Predicting the Current and Future State of Batteries using Data-Driven Machine Learning

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Machine learning is a specific application of artificial intelligence that allows computers to learn and improve from data and experience via sets of algorithms, without the need for reprogramming. In the field of energy storage, machine learning has recently emerged as a novel approach for battery modelling, not only to determine the current state-of-charge of batteries, but also predict their future state-of-health and remaining useful life. In this review, we first discuss the two most studied types of battery models in the literature for battery state prediction: the equivalent circuit and physics-based models. Based on the current limitations of these models, we showcase the promise of machine learning techniques for fast and accurate battery state prediction, as well as the major challenges involved, especially in high-throughput data generation. In addition, we propose the incorporation of physics and domain knowledge to develop machine learning models that are more explainable and interpretable. Overall, we see data-driven machine learning as a promising modelling technique that can open up new, exciting opportunities in battery manufacturing, usage, and optimization in the future.

1 Introduction

With rising concerns about global warming, electrification of transport has emerged as an important vision in many countries in recent years. The successful development of electric vehicles (EVs) depends highly on the cycling performance, cost, and safety of the batteries. Rechargeable lithium-ion (Li-ion) batteries are currently the best choice for EVs due to their reasonable energy density and cycle life.[1] Further research and development on Li-ion batteries will lead to even higher energy density and more complicated battery dynamics,[2] where the efficiency and safety of such batteries will become a concern. An advanced battery management system (BMS) that can monitor and optimize battery behavior and safety is thus essential for the entire electrification system.

Today, one of the major barriers to widespread adoption of EVs is range anxiety. The ability of a BMS to accurately determine the state-of-charge (SOC) and state-of-health (SOH) of batteries, and hence the estimated driving range, will alleviate this problem. In addition, reliable prediction of remaining useful life (RUL) will allow batteries to be used to their fullest potential and maximum life expectancy before replacement or disposal. Knowledge of the RUL of spent batteries will also enable their re-deployment in less demanding, second life applications such as stationary grid storage. If we are able to sort manufactured cells based on their expected lifetime using early-cycle data, we can further accelerate the testing, validation, and development process of new batteries. In summary, accurate prediction of the current and future state of batteries will open up vast opportunities in battery manufacturing, usage, and optimization.[3]

SOC and SOH are the two most important parameters in battery management and are generally defined as:

$$SOC = \frac{C_{rem}}{C_{act}} \times 100\,\%$$

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where  is the remaining capacity of the battery in its current state,  is the actual capacity of the battery at full charge, C_{nom} is the nominal capacity of the brand new battery, and  is the capacity of the battery at end of life (EOL).[4]

In essence, SOC denotes the remaining capacity of the battery in its current state compared to its actual capacity at full charge (equivalent of a fuel gauge), while SOH describes the actual capacity of the battery at full charge compared to the nominal capacity when new. By definition, SOC is 100% when the battery is fully charged and 0% when it is empty, while SOH is 100% at the time of manufacture and reaches 0% at EOL. In the battery manufacturing industry, EOL is often defined as the point at which the actual capacity at full charge drops to 80% of its nominal value, i.e. $C_{EOL} = 0.8 \times C_{nom}$. The remaining number of charge/discharge cycles until the battery reaches EOL is the RUL of the battery. Current BMSs can determine the SOC of Li-ion batteries within 0.6% to 6.5%,[5] but are unable to predict the SOH and RUL of batteries accurately.[6]

The traditional methods for SOC estimation include ampere-hour (AH) counting estimation; open circuit voltage (OCV) based estimation; impedance based estimation; model-based estimation; Fuzzy logic; Kalman filter and observer.[4–14] Among all these methods, the major advantage of the model-based method is its ability to be used for on-line applications. In fact, equivalent circuit models (ECMs) are currently the main battery models that are widely used in the BMS of EVs for on-line SOC estimations due to their low computational demand. But the accuracy is usually limited to the range that the model has been parameterized. A further improvement on model-based method is to develop physics-based models (PBMs). The most studied PBM model is called the pseudo 2D (P2D) model which provides insights into the internal dynamics of the batteries. However, the governing equations are complicated and require a high computational cost to solve, making it less practical for on-line applications. In section 2, we will discuss in detail the intrinsic characteristics of these two most studied models (ECM and PBM) in the literature.

Despite the progress in developing more accurate and fast models for on-line SOC and SOH estimations, there remains a clear tradeoff between the computational efficiency and the accuracy of model-based predictions. Recently, data-driven models (DDMs) have drawn

much attention. Combined with machine learning techniques, these models are able to make predictions without prior knowledge of the system (Figure 1). Machine learning techniques including neural network, support-vector machine, random forest, and regression techniques have been applied to predict the SOC, SOH, and RUL of batteries. In section 3, we summarize the recent works on how various machine learning techniques can be applied for battery property predictions and provide insight into the predictabilities of these machine learning techniques. In addition, the fidelity of the machine learning techniques depends highly on the size and quality of the data set. High-throughput experimentation is one approach that can produce huge volumes of precise data within well-controlled conditions. The current status and challenges of high-throughput experimentation, together with our perspective on the future development of data-driven machine learning for battery state predictions, will be discussed in section 4.

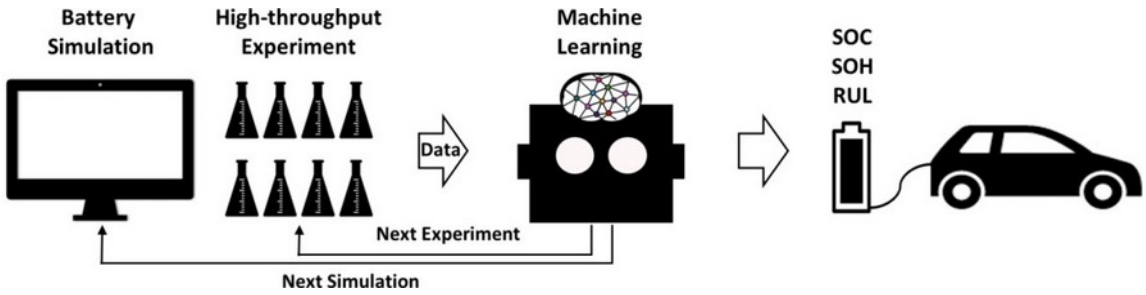

Figure 1. A machine learning approach for state-of-charge (SOC), state-of-health (SOH) and remaining useful life (RUL) predictions of Li-ion batteries.

2 Current Battery Models

Battery modelling is the core part of a BMS and is vital for maintaining safe and optimal operation of the battery pack. A battery model combining various estimation techniques can be used not only to determine the current state of an operating battery (e.g. SOC) but also predict its 'future' state (e.g. SOH and RUL). In the literature, the most studied battery models for Li-ion batteries are ECMs, PBMs and, more recently, DDMs with machine learning techniques. Each model has its own merits and challenges. For example, ECMs are computationally efficient and thus suitable for online battery status predictions (e.g. SOC), but attaining high accuracy remains a challenge. PBMs provide internal information about a battery that is often hard to measure in an experiment such as the Li-ion concentration within the electrodes and electrolytes. However, solving the governing partial differential equations (PDEs) of PBMs requires significant computational resources and a large number of input parameters. In this section, a brief review of the intrinsic characteristics of ECMs and PBMs, and the strategies commonly used to improve their adaptability and predictability will be given.

ECMs[15–25] are currently the major models that are widely used in the BMS of EVs for online SOC estimations due to their practically low computational demands and ability to predict battery behavior in real time. The models are essentially derived from empirical knowledge and experimental data in which the batteries are represented by groups of electrical components such as resistors and capacitors, forming resistor-capacitor (RC) networks (Figure 2) that are used to monitor the battery's behavior at different time constants associated with the diffusion and charge-transfer processes.[15] Typical ECMs are the Rint models,[16] the hysteresis models,[17,18] the Randles models,[19–21] and the RC or Thevenin models.[22–25] Despite their computational efficiency, ECMs generally show limited accuracy in

predicting battery characteristics across a range of operation conditions such as ageing and dynamics environments in real-life applications, due to parametrization of model parameters based on laboratory conditions. In addition, the lack of physics-based information of the system states and parameters limits its ability to provide insight into the battery internal conditions, making it hard to predict the SOH and RUL of batteries precisely.

PBMs should offer more accurate battery models. The pioneering work of full physics-based Li-ion battery models is the development of a P2D porous electrode model, which is based on porous electrode theory, concentrated solution theory, and the Bulter-Volmer kinetic equations (Figure 2).[26,27] The P2D model is named because it allows for variation in the concentration of lithium ions and electric potential throughout the thickness of the battery, as well as radially through the spherical particles of the active material. The model delivers insights into the internal dynamics of batteries such as lithium ion diffusion, Ohmic effects, and electrochemical kinetics. This opens the possibility of analyzing the battery's degradation mechanisms, predicting the SOC and SOH with ageing effects, and designing optimal charging strategies. However, the P2D model is generally described by a number of PDEs and is considered a full order PBM. Solving the PDEs require intensive computations as compared to the ECMs, which makes it impractical to embed the P2D model into a controller of a BMS for real-time applications.[28]

The bottleneck of applying the full PBM in the BMS for EVs lies in the computational complexity. As such, simplifying the PBMs is the main strategy to reduce the computation demand, but approximations must retain sufficient physical information to accurately predict battery behavior. One of the most studied simplified models is the single particle model (SPM) (Figure 2).[29–31] The key assumptions of the model are that a spherical particle represents each electrode, and the concentration and potential effects in the solution phase are neglected. With such approximations, the computational time is reduced significantly. However, the SPM model is inaccurate for high-rate simulations,[32] though efforts to improve this limit are ongoing.[33–36]

The PDEs that govern battery behavior in the P2D model are non-linear, so reducing the order of the equations is another approach to build a practical PBM. The models are commonly known as reduced order models (ROMs), which comprise fewer ordinary differential equations (ODEs). Typical approaches to construct ROMs are parabolic profiles approximations,[37,38] proper orthogonal decomposition;[39] residue grouping technique;[40] the Padé approximations;[41] or polynomial profiles[42]. Using polynomial profiles for solid concentration is the most common method; it is mathematically simple and computationally fast, but prediction accuracy is reduced by the assumption that the profile coefficients are temperature and age independent.

In summary, the main challenge lies in developing a battery model that can achieve an appropriate balance between model fidelity and computational complexity. Recently, DDMs with machine learning techniques are gaining importance due to their immense potential in achieving high accuracy with low computational cost (Figure 2). In the next section, we will discuss state-of-the-art machine learning techniques for battery state prediction.

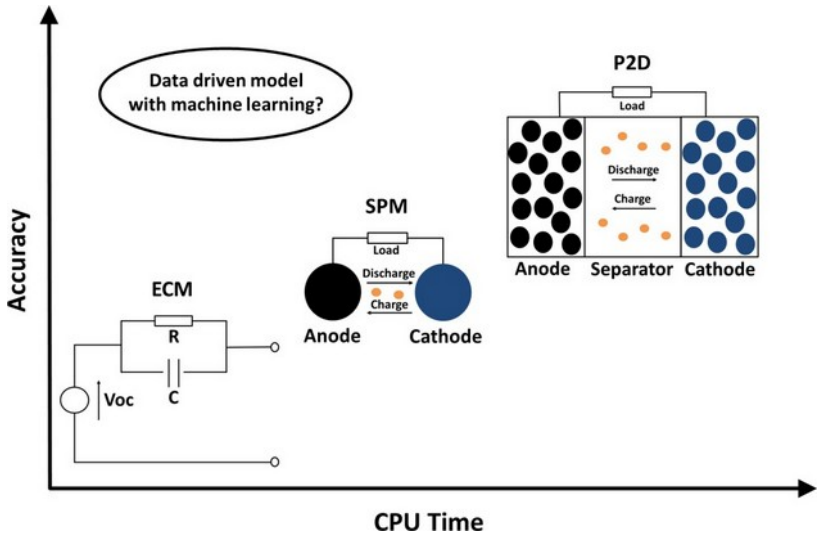

Figure 2. Accuracy vs. CPU time for equivalent circuit model (ECM), single-particle model (SPM) and pseudo 2D model (P2D). Data-driven model (DDM) with machine learning is a new type of battery model that is promising for fast and accurate battery state predictions.

3 Machine Learning for Battery State Prediction

We often want to predict the future behavior of a battery, for example to understand how much further an EV can drive, or how to design a battery that will have the best behavior in the field. Often, we are interested in the SOC of the battery within a single charge/discharge cycle, or the SOH of the battery spanning many charge/discharge cycles. Having two relevant time-scales will make predictions particularly challenging. All of these problems can be summarized as the fact that we need a function that inputs the current state of the battery to predict future behavior. A promising approach is machine learning - a flexible but efficient fitting function with no underlying physical knowledge. Table 1 summarizes the approaches taken by a range of authors over the past few years.[3,4,43–67] We first summarize the input and output parameters captured by the different modelling approaches and battery systems analyzed, before we focus on the advantages and disadvantages of the various machine learning techniques for predictive analytics of batteries. Finally, we offer a perspective on the future outlook and opportunities in modern machine learning and data generation to better understand and predict battery behavior.

3.1 Battery parameters: inputs & outputs

In order to understand, design, and predict battery properties, a range of variables that captures their full behavior must be incorporated. Usually some variables are either ignored or held constant to simplify the model. The possible input variables for a machine learning model can be split into continuous and categorical. Continuous variables can take any value and include the number of charge/discharge cycles that the battery has gone through, the current flow, the internal structure, the geometry, and the temperature. Categorical variables take particular values that cannot be sorted into a list, examples include the type of battery: Li-ion, nickel-metal hydride (NiMH), or lead-acid. A machine learning method should ideally be able to input both continuous and categorical variables in order to make predictions.

The outputs can be classed into two main categories: (1) short-time scale over a single charge/discharge cycle to understand the SOC, and (2) long time-scale over many charge/discharge cycles to understand the SOH. The first approach is to predict the evolution of the battery during a single charge/discharge cycle. Endpoints predicted can include the SOC, the current rate, and the concentration and size of defects formed within the battery. By tracking the evolution during a charge/discharge cycle, the model can address any point in the lifetime of a battery and extrapolate forward in time, but it is susceptible to accumulating errors if applied over too many charge/discharge cycles.

The second approach is to predict the evolution of the battery from the same point cycle-to-cycle over many cycles. This approach can be readily applied across hundreds of cycles covering the entire lifetime of the battery, but cannot be applied during a given cycle, and can start from and propagate to only a particular defined point during the cycle, for example when fully charged. In Table 1, machine learning models are seen to successfully predict the evolution of battery properties. The typical accuracy level attained is a correlation coefficient of 0.93 for SOH/RUL[3] and 0.98 for SOC[45].

Table 1. Summary of recent work on machine learning for battery state predictions.

Article		Method						Input							Output		
		Neural network	Support-vector machine	Gaussian / Bayesian	Regression	Random forest / Tree	Kalman filter	Voltage	Current	Temperature	Cycle number	Capacity	Power	Geometry	SOC	SOH	RUL
Severson et al.	3				✓			✓	✓		✓	✓					✓
Nuhic et al.	4		✓					✓		✓	✓	✓				✓	✓
Guo et al.	43			✓				✓	✓		✓					✓	✓
Wu et al.	44	✓							✓					✓		✓	
Zahid et al.	45	✓						✓	✓	✓			✓		✓		
Chemali et al.	46	✓						✓	✓	✓					✓		
Jiménez-Bermejo et al.	47	✓						✓	✓	✓					✓		
Mansouri et al.	48	✓	✓		✓	✓		✓									✓
Donato et al.	49	✓				✓		✓	✓		✓				✓		
Huang et al.	50						✓	✓	✓	✓					✓		
Ren et al.	51	✓						✓	✓	✓							✓
Khumprom et al.	52	✓						✓	✓		✓					✓	✓
Sahinoglu et al.	53			✓				✓	✓	✓					✓		
Álvarez Antón et al.	54		✓					✓	✓	✓					✓		
Tong et al.	55	✓						✓	✓	✓					✓		
Kang et al.	56	✓						✓	✓			✓			✓		
Hu et al.	57	✓						✓	✓						✓		
Wu et al.	58	✓						✓	✓	✓					✓		
Wu et al.	59	✓						✓			✓					✓	
Hu et al.	60		✓	✓				✓	✓			✓			✓		
Berecibar et al.	61	✓	✓					✓	✓		✓	✓				✓	
Richardson et al.	62			✓				✓	✓		✓	✓				✓	✓
Zhang et al.	63	✓						✓			✓	✓					✓
Hu et al.	64		✓					✓	✓	✓	✓		✓		✓		
Tseng et al.	65				✓			✓	✓		✓					✓	✓
Hussein et al.	66	✓					✓	✓	✓						✓		
Yang et al.	67	✓						✓	✓							✓	

3.2 Machine learning techniques

Machine learning uses a general fitting function with optimizable parameters tuned to deliver the desired behavior, usually a fit to experimental training data. The function can then make predictions for other battery systems. Like all fitting functions with optimizable parameters, machine learning models can be susceptible to over-fitting. Therefore, a standard protocol is cross-validation: the model is trained on a fraction of the total available training data (typically 80%), and then the accuracy is gauged by testing against the remaining (typically 20%) data that was withheld from the training process. This allows the correct hyper-

parameters to be obtained, including the number of optimizable parameters. We now review the fitting functions previously used to model the behavior of batteries, which are summarized in Table 1.

3.2.1 Linear and non-linear regression

Regression is the straightforward fitting of a straight line (one input dimension) or a hyperplane (multiple input dimensions) to the data. The robustness can be further improved through singular value decomposition, which circumvents singular solutions. This approach is clear, robust, and fast, and furthermore requires a minimal amount of training information to form a model. The method can be further extended with additional functionality to capture non-linear behavior.

A linear model that combined nine battery descriptors was used by Severson et al[3] to predict the SOH of lithium iron phosphate/graphite cells after 100 charge/discharge cycles with an error of 9.1%. The simple linear model allows fast computational time for training and predictions that can be deployed in-situ in devices.

3.2.2 Random forest / tree

Random forest involves a set of generalized classification trees, each trained with randomly selected data. A new query passes down the trees to deliver an ensemble of predictions that are averaged to give the expected value alongside an uncertainty. A random forest is most straightforward to train with categorical data. The random forest is accurate, easy to train, and robust against outliers, but the function delivered is not smooth.

An example of the successful application of a tree method to predict the RUL of a Li-ion battery is demonstrated by Mansourei et al.[48] Focusing on batteries in unmanned aerial vehicles, the authors aimed to extend the flying time window. The authors found that the random forest approach delivered a typical prediction error of 2.5%, outperforming linear models, a support-vector machine, and a neural network.

3.2.3 Support-vector machine

Support-vector machine is a generalization of the random forest where the functions trained are simultaneously classified in a multidimensional space rather than split along one input direction. Where the training data is scarce, this approach can improve the quality of the fit, but it comes at the cost of significantly increased computational demands.

Nuhic et al[4] used a support-vector machine to predict both the SOH and RUL of lithium ion batteries. The support-vector machine could estimate SOH between successive cycles within 0.3% for new cells and 0.6% for aged cells, and showed that the SOH and RUL was strongly influenced by environmental and load conditions.

3.2.4 Gaussian / Bayesian process

This is a stochastic method that necessitates storing all of the training data as the foundation of the model. At run-time, once given the input parameters, it calculates the joint probability distribution of the underlying fitting functions, usually Gaussian distributions, and the training data. The approach is Bayesian, so it calculates the best possible prediction given the training data, but can also be prohibitively expensive.

Sahinoglu et al[53] used Gaussian process regression to estimate the SOC of Li-ion batteries. The model uses battery parameters, including voltage, current, and temperature, as inputs. The Gaussian processes are shown to deliver predictions for SOC within 0.2% and outperform support-vector machine and neural network predictions.

3.2.5 Neural network

The linear fitting method could be extended with a Taylor expansion to capture non-linear behavior. However, a more efficient approach is to use several locally non-linear basis functions to build a composite function in a neural network. The neural network is more expensive to train, but when a large amount of data is available, it often gives the highest possible quality fitting function, hence its widespread use in industry.

In batteries, we are often interested in predicting the evolution of the SOC over a single charge/discharge cycle or the evolution of the SOH over several cycles. For these problems that focus on the passage of time, a convolutional neural network is helpful. This is a specialist fitting function useful on systems that display temporal invariance, fundamentally capturing that, for example, the behavior of a battery is independent of the time of day that it was used.

Yang et al[67] used a neural network to predict the SOH of Li-ion batteries for EVs. Taking in parameters from a first-order ECM, a three-layer neural network could predict the SOH within 5%. In fact, the majority of studies so far focus on the most commercially important system of Li-ion batteries, with only a couple addressing NiMH and lead-acid batteries. A single study by Zahid et al[45] presents a generalized neural network model that can address all three battery families. This is a valuable direction as it allows information on one battery system, e.g. Li-ion, to inform the behavior of other systems that are less well-studied, and furthermore provide guidance for future possible battery families.

4 Future Outlook and Opportunities

4.1 Data-driven machine learning

Machine learning is a rapidly developing field. Although significant strides have already been made in its application to predict battery SOC, SOH, and RUL, harnessing the latest developments in machine learning will open future prospects to improve the accuracy of predictions and also deliver deep insights into the underlying physics.

4.1.1 Juxtaposing physics-based modelling with machine learning

Machine learning models, being a generalized fitting method, are best used when the underlying functional dependence is not known from a PBM. Because of this, machine learning is often referred to as a ‘black box’, where datasets enter and predictions emerge, but the process between input and output is opaque. The incorporation of physics and domain knowledge (e.g. known battery degradation mechanisms) into machine learning will help in the development of models that are more causal and explanatory. Moreover, if a PBM is available, then machine learning can be applied to capture the remaining difference from the experimental data. Although this hybrid approach introduces additional computational cost, it can deliver more accurate and insightful models with less risk of over-fitting the training data.

4.1.2 Combining techniques over different time-scales

The models presented from the literature focus either on the prediction of SOC within a charge/discharge cycle, or the SOH/RUL over many cycles. There is however a more general problem: to predict the long-term SOH, but starting from an arbitrary point in the charge/discharge cycle. Machine learning could first use a detailed model to predict until a

fixed point in a cycle, for example, the state of being fully charged. Next, a SOH model that covers integer cycles could be applied to predict the final SOH. This hybrid approach would achieve the best of both worlds, and as both the short and long-term behavior models have now been developed, there is an opportunity to juxtapose them into a holistic model of battery evolution.

4.1.3 Handling sparse data

Experimental data is often sparse: for every battery not every single design parameter or property has been measured. This can often be because of cost: first-principle simulations are cheaper than, for example, nuclear magnetic resonance (NMR) experiments, so often only simulations have been performed. Specialist machine learning techniques[68,69] are able to train from sparse databases, and then use readily available properties, for example first-principle simulations, to guide the extrapolation of more expensive properties, for example experiments.

4.1.4 Shortcut first-principles simulations

Detailed first-principles simulations are costly. One shortcut is to build a database of historic results from first-principles simulations and then train a machine learning model. This model is then used as a proxy for first-principles simulations, except if the machine learning reports a large uncertainty, when an additional first-principles simulation is performed, added to the database, and the machine learning model retrained. This cycle of reinforcement learning can significantly reduce the number of simulations required to understand a system. Machine learning can be used in a similar way for experimental design and to shortcut costly experiments.

In fact, every battery in service is different. Due to its particular usage, the behavior of a certain battery is unique, and evolves throughout the battery's service. Therefore, one could also develop a bespoke machine learning model for that particular battery, perturbed from the default, refined by data gathered in service to capture that particular battery's characteristics for accurate on-line predictions.

4.2 High-throughput data generation

Databases underlie all machine learning and data-driven approaches. Compared to the traditional one-by-one approach, high-throughput technologies can generate a large but high quality database in a short time at low cost. Today, high-throughput technologies have been widely employed in various fields, e.g. biological and medical sciences, due to the rapid progress in automation, robotics, and computational technologies.[70–76] In the field of Li-ion batteries, high-throughput data generation involves several aspects, namely material synthesis, material characterization, battery fabrication, and electrochemical testing.[77–82]

4.2.1 Material synthesis

The development of Li-ion batteries is driven by breakthroughs in advanced electrode materials. With high-throughput synthesis, electrode materials with different and optimized compositions can be rapidly prepared for subsequent structural and electrochemical analysis, which can speed up the discovery and optimization of electrode materials. Currently, thin-film sputtering, pulsed laser deposition, combinatorial robotic, and microplate techniques have been developed to synthesize/screen electrode materials and electrolytes, as well as optimize the content of additives, in a high-throughput manner.[77,83–88] These methods are still limited to modulation and tuning of material compositions, which is below the typical requirement for diverse machine

learning datasets. Currently, high-throughput material synthesis remains to be explored for diverse materials with novel microstructures, different crystal structures, controllable dopants, interfaces, and defects.

4.2.2 Material characterization

Material characterization will be carried out sequentially to measure and ascertain the key properties of the electrode materials before incorporation into batteries. In recent years, a push to develop new characterization techniques for battery research has motivated the development of high-throughput diagnostic tools across a range of methodologies. Today, high-throughput X-ray diffraction (XRD) and X-ray fluorescence (XRF) techniques have been developed to collect the crystalline phase and elemental information of electrode materials.[78,88–91] However, ex-situ characterization may not reflect the true information of the actual charge/discharge states due to changes in the thermodynamic non-equilibrium phase after relaxation. With in-situ techniques such as XRD and X-ray absorption spectroscopy (XAS), the chemical, structural and thermal evolution of materials, as well as the pressure within Li-ion batteries can now be properly monitored.[81,82,92–99] More work is required, however, to further spur the development of high-throughput characterization methods for Li-ion batteries, e.g. by directly coupling the characterization tools to the synthesis process so as to speed up the screening of materials and employ reinforcement learning to drive methodical experimental design. Moreover, advanced robotic tools need to be developed and new algorithms need to be created to take advantage of the current characterization techniques.

4.2.3 Battery fabrication

Automated high-throughput battery fabrication is crucial as it can accelerate subsequent battery optimization and testing based on realistic operating conditions.[100] Conventional battery development usually starts with small-scale, simplified and discontinuous laboratory equipment, as well as manual processes. The electrodes, associated components and entire cells generally have non-optimized internal structures and often low mass loading. This is far below the requirements of real-life commercial applications and cannot provide reliable data for machine learning. Hence, highly integrated Li-ion battery production processes from the initial automatic electrode synthesis to the final battery testing systems are necessary for high-throughput precise data generation (Figure 3). Ideally, by using the highly integrated battery fabrication system, the anode, cathode, binder, and conductive additives can be selected and optimized automatically, followed by automatic mixing to prepare electrode slurries. The slurries are then coated onto current collectors, carefully dried, and calendared into anode and cathode films for automated assembly into batteries, together with electrolyte and separator.

4.2.4 Electrochemical testing

High-throughput electrochemical testing of batteries holds the key to generating huge and reliable datasets for machine learning. A variety of electrochemical techniques, including cyclic voltammetry (CV), galvanostatic charge/discharge (GCD), and electrochemical impedance spectroscopy (EIS), can be used to measure the cycle life, rate capability, capacity and impedance of batteries with high precision and accuracy (Figure 3). Batteries should be screened quickly in parallel based on realistic working conditions (e.g. different current, voltage, power, temperature, mass loading, and cell design) to generate huge volumes of meaningful data. Once the machine learning models are trained with these data, they can further accelerate the process of battery testing, by weeding out potential poor-performing batteries based on their initial cycles. For instance, by using the first five cycles, Severson et al[3] managed to use a trained machine learning model to classify cells into two groups: a ‘low-lifetime’ and a ‘high-lifetime’ group, with 4.9% test error. In essence, integrating smart automation systems with advanced

computing and machine learning would open up the prospects of automating the entire Li-ion battery industry, from material synthesis and characterization, to battery fabrication and testing.

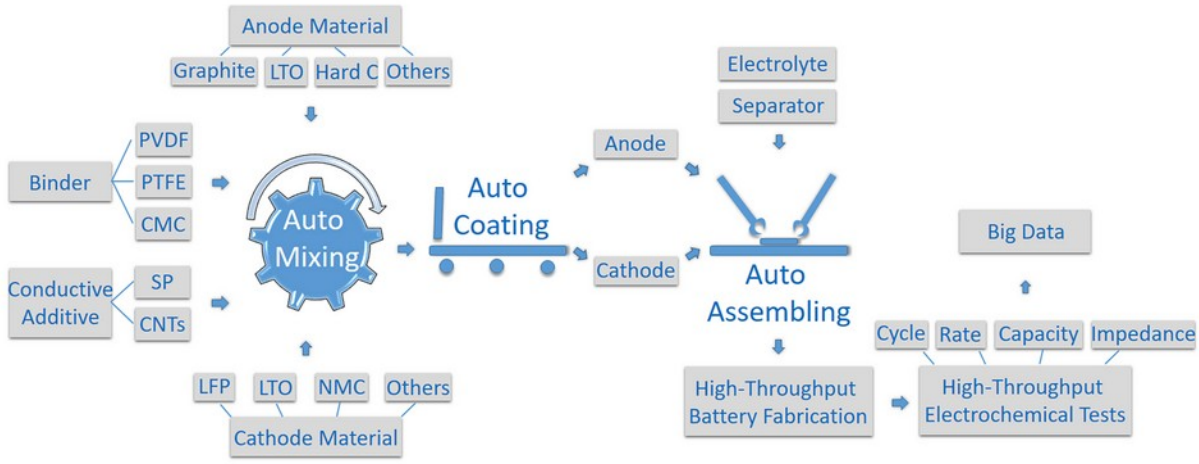

Figure 3. High-throughput battery fabrication and testing. Abbreviations: PVDF: polyvinylidene fluoride, PTFE: polytetrafluoroethylene, CMC: carboxymethyl cellulose, SP: Super P, CNTs: carbon nanotubes, LTO: lithium titanate, Hard C: hard carbon, LFP: lithium iron phosphate, LCO: lithium cobalt oxide, NMC: lithium nickel manganese cobalt oxide.

5 Conclusion

Currently, the two most studied models for battery state prediction are the ECMs and PBMs. Despite their popularity and continuous development, there remains a clear tradeoff between computational efficiency and accuracy when using these models for on-line battery state prediction. DDMs with machine learning is a novel way to model batteries that can potentially address the dilemma faced by traditional modelling using ECMs or PBMs. Currently, most of the studies use experimental data only for machine learning, which is usually defined as ‘black box’ prediction. We see the opportunity of juxtaposing physics-based modelling data and high-throughput experimental data with machine learning to develop a novel type of battery model. Physics-based modelling data can be obtained from multi-scale simulations from atomistic all the way to continuum level. Machine learning can combine models with different time and length scales. Moreover, high-throughput experimentation, perhaps guided by preliminary machine learning results, is the key to provide real-life and high-quality datasets on battery performance for machine learning. Combining all these pieces together with domain knowledge, the resulting physics-based machine learning technique paves the way for explainable ‘white box’ prediction. With the advancement of computational technologies and mathematical algorithms, together with the reduced costs of data storage devices and high-throughput experiments, we envision data-driven machine learning to be a promising technique for advanced battery modelling in the future.

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Author contributions

This work was written through the contributions of all authors.

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