introducing machine learning in batteries will be discussed, and finally, the challenges and perspectives of artificial intelligence in this field will be examined. The increasing demand for energy in everyday life has led to more demand for advanced lithium batteries to meet these needs, including high energy density, high power density, longer life cycle and acceptable cost and cheap pointed out. Discovering new materials for lithium batteries is one of the key factors in improving these functions, including electrodes, electrolytes and other new and advanced materials.

Experimental measurements and computational simulations are two common methods for material discovery and realization. However, these methods have a long time period and analysis of material properties strongly requires equipment conditions, experimental environment and researcher expertise. Each of them can face a percentage of error. With the spread of laboratory information and data, the big data age is approaching and databases have been created, including the Mineral Crystal Structure Database (ICSD), the Cambridge Structure Database, the File and Material Project Database (MP), and the Open Material Database. Quantum is an effective way to accelerate the discovery and design of new materials for lithium batteries.

Machine learning is a powerful tool for detecting and predicting the performance of new materials in large dimensions. This tool is divided into three parts: input, model and output, which are optimized through training data and algorithms, and then build the interface between input and output. Achieved. And then the machine will predict and discover new



materials according to them. Further promotion and development of materials in lithium batteries requires a comprehensive overview of the application of machine learning in lithium batteries and components in batteries such as electrolytes, cathodes and anodes, which will be discussed in other sections.

Figure 1: The difference between the human brain and the computer

The latest UN reports on climate change show that humanity has a multi-year budget for CO_2 emissions at current rates to keep temperatures rising below 1.5 degrees Celsius by 2050. Renewable energy sources fluctuate, hence they must be associated with an efficient energy storage source, where rechargeable batteries are at the forefront of energy storage due to their efficiency and flexibility of operation. Among them, lithium-ion batteries are one of the most influential technologies in modern society, which has made possible the widespread emergence of portable electronic devices and is driving the growth of the electric vehicle market. Even though LIBs have improved significantly, they have greatly improved their energy density since their first LIB cells were successfully commercialized by Sony in 1991, their widespread use for EV or fixed applications requires Is even more optimized in terms of performance, durability, safety, cost, as well as reducing CO_2 and increasing their reusability and recyclability. This is true for current LIBs and any next generation batteries that are currently being developed or manufactured. Several initiatives have been developed

to develop new tools and protocols to reduce the number of experiments in battery research to accelerate the discovery of materials for energy applications. Artificial intelligence, and especially its prolific branch called machine learning, stands out as a promising approach that could lead to a pattern change in battery research and development.

Battery research and development is a complex multivariate issue in which there are many different characteristics such as performance, life cycle analysis, safety, cost, environmental impact and resource issues. In addition, the circular economy of the overall battery should range from the extraction, production, and assembly phase through the long use phase to the reuse and final recycling processes. However, the workflow of the present study relies heavily on a trial-and-error approach that includes material synthesis, fabrication of electrolytes and electrodes, assembly of cells, and ultimately performance appraisal. Even with just these aspects in mind, there are more than a thousand possibilities for synthesizing active ingredients and preparing electrolytes. There can be an almost infinite number of possibilities for selecting electrode production parameters and hundreds of possible cell formats, which is much larger than the human brain, leading to the advent of reverse design tools that can predict the characteristics of battery components needed for a performance goal. Makes it possible and determines the cellular form, makes it difficult.

Battery research and development data is growing exponentially, following the global data field trend. For example, BASF, the world's second-largest chemical producer, recently announced that it generates more than 70 million battery-specific data points per day, and in one academic context, for example, the French network in electrochemical energy storage (RS2E) With about 17 college partners, it produces about 1 petabyte of battery data per year. This huge data set is not currently available to the scientific community as a comprehensive system, but steps have been taken to create open battery and FAIR databases. In addition, huge volumes of data are already being disseminated in scientific journals: there are currently approximately 30,000 publications on lithium batteries, and that number is growing rapidly. A researcher who reads 200 articles a year takes 150 years to read all the LIB publications available today. Therefore, AI and ML should help researchers to effectively solve the parameters and data challenges of LIBs, as well as to research and develop battery technologies beyond LIBs - such as Na-ion, solid-state, and Li-S and others. Batteries and electrochemical capacitors (super capacitors) help. To achieve this, several challenges need to be addressed, for example, defining widely accepted standards in battery research and development along with systematic data disclosure, identifying the most appropriate descriptor (s) for a particular ML model, or determining the associated error. In addition, different battery technologies pose different challenges, and AI and ML-based approaches can be useful in many ways, as ML-assisted operando imaging techniques aim to study the formation and growth of lithium dendrites for all-solid batteries. Other examples could be the increase in time scales and length of current physics-based simulations or the development of innovative multiscale approaches. The aim is to provide a comprehensive, authoritative, and critical, yet easily understood, review of artificial intelligence and machine learning of public interest to the chemical and electrochemical energy community. Concepts, approaches, tools, results and challenges of

using them as an accelerator for battery design and optimization are discussed. More access to booming and highly dynamic articles related to artificial intelligence is crucial for the battery community as an end goal. A strong collaboration between empirical researchers, modeling specialists, and artificial intelligence experts is needed to transfer the artificial intelligence used in batteries. Therefore, AI and ML must be properly explained and examined in a way that is appropriate for the audience. Our goal in this book is to provide better access to these tools and to be complete in terms of various aspects of battery research and development.

In addition, the breadth of battery research and development that uses artificial intelligence and ML has led to inconsistencies in terms used and ambiguity in the direction AI / ML applies to batteries, and major challenges to be addressed. The first goal is to give researchers, with little or no knowledge of the subject, a simple but understandable idea of how artificial intelligence works, and more specifically ML. We hope this will help them critically study modern scientific papers in which artificial intelligence or ML is used for battery research, as well as facilitate collaboration between AI / ML experts and other researchers in the field. Readers interested in a more detailed discussion of AI / ML in general can refer to many of the great books that have already been published on the subject. We first define artificial intelligence and ML, and provide a brief historical perspective. Then, the importance of data and the difference between monitored and unsupervised ML methods along with the importance of their meta-parameters are discussed. Next, we explain in an accessible way the basics of the most widely used ML techniques and the programming languages and software available for their development. Finally, an overview is provided.

What is artificial intelligence?

Artificial intelligence is ubiquitous in our modern world and equips many modern digital devices. Artificial intelligence equips Internet search engines like Google to learn from our search habits and offer us the most relevant results. It is used in social networks such as Facebook or Twitter and Amazon to personalize news feeds, identify people or objects in photos, provide machine translations, or detect inappropriate content, etc. On-demand video services, such as Netflix, use artificial intelligence to personalize suggested videos, and our cell phones use artificial intelligence as personal assistants (such as Siri, Google Now, and Bixby. Other widely accepted artificial intelligence applications). They have capabilities ranging from spam sorting and speech recognition to personalized e-commerce sales offers. Another well-known example is the game, whose major improvements are the Deep Blue, Alpha Go, and Watson chessboards. Located at the center of modern robotic development, automated driving and smart grids, the chemical industry is investing in artificial intelligence and digitization to accelerate its research and development in order to reduce costs and increase the quality of its products. They are using artificial intelligence and ML to expedite research into substances, drugs, catalysts, and so on.

Despite this, artificial intelligence was not as widely accepted as it is today. Even though it is typically associated with the fields of informatics and computer science, the concept of artificial intelligence belongs to fields such as philosophy and psychology that investigate the relationship between humans and machines. From the beginning of human history, the development of new machines and tools ensured the survival of mankind, and as a result, a strong relationship between man and machine was established from ancient times. An example of this can be found in Egyptian society, where the announcement of the next Pharaoh was shown to the people by a statue of the god Amon through a moving mechanical arm. However, the advent of the concept of artificial intelligence and the development of computers, both of which originated with the English mathematician Alan Turing, revolutionized the field. For the first time in human history, the question of the ability to develop machines capable of reasoning like humans is posed by the philosophical question "Can machines think?" Recognized. In his 1950 paper, Alan Turing proposed an experiment now known as the Turing Test, which aimed to examine whether the person being asked interacted with a human or machine through multiple questions without knowing it. Be or not. His identity can distinguish machines from humans. Despite the limitations of such an experiment, Turing was able to guess at a time when machines would be smart enough to reproduce human intelligence, ushering in the age of modern artificial intelligence.

The idea of Turing quickly gained the attention of the scientific community and led to the Dartmouth Artificial Intelligence Summer Research Conference in 1956, which was widely regarded as the founding event of the discipline, and the term artificial intelligence was first coined. The purpose of the conference was defined by its organizer, John McCarthy, who stated: "Every aspect of learning or any other feature of intelligence can in principle be described so precisely that a machine can be built to simulate it." Given this as a starting point, it is not surprising that the first attempts to develop artificial intelligence algorithms were made to simulate the behavior of the human brain.

Historically, artificial intelligence has been defined as making machines think human, act human, think logically, or act rationally. The Turing test, for example, required a machine to operate humanely. However, the clear definition of what is human / rational action or thought is constantly evolving, and not just computer science. It is related to other disciplines such as philosophy, psychology, neurobiology, logic and mathematics. Artificial intelligence can be defined as "the science and engineering of building computers in a way that we thought until recently required human intelligence." However, as in the previous case, whether or not we consider the behaviors we need human intelligence to depend on time and society. Decades ago, many believed that playing games or interpreting human behavior to send personal feeds required human intelligence, while today these are tasks that we know machines can do. All of the above make artificial intelligence a moving target whose exact definition is not insignificant. However, most AI systems are now capable of learning from experience. The most common approach to building machines that do this is through the algorithm architectures known as machine learning, which are used today in battery research and development and will be the main topic of this study. These algorithms have tremendous capabilities for evaluating multidimensional datasets (for example,

datasets containing multiple variables), discovering patterns in data, and unlocking applications that are difficult to exploit using other methods. This is especially true in the areas of battery exploration or battery optimization, where many parameters must be considered simultaneously. The detection capabilities of modern ML algorithms depend on the quantity, quality and accuracy of the data. Therefore, the first step for any ML-based approach is to create a complete and complete dataset. After that, the ML model should be trained and evaluated if possible. In the most common case (supervised models), this is done by using a part of the data set to teach the algorithm (training phase), which can be predicted by comparing the values predicted by the model and the data for the training phase is generally called the experimental phase. Be. If the model obtained during this step is reliable, the monitored ML algorithm is ready to use.

Machine learning algorithms can be classified into supervised, unsupervised or semi-supervised methods. Supervised approaches use datasets that are pre-processed to define certain variables as input and others as output. This is not previously the case for unsupervised ML algorithms, which aim to find patterns in datasets. In supervised ML, a distinction can be made between regression and classification, where the latter shows the ML approach that analyzes the data set by classes, while the former by continuous values. Analyzes. The classes used for a supervised ML can be from the operator or from an unsupervised ML. Semi-regulated methods are somewhere between the two and use datasets that contain labeled and unlabeled data. In addition to the type used, classical ML algorithms rely on data and are relatively agnostic to physics, meaning that they can, for example, instead of providing any physical interpretation of such a relationship, relate the various variables that intercept the training data. They do, they determine. However, there are ML approaches with physical information, for example, when using ML algorithms to solve or discover partial differential equations.

Basic machine learning procedure in lithium batteries

The machine learning method is somewhat similar to the human learning method. The difference is that human intelligence relies on the brain, while machine learning relies on computer algorithms. In general, there are four main steps in the machine learning method: data collection, feature engineering, model construction, and model application. Data are first collected in experimental measurements and simulation calculations or obtained from open databases. The main data features should then be extracted and selected as training data to teach a machine learning model. Third, machine learning algorithms are selected to build a model and learn from training data. Finally, it can be used to guide the discovery of new materials or to predict the properties of lithium batteries.

Machine learning methods in lithium batteries

Machine learning methods play a key role in the results predicted by artificial intelligence and computers. Choosing the right machine learning model can not only achieve reliable results, but also shorten the calculation time. Although there are thousands of artificial intelligence algorithms, they can be divided into three categories based on learning progress, which include supervised learning, unsupervised learning, and reinforcement learning.

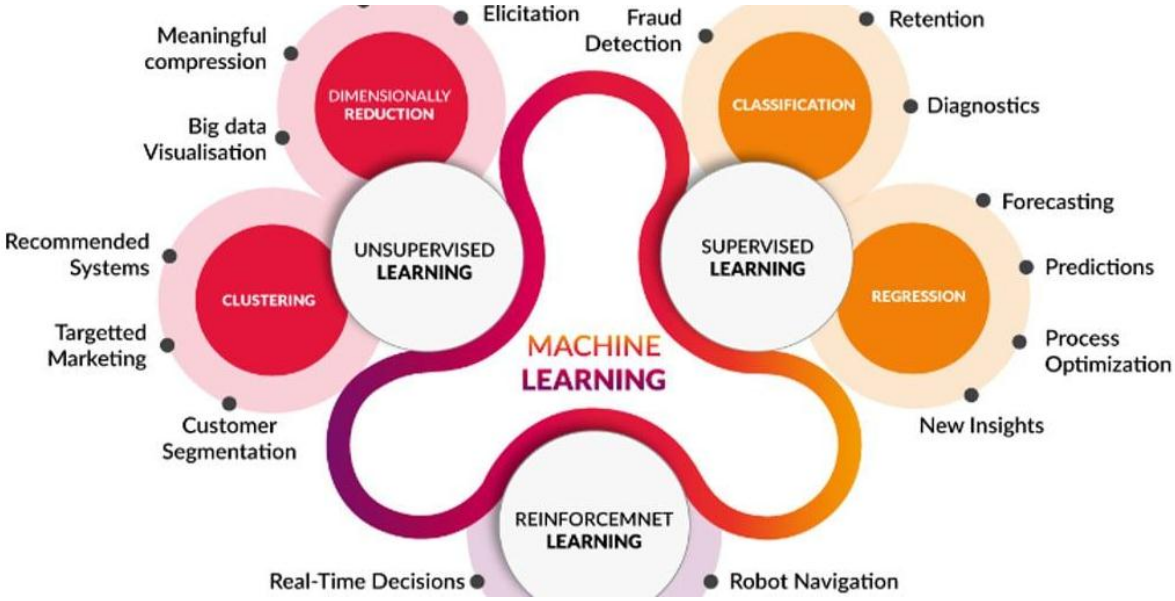


Figure 2: Machine learning methods

Classification of machine learning algorithms in lithium batteries

1. Supervised learning

Supervised learning is the most widely used effective tool among machine learning methods in lithium batteries. Requires a complete set of training data, including relevant input and output data. Supervised learning can create a learning model from educational data and then infer new examples according to the model. The output of the learning model can be a continuous value or a predicted label. Depending on the type of output, supervised learning can be divided into classification problems and regression problems. The purpose of the classification problem is to predict the batch of samples through input. Support vector machine (SVM) is one of the most widely used models in supervised learning. And regression is mainly used to predict the true value of a variable whose output is not the result of classification but a real value.

2. Learning without supervision

Unsupervised learning is another type of machine learning method that can automatically classify input data without labeled instructional examples. Unlike supervised learning, it does not require a complete set of input and output data, and its output is usually uncertain. There is no human intervention in unsupervised learning. Can interpret data independently

and seek solutions. Some new patterns and information can be found by unsupervised learning but not by other methods. Analysis, clustering problems, and data size reduction can be solved by unsupervised learning. There are many methods for unsupervised learning, such as automated encryption, principal component analysis, K-means, noise-based spatial clustering of programs, and maximizing algorithm expectations.

3. Reinforcement learning

Reinforcement learning with continuous rewards and punishments solves problems and can achieve an optimal strategy after continuous strengthening of operations. It is a trial and error learning process to maximize long-term returns. Reinforcement learning can improve your behavior and algorithm through reward function feedback. Unlike supervised learning and unsupervised learning, the reinforcing learning process is dynamic and interactive, and data in reinforced learning is generated through continuous interaction with the environment. However, reinforcement learning is not simple in practice and its implementation requires a variety of algorithms.

Machine learning algorithms in lithium batteries

1. Linear regression (LR)

Linear regression is one of the simplest models in machine learning. There is a set of input variables (x) to determine the output variables (y) in linear regression. The purpose of linear regression is to quantify the relationship between input variables (x) and output variables (y). In linear regression, the relation is expressed as the equation $y = bx + a$ in which b is the slope and a is the width of the origin. As shown in Figure 3 (a), the goal of linear regression is to match the nearest line to most points. The benefits of linear regression lie in two aspects. One is that it requires low computational costs. Another is that it is easy to interpret its physical meaning. However, the relationship between input and output for lithium batteries is often nonlinear. Linear regression leads to nonlinear result if incorrect prediction is applied.

Gaussian process regression (GRR)

Linear regression uses a linear equation $y = bx + a$ to express the relationship between input and output, which in nonlinear cases leads to incorrect prediction. Nonlinear equations can be adopted to predict the result for nonlinear cases known as nonlinear regression. However, these predetermined equations may not be able to accurately describe the target cases. The Gaussian process (GP) considers all possible equations. Gaussian process regression is a nonparametric model that uses GP before analyzing data. If the form of the nucleus equation is not finite, the Gaussian process regression is a theoretical approximation of any continuous equation in compact space. In addition, Gaussian process

regression can provide a posteriori prediction results, and when the distribution is likely to be normal, a posterior is analytical. Therefore, Gaussian process regression is a global and analytical probability model.

3. Nearest neighbors point k (kNN)

The kNN algorithm is one of the most complete algorithms in machine learning. The principle of this algorithm is to identify samples with the majority of their nearest neighbors to their point k. As shown in Figure 3 (b), a series of data is classified into a yellow class and a purple class. When a new sample is imported (red sample), the model calculates the distance from the red sample to each yellow and purple sample. Then, the nearest point k can be selected from the training data, where the majority type is the new sample type. kNN is a supervised learning algorithm that can be used for classification and regression. However, when the training dataset is large, kNN prediction is time consuming.

4. Support Vector Machine (SVM)

The backup vector machine is a generalized linear classifier for binary classification of data. The decision limit of this method is the maximum level of margin of learning examples. As shown in Figure 3 (c), the SVM must first find the data at the edge of the set (called the backup vector) and then use these points to obtain a page (called the decision page). Slow, where the distance between the backup vector and the plate is maximized. In the matter of classification, there are usually many levels of decision-making. The basic backup machine model is to find the best decision page in the feature space that can maximize the distance between positive and negative samples in the training dataset. Backup machine vector is a common machine learning algorithm in lithium batteries. One of the advantages of SVMs is that they can deal with more complex problems than other simple models such as decision trees, and can be integrated seamlessly by merging different decision trees for a problem or adding random factors. Avoid over-construction. Another issue is that less meta-parameters need to be set and the result of the prediction is not sensitive to changes in meta-parameter values and the data set scale.

4. Artificial Neural Network (ANN)

An artificial neural network is a nonlinear and adaptive information processing system consisting of a large number of interconnected processing units. This is an algorithmic mathematical model that mimics the neural-behavioral properties of animals

The typical structure networks of an artificial neural network are shown in Figure 3 (d), which includes an input layer, an output layer, and n hidden layers ($n \geq 1$). ANN methods can effectively find complex nonlinear relationships from large-scale datasets. However, these methods usually require large amounts of training data for accurate prediction. They are "black boxes" in which physical importance is neglected. ANN is a commonly

supervised learning algorithm. It is well accepted that the artificial neural network is a typical nonlinear learning model that can fully approximate complex nonlinear relationships in lithium batteries. It has strong robustness and error tolerance against noise in the data. However, it needs to determine a large number of parameters such as network topology, initial values of weights and thresholds. The training process requires a large amount of data and computational time.

5. Simple Bayes (Naïve Bayes)

Bayesian simple classification methods are based on Bayesian theorem. Meanwhile, the terms between the features in the simple Bayesian are independent. The simple Bayesian mathematical principle is as follows: To classify the samples, the probability of occurrence of each category can be calculated with a conditional probability formula. The samples will belong to the category most likely. A simple example of a simple Bayesian classification is shown in Figure 3 (e). There are two categories y1 and y2 that each person has four main characteristics. The color represents the value of each attribute. Then, f (x) is taught by a simple Bayesian algorithm. It is the output handle of this model that makes the function have the maximum value.

The simple Bayesian algorithm has the advantages of simple implementation, without repetition, high learning efficiency and good performance in large sample sizes. However, it assumes that the characteristic conditions of the input data are independent, which is a very strong assumption. Therefore, it is not applicable when the input data feature conditions are relevant.

6. Decision tree

The decision tree has a tree structure similar to a flow chart (Figure 3-Section (f). Classification is mainly based on the prediction of each leaf node, where the final decision is made through continuous prediction. The decision tree can provide the result of high accuracy prediction with low computational cost The biggest disadvantage of decision trees is that the trees are too complex which can lead to excessive integration Statistical methods are commonly used to reduce the complexity of trees.

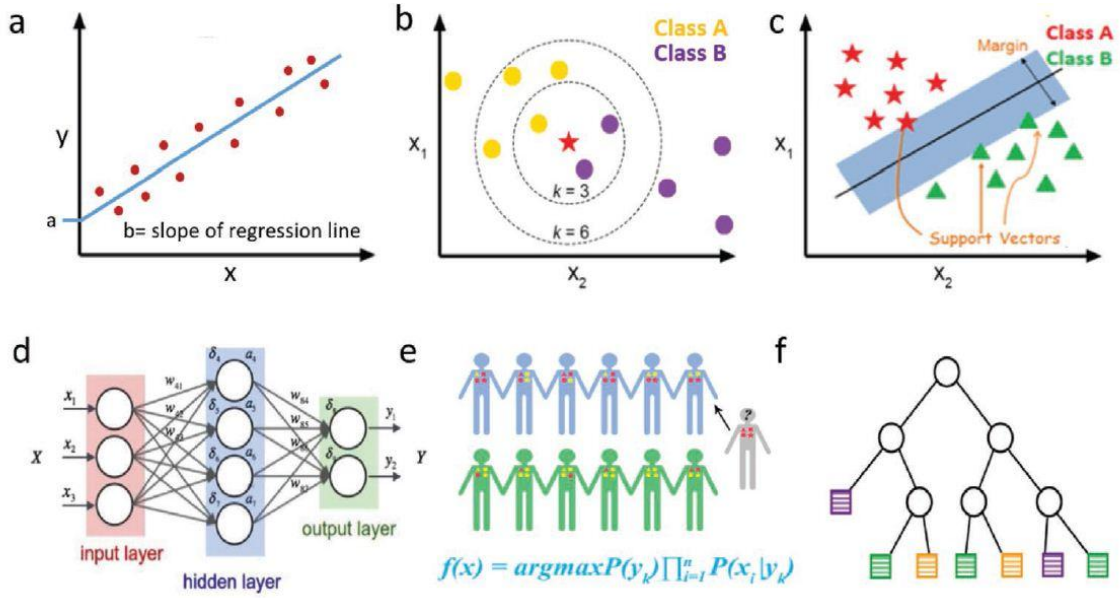


Figure 3: Machine learning algorithms in lithium batteries

7- K-Means

K-means is a well-known clustering algorithm that can find K centers that represent the clustering structure. As shown in Figure 4, the green dots are the raw data set, the red X and the blue X represent the center of the cluster in Figure 4 (b). If a point is closer to other centers than one center, that point is assigned to the cluster denoted by the nearest center (Figure 4-Section (c). Then, define the center of the cluster with the current clustering points as the new center. (Figure 4- (f) The principle of K-means is simple and can easily be applied with a clear physical meaning. However, the center K must be determined correctly before performing K-means. Prediction is sensitive to noise and throw points in the input data.

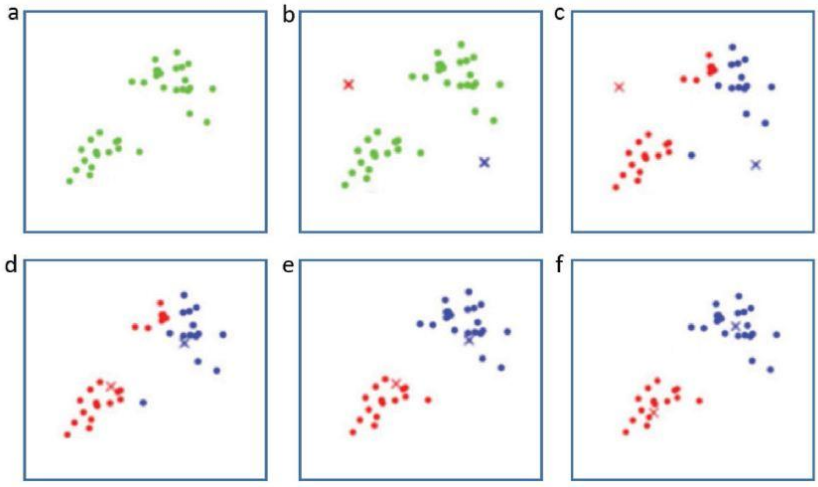


Figure 4: Diagram of K-Means algorithms

Application of machine learning in lithium batteries

Machine learning is widely used in lithium batteries and has been proven to have both time efficiency and predictive accuracy. Predicting performance and discovering materials are the two main directions of machine learning in lithium batteries. Through machine learning methods, it is necessary to establish a quantitative relationship between structure and activity between descriptors and decision characteristics in both directions. Among them, regression analysis methods are generally used to predict performance, which requires considering many of the basic properties of materials as descriptors. Classification and clustering algorithms are commonly used to discover new materials that require large amounts of data from open access databases. In this section, recent advances in machine learning applications related to electrolytes, cathodes, anodes, and lithium battery performance are reported.

Electrolytes

Electrolytes are essential components of lithium batteries and play a dominant role in determining the performance of lithium batteries. Electrolytes are used to conduct lithium ions in batteries and therefore must be both ionically conductive and electronically insulating. In addition, the compatibility of the electrode / electrolyte interface is determined by the chemical and electrochemical activities between the electrolyte and the electrodes. Therefore, finding high-performance electrolytes is a key issue in the development of advanced lithium batteries. There are currently three major types of electrolytes in lithium batteries: liquid electrolytes, polymer electrolytes, and solid-state inorganic electrolytes. Many machine learning methods have been developed to discover new electrolyte materials and predict their properties. The redox potential of electrolytes is also an important indicator of the activity of the electrochemical reaction between the electrodes and the electrolytes. The machine learning approach was combined with initial calculations to predict oxidation potentials and reduce new additives in electrolytes. Solid electrolytes (ISEs) have attracted a great deal of attention in recent years. Compared to conventional liquid electrolytes, lithium batteries that use solid electrolytes can have higher energy densities, superior safety performance, and longer life. There are many promising solid electrolytes that have been studied. For these solid electrolytes, ion transfer property is one of the most important features that various machine learning methods have been developed to accelerate the prediction of ion transfer properties in solid electrolytes. In general, DFT has been widely used to study the ion transfer properties of ISEs. However, this method is not only time consuming, but also impossible for large systems containing more than a hundred atoms. Combining a machine learning approach with DFT can effectively speed up computation and encourage the discovery of new ISE materials.

Compared to solid electrolytes, polymer (PE) electrolytes have advantages in terms of safety, cost, and flexibility that make them one of the most promising electrolyte materials for lithium batteries. However, PEs generally have low ionic conductivity, which limits their practical application in lithium batteries. To address this key problem, researchers

have conducted many experimental studies since its discovery. However, many factors affect ionic conductivity due to the complex composition of polyethylene's, which dramatically slows research progress. The machine learning approach can quickly predict the ion transfer properties of polyethylene, which effectively accelerates research into advanced polyethylene materials.

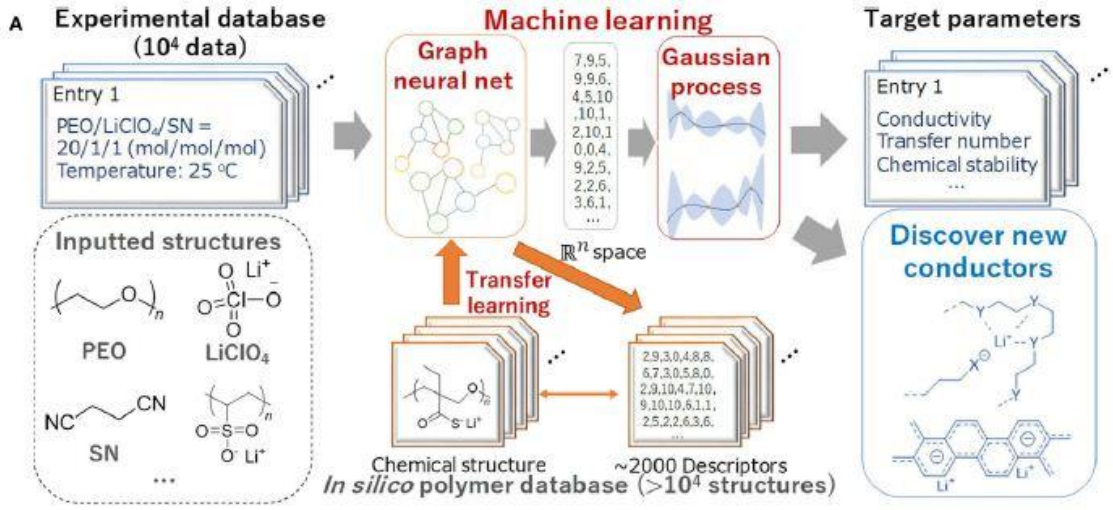


Figure 5: A scheme for using artificial intelligence to predict the conductivity of solid polymer electrolytes

Cathode

Cathodes are very important in lithium batteries, they are one of the key factors in determining energy density, output power, cycle life and user safety of lithium batteries. Voltage, redox potential, changes in volume, capacity and thickness of the cathode material layer are closely related to the above functions, which are commonly used in predicting cathode material performance. High voltage cathode materials can increase the voltage platform of lithium batteries, which is a key component for high energy density lithium batteries. To evaluate the voltage platform, an ANN was integrated with DFT calculations to predict the electrochemical potential of the cathode material. The prediction results were in good agreement with the known experimental results. However, there were only small data (31 samples) that limited the accuracy of the ANN model. To increase the prediction accuracy, the combination of different algorithms was increased to 4250 data samples.

The results showed that machine learning models could reproduce DFT processes, which were successfully used to detect electrode materials in terms of voltage. In addition, the ANN-DFT framework was used to predict the redox potentials of carbon-based molecular electrode materials.

The crystal structure of cathodic materials had a significant effect on the physical and chemical properties of lithium batteries. To investigate the crystal structure of cathodic materials, five classification algorithms with DFT calculations were performed to predict crystal systems based on artificial intelligence (machine learning).

Volume changes in cathodic materials during the charging and discharging process have a very significant effect on the cycle performance and longevity of lithium batteries. Artificial intelligence-

based regression algorithms and amplification algorithms have been very effective in predicting volume changes in cathodic materials.

The mass charge of the electrode determines the energy density of the battery, which must be precisely controlled during the manufacturing process. A GPR-based learning model was proposed to analyze the importance of variables, their characteristics and their effects on mass load. As a result, it is possible to predict a satisfactory mass load of the electrodes.

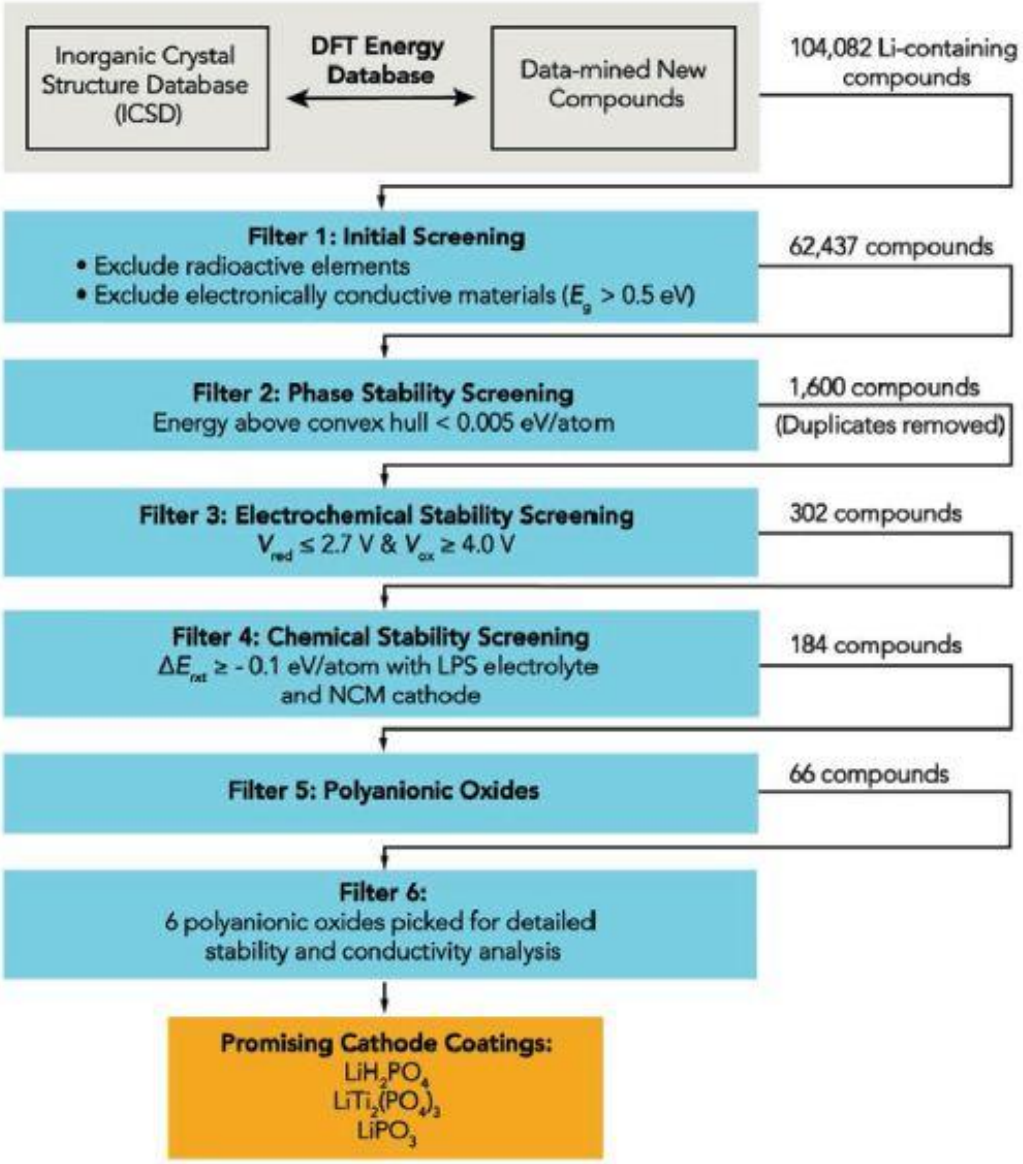


Figure 6: Flowchart describing computational screening of cathodic coating materials

Anode

Lithium metal has an extremely high theoretical specific capacity (3860 mAh / g) and electrochemical potential

(3.04 V vs. standard hydrogen electrodes) is the "holy grail" anode for high energy density lithium batteries. However, there are some serious problems with lithium metal anodes, such as dendrites and high reactivity, which lead to low Coulomb efficiency, rapid capacity reduction, poor lifespan, and severe safety hazards. In recent years, machine learning approaches to accelerate correlation studies have begun to use lithium metal anodes. As a result, it was found that there are few applications of machine learning in the anode, and most of them focus on the lithium metal anode. In fact, silicon electrodes, graphite electrodes, and organic electrodes are promising anodic materials for advanced lithium batteries, all of which have advantages and disadvantages that machine learning can use in these anodic materials to solve some of the classic problems of these materials, such as electrode volumetric expansion. Silicone, used.

Battery performance

Battery performance, such as battery life and heat volatile performance, is important for the practical application of lithium batteries, which are obviously influenced by many experimental parameters. However, performing experiments with different parameters requires a lot of time and money. Machine learning techniques can effectively speed up battery performance forecasting while saving time and money.

Choe and Bratz developed a cycle-life prediction model using initial cycle discharge data to detect capacity reduction. It ranged from 150 to 2300 cycles. As a result, a 9.1% test error was obtained to quantitatively predict cycle life using only the first 100 cycles in the best models. A test error of 4.9% was obtained using the data of the first 5 cycles in adjusting the classification of the predicted models. In addition, to reduce the number and duration of experiments, a very fast CLO system was developed, as shown in Figure 7. An initial prediction model in the CLO system was used to predict the final cycle life using data from the first 100 cycles, which can effectively reduce test time. Using this method, high-cycle charging protocols among 224 candidates in 16 The day was quickly identified, which required more than 500 days to conduct a comprehensive search without prior forecasting. The accuracy and efficiency of our optimization approach was confirmed by experimental data. This method can be extended to other design spaces with fast charging as well as other purposes and will have a wide impact on the development and production of energy storage devices.

In short, a good prediction of battery performance can be achieved by using appropriate machine learning methods, especially nonlinear methods. However, those nonlinear models, such as ANN and Bayesian, where physical significance is usually avoided. Therefore, the development of interpretable algorithms beyond these models is an effective

way to discover the scientific laws of lithium batteries. But these questions must be answered before anything else.

Is the machine learning algorithm suitable for the job? Which machine learning algorithm is better for processing work? We do not know the answers. Therefore, automatically designing a machine learning model or modifying its algorithm for a specific task will lead to adopting the model to help further applications in the future.

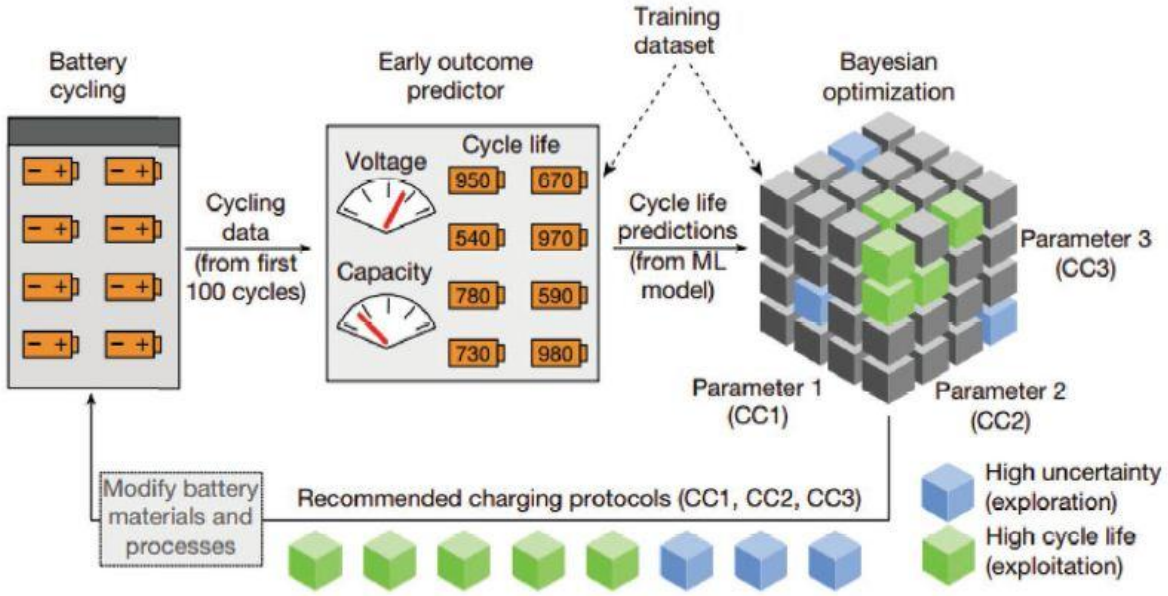


Figure 7: Schematic of the CLO system where the batteries are tested first. Cycle data from the first 100 cycles is used as input to predict the initial outcome of the cycle life

Challenges and prospects

Machine learning technologies are now widely used in lithium batteries. In particular, with calculations or experiments, machine learning technologies can effectively save time and money and significantly accelerate the discovery of new materials. This is a great impetus for the development of lithium batteries and a fast track to research into energy storage technology. However, many new problems and challenges arise with the growing demand for machine learning technologies. Some of the challenges and problems are as follows:

1. Machine learning is a data-driven science whose quality depends abnormally on the size of the database. To improve forecasting accuracy, a more open database for high-throughput screening is urgently needed. In addition, the information in the current database is fragmented and not comprehensive enough. Therefore, many more material properties should be available in the database, such as electronegative, HOMO, LUMO, first ionization energy, coordination energy, chemical bond energy and implicit correlations, etc.

Different data must be found by machine learning to form a network knowledge structure. In addition, a small number of "failed data" are included in current databases, which usually produce

many experiments but are not obtained from the published literature. Collecting that "failed data" in the data set can effectively improve the accuracy of machine learning methods.

2- Data quality can significantly affect the accuracy of machine learning. Free-access database data has been collected from various publications and may be biased. Combining this data with machine learning methods can also reduce the accuracy of prediction results. How to improve the quality of databases is an important problem in improving it?

3- Selecting features is another important way for machine learning models to succeed. Currently, most feature selection is determined by the experience of researchers, which may omit some useful features. To solve this problem, automated feature engineering should be used to teach machine learning models and reduce artificial errors.

4- Predicting machine learning methods is sometimes in conflict with specialized knowledge. To reduce this problem, we can integrate more professional knowledge into feature selection or computing. Recently, a group of researchers proposed a data-based multi-layer feature selection method that incorporates specialized field knowledge. This method can represent objective properties with a smaller and more interpretable set of features, while ensuring equal or better prediction accuracy, which is important for feature optimization.

Interpretability of machine learning models is also a key challenge. Due to the complex electrochemical behavior of lithium batteries, linear algorithms can generally not be used to establish the relationship between microstructure and material properties.

Nonlinear models, such as ANN and SVR, can create complex nonlinear relationships between various factors and targets that are widely used in lithium batteries. However, those nonlinear models are usually "black boxes" in which physical significance is avoided. Therefore, the development of interpretable algorithms beyond these models is an effective way to study the scientific laws of lithium batteries.

6- With the development of lithium batteries, more material performance of lithium batteries is considered and required, such as mechanical properties and self-healing properties of solid electrolytes, volumetric expansion of silicon electrodes, separation of graphite electrodes under fast charge, and dissolution of negative electrodes. To. It is believed that machine learning can play an important role in this research.

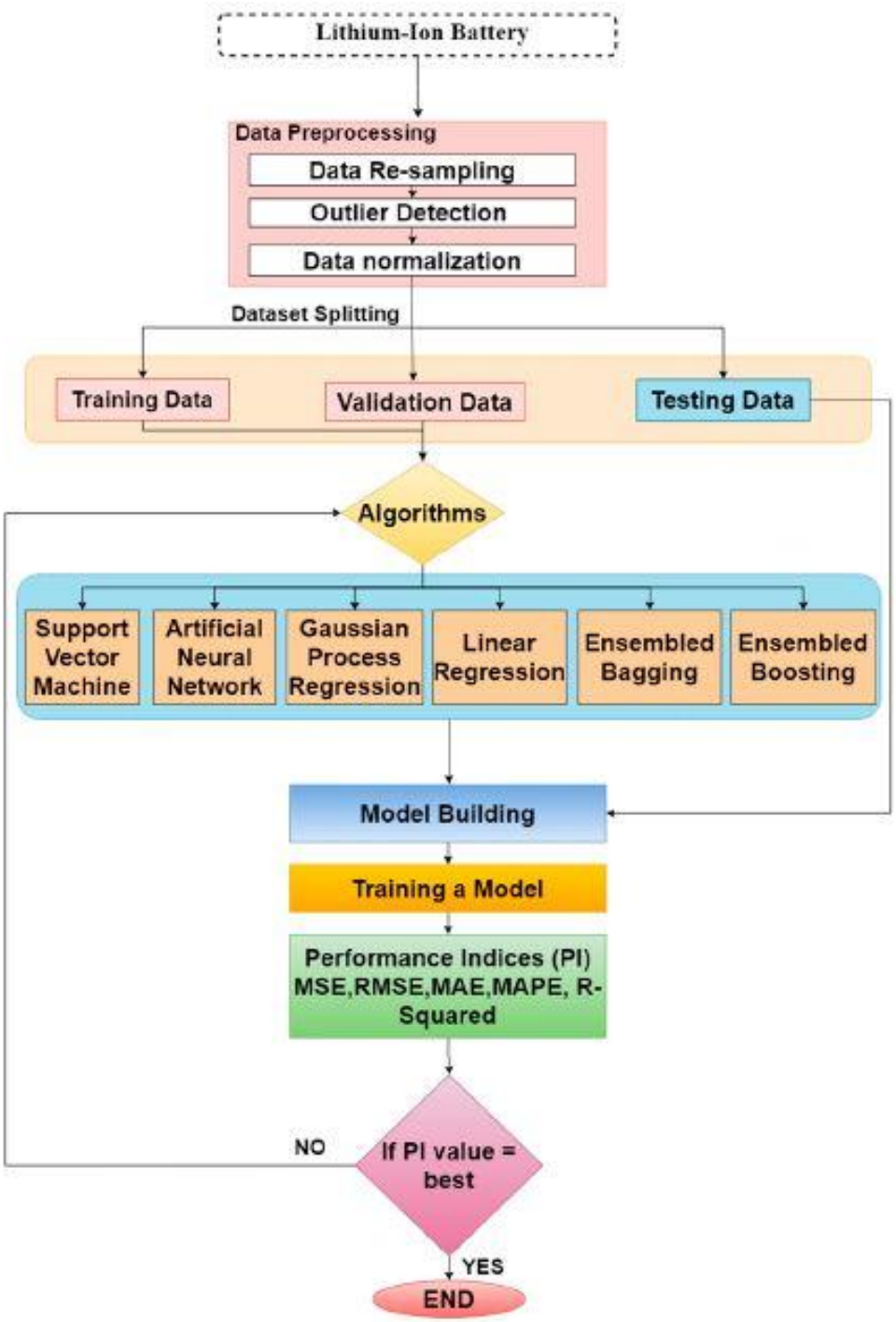


Figure 8: General flowchart of machine learning in lithium batteries

Battery testing process

Inside a lab at Stanford University's Récourt Energy Institute, there are twelve refrigerator-sized cabinets designed to consume batteries as quickly as possible. Each has about 100 lithium-ion cells stored in trays that can charge and discharge batteries dozens of times a day. Typically, batteries housed inside these electrochemical chambers are used inside electrical appliances or devices. But when they are placed in the holding devices, they do not receive any force. Instead, energy flows in and out of these cells as quickly as possible to generate performance data that teaches AI how to make better batteries.

The introduction of artificial intelligence to test batteries

In 2019, a team of researchers at Stanford, MIT and the Toyota Research Institute used artificial intelligence trained on the data generated by these devices to predict the performance of lithium-ion batteries during cell life before they began to slip. Typically, artificial intelligence needs data from the start of battery life to predict future performance. It may take months for the battery to charge enough. But AI researchers can predict lifespan performance after just a few hours of data collection, while the battery is still at its peak. "Before we came here, no one thought it was possible," said Stanford materials scientist William Choue. And earlier this year, Chouh and his colleagues did it again.

Fast battery charge

In a February paper published in Nature, Chueh and colleagues described an experiment in which artificial intelligence was able to find the optimal way to quickly charge a lithium-ion battery for 10 minutes. Many experts think that fast charging batteries are very important for the acceptance of electric cars by the general public. But it should be noted that the speed of discharging the charge of these batteries also contributes to the performance of these cars. Leaving fast-charging batteries out of the lab and entering the real world means finding the point between charging speed and battery life. The problem is that there is an infinitely efficient way to charge the battery. These methods were compared in the laboratory. Experimental screening All of these methods to find the best charging method can be tedious and tedious, but this is where artificial intelligence comes in handy.

The impact of artificial intelligence on the testing process

In less than a month, Chueh and his colleagues were able to optimize the fast-charging lithium-ion battery protocol. Achieving the same results without the help of artificial intelligence took about two years.

"With the help of artificial intelligence, at the end of the day, we were speeding up battery research and development," says Chueh. "Both the discovery of new chemicals and finding

the best way to make batteries safer were both time-consuming tasks. "Battery performance has grown dramatically over the past decade or so. Their cost has dropped dramatically. For researchers like Chueh, the speed of battery innovation did not happen fast enough. The reason is simple: batteries are very complex. Making a better battery means brutal optimization at every stage of the production process. It's all about using cheaper raw materials, better chemistry, efficient production techniques. But there are many parameters that can be optimized. Improvements in one area - such as energy density - often come at a cost of increasing profits in another area, such as charge rates. Finding optimal solutions in a huge search space is exactly the kind of problem that AI has created to solve. Until recently, however, artificial intelligence made it difficult to build batteries due to a lack of information.

Lack of information

"In the past, it was very difficult to get information on battery life because researchers and companies did not share that information," said Bruis van Vlijmen, a battery analyst at Stanford.

"There is a high level of confidentiality or proprietary information."

Following their 2019 paper, Chueh and colleagues made all of their battery data available to the public to be used by other researchers to teach artificial intelligence algorithms. At the time, this was the largest battery performance database ever released.

According to Ian Foster, director of data science and learning at Argonne National Laboratory, the lack of quality data is a long-standing issue. Over the past few years, Foster and his colleagues at the lab have been building a database of elements that can be used by machine learning algorithms to capture chemicals that may improve battery electrolyte performance. A substance that lies between two parts.

Electrodes, like other elements in a battery, can modify electrolyte chemicals to increase desirable properties such as energy density or reduce undesirable properties such as toxicity.

"From the past until now, the identification of new electrolyte materials has been a process of trial and error," says Foster. "Our goal is to use artificial intelligence techniques to explore the infinite space of possible materials."

Application of machine learning

In late 2019, the Argon team published an article on how to use the existing database of 133,000 organic molecules and laboratory supercomputers to create highly accurate simulations of the properties of these molecules to "heavy" or "non-hydrogen" molecules. harvest.

Their idea was to use this database to teach machine learning algorithms to find molecules with desirable properties in a relatively small data set so that they could discover a much larger database of potential material.

The molecules in most battery electrolytes may be as heavy as 20 atoms. There are many ways to combine these atoms. For example, another database of organic molecules with a maximum of 17 heavy atoms consists of 166 billion samples. This is an unreasonably large space for an AI to look for promising examples without having a good idea of what it is looking for. Foster says the argon electrolyte search algorithm is still in its infancy. No new material has been identified yet. But the next step is to create a physical cell using that electrolyte substance for testing. The data from these experiments can then be used to further refine the algorithm and help search for better examples.

"The process of finding the right electrolyte and moving from a large number of electrolytes to one electrolyte for car batteries is really long," says Foster. "The purpose of machine learning is to speed up the testing process."

Data retention

Foster teamed with battery scientists at ten research institutes and companies to facilitate the sharing of statistics across organizations. The group hopes to use a platform developed at the University of Chicago called the Data Station. This platform allows researchers to teach machine learning models based on information sets that different groups help with. Without direct external access to their data. A machine learning model is loaded on the platform. Learns about data. It then provides output to researchers.

Those scientists do not know the specifications of the data, but they can determine whether exposure to the data improves the model's ability to predict batteries. Foster and his colleagues hope that this will reduce people's fear of losing proprietary data to competitors while allowing them to create large data sets.

Other applications of artificial intelligence and machine learning

But even without massive shared databases, the use of artificial intelligence in battery development is booming. As reported in an article in Frontiers in Energy Research, artificial intelligence has been used for a significant number of applications in battery research over the past year.

On the material side, molecules have been used to study lithium metal anodes that can stabilize energy densities dramatically but are currently of great safety concern. Machine learning has also been used to discover possible cathode coatings to improve the performance of solid electrolyte batteries. Which is more safe than liquid electrolytes in batteries?

Artificial intelligence has also been used to optimize researchers' understanding of existing batteries by optimizing battery management systems and creating accurate mathematical models of batteries to simulate their performance in electronic vehicles.

Artificial intelligence researchers have even written a book summarizing current research on lithium-ion batteries.

"There is a lot of untapped potential in existing battery materials that we can use to better use software for "Plan to use the battery".

"New Battery Health Predictions will benefit from the scalable battery software innovation we saw in the digital revolution, ushering in a new era of energy storage technologies."

The next step is to take these machine learning techniques out of the lab and use them to build the batteries that power our gadgets and cars. InfoBar, a Slovak-based company founded in 2018, is a pioneer in this field. Using artificial intelligence research platform developed by California-based Wildcat Discovery Technologies, the company is rapidly producing prototypes of new battery chemistry to build custom cells for electric vehicles.

According to InfoBar CEO Marianne Bukk, the Al platform will allow for a comprehensive investigation into the new lithium-ion chemistry, which could speed up the discovery process. In other words, artificial intelligence can simulate the performance of a battery when several different variables are modified simultaneously. Instead of manipulating one part of the battery at a time and testing all the repetitions completely.

"The way to discover new cellular chemistry is 10 times faster than a traditional laboratory," says Bocek, who compares research into InfoBar artificial intelligence fuel using automated drug discovery in the pharmaceutical industry. "We are moving away from the 'one size fits all' model that dominates the EV industry." InfoBar last week unveiled its first "smart battery" designed with artificial intelligence. During the announcement, Bocek claimed that the battery could increase the range of the "best" option in the EV class by almost 20%.

But do not expect to find it in an average EV battery pack anytime soon. Unlike large manufacturers of lithium ion cells, such as Panasonic or Samsung, InfoBar is more of a battery boutique.

The company focuses on specialized vehicles such as high-performance electric cars or electric aircraft, and can produce small volumes to produce cells that meet customer-specific needs. "We are the only player in this market that has the ability to create a custom solution in terms of cell format and energy density," says Bocek.

Bocek says the company's first test plant will start working on batteries by the end of next year. Initially, the plant produced only 100 megawatt hours of Al-designed batteries per year. That's about half of Tesla's Gig factory production volume in Nevada. Bocek says the company plans to increase its production to 10 gigawatt hours in five years.

Conclusion

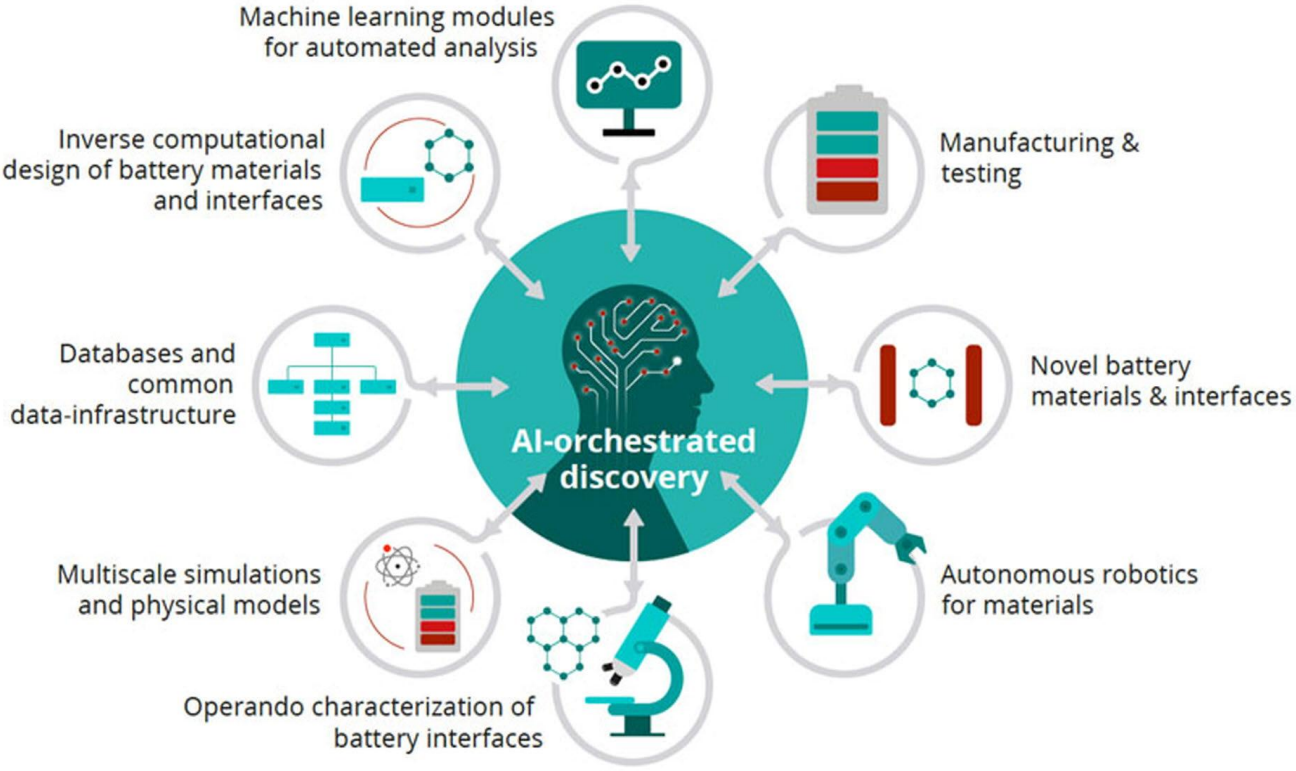
Currently, the long research and development cycle is the most important challenge for the development of new materials. It takes about 20 to 30 years for a new material to develop from discovery to practical application. For products with high requirements, such as aviation equipment, the development time will be longer. Four reasons for the time-consuming and laborious development of new materials:

(1) The subject of research is complex.

(2) Research relies on accumulated personal experience.

(3) The research method is repetitive and based on trial and error.

(4) After completing the development of new materials, it takes a long time to determine the production process and operational parameters.



The use of artificial intelligence in material research and development is a new solution to the problem of long research and the current material cycle. Materials research, prototyping, testing, validation, and cycle evaluation, which used to take a long time in laboratories, can now be performed in a virtual laboratory. Therefore, it can increase the speed of material development.

However, the use of artificial intelligence in material research still has certain drawbacks. The first problem when using artificial intelligence to discover materials is to create a database. The database created by the researchers should include a wide range of material data such as electronegativity, first ionization energy, chemicals, bond energy, single cell parameters, and so on.

It should also allow different data to have implicit correlations to form a network knowledge structure. On the one hand, the current database information is fragmented and not comprehensive enough.

Therefore, the integration of artificial intelligence algorithms and finding new algorithms will be the solution to use this technology in lithium batteries to discover new materia