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**State of Charge Prediction for Electric Vehicle’s Power Battery**

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# Abstract

Due to the dramatic increase in the number of fuel vehicles and the consequent environmental pollution and energy crisis, countries around the world are beginning to focus on electric vehicles that are both energy efficient and environmentally friendly and can be recycled. The key technology for electric vehicles is the power battery and the battery management system. Li-ion batteries are the battery type of choice for electric vehicles due to their unique advantages: long cycle life, high specific energy, safety and reliability, high energy density and adaptability. The study of the remaining state of charge is the core component of the battery management system. The aim of this paper is to establish and compare the accuracy and convergence of different models for remaining charge estimation. This study uses a lithium iron phosphate battery as the target, uses the Thevenin equivalent circuit model and builds battery model, which in turn performs parameter identification of this circuit model. After that, the extended Kalman filter is chosen for estimation adjustment. The following is the main work and results of this paper: Firstly, the chemical reaction of Li-ion battery is discussed, the mechanism of battery chemical reaction and its ageing mechanism and influencing factors are given, the definition formula of state of charge is given, the electrochemical model equivalent circuit model and neural network model are analysed. Based on this, the current commonly used methods for state of charge estimation are analysed, Kalman filter is chosen as the representative of the equivalent circuit model and the long and short term memory as the representative of the neural network for estimation. Based on the HPPC experiments of constant-current charging and discharging of lithium iron phosphate batteries at the University of Maryland, USA, the model parameters were identified by the corresponding formulae, and the mathematical function relationship between each model parameter and state of charge was fitted using Matlab's cftool tool. Then use Matlab's Simulink software to establish the Thevenin battery model and apply filter algorithm. It demonstrates the accuracy of the second-order Thevenin battery model is higher than 98%, which meets the requirements of this battery model. The paper also describes the principle of the extended Kalman filter, the recurrence formula. In addition, this paper investigates another comparison method, a kind of deep learning method, long-short term memory, describing the working principle of LSTM and implementing it. In contrast, the neural network model has higher accuracy, but requires a large amount of data as a training set and is significantly slower than the filtering method in terms of computational speed. In practical applications in industry, neural network models are not as well used as the filtering method.

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# Introduction

Global sales of electric vehicles (EV) have increased dramatically in recent years. Despite experiencing the global covid-19 pandemic last year, sales in 2021 are still up 109% on the previous year, with an absolute figure of 6.5 million. There is 85% of EVs which were sold to the mainland Chinese and European markets. With a series of incentives from the Chinese government, such as subsidies for purchasing electric vehicles and charging subsidies, an increasing number of ordinary users choose electric vehicles as their first choice and alternative for personal mobility, and electric vehicles are playing an increasingly important role in daily life.

Due to the global trend of energy saving and emission reduction and the dividends in some countries, more and more established car manufacturers with good reputation and emerging car companies are joining in the production and development of EVs, including world giants, BMW, Mercedes-Benz and Audi, emerging manufacturers Tesla, Chinese traditional companies BYD, GAC, BAIC, start-ups NIO, Xiaopeng, etc. they launched distinctive models which satisfies different requirement of consumer segments.

EVs look like a fuel car, but the power is delivered in a very different way. The power battery pack is one of the most critical components and two most important building blocks in a battery pack are the cells for discharging (heart) and the battery management system (BMS) (brain). The main function of the BMS is to manage and monitor the status of the battery pack. The main purpose of monitor is to prevent over-charging and over-discharging of the battery, as well as to monitor the ageing of the battery to ensure that the battery is used for a certain period of time. A poor implementation of any of the above functions can be fatal to the battery. The R&D costs for the battery management system account for approximately 20% of the overall battery pack. There are currently three main bodies of the design and production of BMS in the world, battery manufacturers, original equipment manufacturer (OEM) and third parties. Leading Chinese battery manufacturers include CATL, CITIC Guoan and others. Unlike the single battery application in a mobile phone, third parties always have many problems with the BMS development due to their research capabilities because of the intricate charge/discharge relationships and balance within the battery pack, therefore EVs equipped with BMS developed by these companies are sometimes dangerous for these internal defects.

Accurate prediction of a series of battery indicators, including state of charge (SoC) (remaining charge of battery), state of health (SoH), state of power (SoP) etc. is one of the important functions of the BMS. Based on the feedback from EV charging companies, it is found that the number of burn-in accidents is particularly high in BMS developed by third parties and some models made by the OEM can also suffer burnouts due to problems with the battery cells. On the one hand, an incorrect estimation of the remaining charge by the BMS leads to the BMS continuing to send charging demands to the electric vehicle supply equipment (EVSE), while the charging platform, after parsing the vehicle-side message, gives instructions to the EVSE (chargers) to continue charging. The voltage, current, internal resistance, temperature and other data recorded in the message at this point are all normal. However, the battery is already showing signs of overcharging in reality. As the internal chemistry of the battery is very sensitive to temperature, the significant increase in charging temperature due to overcharging usually occurs at the end of charging and is therefore ignored by the BMS, at which point the situation is no longer controllable. On the other hand, even if BMS is correct in its prediction of SoC, the characteristic of low ignition point in cells may lead to fires, such a problem is easier to solve technically, for example, wrapping the cells in a flame-retardant material.

In the accident of burnout, as EV charging companies, they may have to carry more public pressure, as consumers at one charging station will instinctively assume that there is a problem with the station's chargers, while their usual driving and other charging behaviours are unaffected. Internally they do not know how to improve their own chargers, as the chargers themselves only receive the data sent by the BMS to make the next judgement, and the BMS itself has the incorrect data. For such a dilemma, the only thing that can be done at the moment is to rank the effectiveness of BMS designed by different manufacturers and to take charging restrictions for models that are highly prone to problems. This is a mechanical selection, just as the corpus is subject to a strong time constraint for updating. In order to enhance the performance of BMS and make the prediction more precise, it is necessary to increase the computational power by adding chips and embed some flexible models which are apply the principle of machine learning.

This article will analyse the chemistry inherent in the charging and discharging of Li-ion batteries and explain the aging mechanism of them. It will introduce what theories and models are well established in the world to study the prediction of the remaining charge of Li-ion batteries. In the modelling part, this paper will construct an equivalent Thevenin circuit model and perform circuit parameter identification based on actual tested out data, based on which the filtering method prediction will be performed. In later sections, the neural network model of long and short-term memory will be introduced, its principles will be described, and the model will be trained, and the accuracy obtained under this model will be compared with the equivalent circuit model to analyse which is more appropriate.

# Literature review

This chapter aims to introduce the working mechanism and the ageing mechanism of Li-ion batteries, understand the most important criteria for calculating the remaining charge and service time, and to give examples for some popular estimation models currently available.

## The charging and discharging mechanism of Li-ion batteries

Inside a Li-ion battery are the anode (negative electrode), cathode (positive electrode) and electrolyte. There is a membrane between the anode and cathode, with the liquid electrolyte filling the space (Zhong et al., 2015). The materials used in Li-ion batteries are very elaborate. Firstly, cathode material is lithium salt. There are three main types of lithium salt used as cathode material, namely lithium cobaltite (LiCoO2), lithium iron phosphate (LiFePO4) and ternary lithium. Lithium cobaltite is the most expensive to synthesise and is therefore not used in large numbers in EVs, but it also has the highest output voltage. Lithium iron phosphate is less expensive and has the highest number of available charges and discharges, allowing it to be used in EVs, but its output voltage is the lowest. Tritium combines the advantages of these two types of Li-ion batteries, using a manganese (Mn) nickel (Ni) iron (Fe) mixture as the anionic part of the lithium salt.

Anode material is graphite or coke because its laminar structure can hold Li-ions. Electrolytes are liquid and consist mainly of inorganic solutes and organic solutions. The inorganic solute is mainly lithium hex phosphate fluoride (LiPF6), while the organic solute is Ethylene Carbonate (EC, highly conductive but viscous) and Dimethyl Carbonate (DMC, weakly conductive but less viscous), exactly two materials to compensate for their respective physicochemical deficiencies (Zhang, 2018).

The charge/discharge chemistry of a Li-ion battery is a regular movement of Li-ions between anode and cathode. Then, take LiCoO2 as an example, LixC6 (compounds for anode) breaks down into Li-ions (Li+), electrons and carbon ions (C-) during charging. The separator only allows Li+ to pass through but not electrons, so electrons are transferred from the external circuit to cathode, and Li+ move towards the cathode due to the electric field created by the external electron movement, reaching the cathode through the small zigzagging hole inside the separator, where they combine with electrons and cobaltite ions (remains in the anode) (CoO2-) to produce lithium cobaltite, while other ions left in the anode combine with the cations in the electrolyte to form compounds (Roy and Srivastava, 2015). On the contrary, when discharging, lithium cobaltite in the cathode decomposes to Li+, electron and CoO2-, electron still moves from external circuit to anode, and at there, it combines Li+ and CoO2- as lithium cobaltite (Belov and Yang, 2007a).

## The aging mechanism of Li-ion battery

After the battery has been assembled, at low temperatures, the Li-ions on the surface of the two electrodes react with the electrolyte to form a solid electrolyte interphase (SEI), which has both positive and negative aspects. It prevents the electrolyte and Li-ions from continuing to react and blocks electrons and bulky solvent molecules from entering the electrodes. However, in order to create it, some of the Li-ions are consumed and the active Li-ions are reduced. Most of the causes of ageing are related to SEI, the following is scenarios.

1. Charging and staying in high temperature (only exceeding 60 degree Celsius): High temperatures lead to the dissolution of the SEI, making it no longer able to isolate the electrolyte from the Li-ion. Electrolytes such as LiPF6 and EC are decomposing at high temperatures, and the products of decomposition react with graphite to change their layer structure, thus reducing the space left for Li-ions (Sarre, Blanchard and Broussely, 2004).
2. Charging in low temperature: The low temperature makes the lithium monolith precipitate, the Li-ions gather on the SEI without passing, get electrons to form lithium atoms stacked on the SEI, over time the lithium atoms deposit and break through the SEI, forming a tree-like lithium dendrite (). The continuous generation of lithium dendrites may puncture the separator (Zhang, Xu and Jow, 2003).
3. Over-current: On the one hand, the thermal effect of the current makes the electrolyte decompose. On the one hand there is an excess of active Li-ions, which leads to saturation of the electrode material and the formation of lithium dendrites from the excess Li-ions. In addition, the resistance of the SEI becomes smaller at higher currents, allowing electrons to pass through and the Li-ions to precipitate directly on the electrode surface before they can diffuse (Belov and Yang, 2007b).
4. Self-discharge: Self-discharge is more likely to occur in winter and summer, at higher and lower temperatures.
5. Aging of battery module: The ageing of single cells leads to an amplification of the ageing of the modules. At the same time, the joints between the individual cells are also being oxidised and ageing, which deepens the ageing of the modules (Ping et al., 2018).

In summary, the liquid electrolyte Li-ion battery is fragile and its internal chemistry is extremely sensitive to current, voltage and temperature. Improper usage leads to accelerated ageing of Li-ion batteries. Currently, the use of solid electrolytes instead of liquid is the industry's direction of development. However, the chemical reaction is a step-by-step process, so if the remaining charge in the last state of the battery is accurate, it demonstrates that the state of the electrodes, the concentration of active Li-ions, and the state of the SEI at the previous moment are accurate, there is, therefore, a theoretical basis for predicting the next state of power based on the previous state's power adjust some parameters that change internally.

## State of Charge and State of Health

The descriptive formula for battery capacity after removal of loss current is:

(1)

If the current is constant during full charging and discharging, the time is the total time required to complete the process, if the current is not constant, the equation is written in integral form:

(2)

The percentage of battery capacity to rated capacitance is the state of charge:

(3)

If letting time to be infinite small, instantaneous SoC will be obtained. Ampere-hour method is using the initial SoC derived from the correspondence between open circuit voltage and SoC at a fixed temperature to minus the current SoC.

(4)

State of health measures the effect of the internal resistance under different charging state. The higher the internal resistance, The more frequent the chemical reactions within the battery, the faster the battery will age.

## Models and prediction methods

### The foundation of models

There are currently three ways to consider the prediction of SoC. The first method uses differential equations to model the internal chemical reactions and measure the changes in lithium ion concentration, the changes in electrode potential and the quantification of the polarisation reaction during the charging and discharging of the battery. The classical electrochemical model is the porous electrode theory developed by Fuller, Doyle and Newman (1993). This theory defines a number of parameters to quantitatively describe the various kinetic and thermodynamic relationships that occur within the cell, such as electrochemical reactions, ion transport pathways, electron pathways, diffusion, concentration distribution and ion distribution. These parameters include structural parameters (electrode material, bulkhead thickness, cell dimensions) linked to physical quantities (voltage, current, capacity) and thermal behaviour. The electrochemical model consists of a series of coupled differential equations. Complex calculations are required in order to solve for these parameters, in addition to some difficult to obtain parameters. In order to improve the electrochemical model, Kandler et al. (2006) consider a one-dimensional model and define the thickness of cell as independent value (collector, electrode, spacer). The design of the parameters of the model tests the chemistry background of the designer. Therefore, Kandler's model is not suitable for generalisation. To increase understandability, model order reduction (MOR) techniques can be applied. a study by Ahmed et al. (2014) presented reduced order model equations and identification of model parameters for lithium iron phosphate batteries. For a single cell, the maximum root mean square error (RMSE) between the measured voltage and the model output is within 55 mV. a study by Fan, Li and Canova, (2018) developed a step-down model based on Galerkin projection for lithium iron phosphate (LFP) and nickel-manganese-cobalt (NMC) cells with a maximum RMSE equal to 15.5 mV. these models were used in battery design are fully considered as the preferred.

The second approach is to use neural networks, built on a large number of HPPC tests on a single type of battery (e.g. lithium iron phosphate as cathode material), to obtain experimental data such as changes in voltage, current, temperature, internal resistance and the charging/discharging capacity under different SoC. Yu et al. (2020) used a neural network combining a genetic algorithm (GA) and a back propagation (BP) algorithm. The genetic algorithm overcomes the disadvantages of the backpropagation algorithm, which is slow to converge and easily falls into local optimum solutions, and speeds up the convergence speed and has strong robustness. They created a dataset which contains charge/discharge current, voltage and positive battery temperature as input values. By training the input and output parameters optimized by the genetic algorithm, and then judging whether the error range is within a reasonable interval based on the output values of the trained GA-BP neural network prediction system, the feasibility of the algorithm for power battery SoC value prediction is finally justified.

In order to make the model more accurate, some modifications need to be made to the fully connected layer to take into account the influence of the SoC of the previous state of the battery on the current SoC prediction, so recurrent neural networks or long and short-term memory are introduced for relationship fitting. This method can be used to obtain relatively reliable prediction curves directly without considering any internal battery chemistry mechanism. Figure 1 is an example of the structure.

图示

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Figure 1. example of radial basis function network

This model basically follows the principle of the radial basis function network (RBF), where the network is divided into is three layers, the input layer, the hidden layer and the output layer. The BRF is now widely used in engineering.

Considering that the SoC has continuity when charging and discharging, and that the SoC values in the previous phase affect the latter phase, simple BP neural networks can no longer meet the needs of prediction, therefore, recurrent neural networks are introduced, but the traditional recurrent neural networks have larger weights for the hidden layers closer to the current hidden layer and smaller weights for the ones further away, with the problem of gradient disappearance. Therefore, Park et al. (2020) introduced a long and short-term memory algorithm to construct a battery power prediction model, and Zhang et al. (2018) used a long and short-term memory recurrent neural network (LSTM-RNN) to learn the long-term dependence of Li-ion battery capacity degradation. This led to a further improvement in accuracy, with an error of less than 5% in the measurements obtained.

The problem of various types of neural networks are obvious, the first requirement is data quality and volume for the training set, and secondly the poor generalisation capability of the model, and the fact that if the cathode material is replaced with another lithium salt, such as ternary lithium, the existing relationship may change.

The equivalent circuit model is now widely used in industry because it is less computationally intensive than the electrochemical and neural network models and more accurate than the ampere-time integration and open-circuit voltage methods. Equivalent circuit models have also undergone many developments. The first was the Rint model, also known as the internal resistance model, which is a linear, purely resistive model containing only a voltage source and an ohmic internal resistance of the battery, and is the most basic physical equivalent model. It is the most basic physical equivalent model.

The parameters of this model are relatively easy to identify, and the overall model is in accordance with Ohm's Law, but the internal chemistry of the power Li-ion battery is a complex and reversible reaction. However, the chemical reactions within the power Li-ion battery are complex reversible reactions with some internal polarisation, which cannot be characterised by a purely linear model. However, the chemical reactions within the power Li-ion battery are complex and reversible, and there are certain polarisation phenomena within the battery.

Based on the previous study, Thevenin equivalent circuit model is an equivalent circuit model based on the Rint model to address the inability of the Rint model to represent multiple polarisations, which is a non-linear model. The model is more accurate and has more practical applications in engineering. The model has therefore been widely adopted by researchers at home and abroad. It is currently the most widely used equivalent model for Li-ion batteries. The research team at Beijing Institute of Technology has studied more than ten equivalent circuit models and has shown that this model has the highest accuracy in modelling ternary Li-ion batteries. The model has the highest accuracy in modelling ternary Li-ion batteries.

The initial Thevenin model is shown in figure 2 below, a resistor and a capacitor are connected in parallel to simulate the variation of the internal resistance of polarisation inside the battery, and another resistor is connected in series to simulate the variation of ohmic internal resistance.

图表

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Figure 2. one-order equivalent circuit model

USCAR published the Partnership for a New Generation of Vehicles (PNGV) battery test manual in 2001, which refers to a standard equivalent circuit model for PNGV. The methodology for determining the model parameters is presented in the Freedom CAR Battery Test Manual published in 2003. The PNGV model takes the effect of changes on battery’s OCV into consideration. In this model is used to represent the ideal open circuit voltage of the battery, is the battery capacitance (representing the change in OCV due to the load from current ), other parts remain consistent with Thevenin model, figure 3 shows below.

图示

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Figure 3. PNGV model

Therefore, will be equal to the summary of , and the voltage in the combination of resistance and capacitor. Inspired by the current idea of adding an series of capacitor and resistance component to the Thevenin model to separately represent different types of battery schedules depending on their polarisation rates, the PNGV model also extends one RC circuit to two, which will make the model more accurate than the extended Thevenin model.

### The method of prediction

The SoC describes the work done by the current in the circuit, therefore, according to the integration of the current in time, it is possible to obtain how much work the current has done during the discharge phase, subtracting the consumed from the initial SoC to obtain the remaining, this method is called the ampere-hour integration method (Li et al., 2019).

(5)

refers to the remaining charge of the battery at the moment , refers to the rated capacitance, and refers to the actual current after taking the loss. The formula describes the remaining power equal to the area of SoC in the initial state minus the area of power consumed in actual use. This method would be the most effective if it were accurate for the measurement of three variables, one is SoC(), which is difficult to measure precisely for each vehicle start. The second is . The rated capacitance of the battery is also a variable because the more the battery is used, the more it ages (CSDN, 2021). Thirdly, this problem of measurement bias is further magnified if not taking into account the years already used and the remaining life of the battery, and environmental factors such as temperature (Hua & Li, 2013).

The Kalman filter was introduced in order to adjust these deviations in time to bring the next step closer to the real situation. It still uses the basic principle of the Ampere-hour method and corrects it at each step. Pang, et.al (2020) used Kalman filtering and weighted the input values in the algorithm, the current of the previous period and the current of the next period, to correct the Kalman gain matrix and obtain a more accurate SoC. in addition, Kalman filtering takes into account the effect of noise and performs noise cancellation by minimising the noise correlation matrix, and after a number of iterations, the noise in the system After a number of iterations, the noise disappears from the system and both predicted and observed values are adjusted to have smaller deviations (Kalman, 1960). The extended Kalman filter uses a Taylor expansion to transform the non-linear relational equation into a linear one, which is then corrected by using the Kalman filter, as the SoC variation of the battery is non-linear and therefore better using the EKF (Pang et al., 2021).

The last method is to use the popular neural network. Although this method requires the use of a large amount of data as a training set and is arithmetic dependent compared to the other three methods, the method does not require an understanding of the internal properties of the battery and has a high accuracy in predicting directly using the trained model. Recursive neural networks (Han, 2017a) were introduced considering that the state data before and after the battery are interrelated. The recurrent neural network had some drawbacks and was later improved continuously by introducing long and short-term memory and then changing the optimiser and introducing genetic algorithms (Han, 2017b). The hyperparameters of the deep neural network need to be set manually, therefore, a grid search can be used to find more suitable parameters.

# models and methodology

This chapter shows the construction of a second order equivalent circuit model and does detailed descriptive statistics using experimental data from a real battery HPPC test. The parameters of the model are identified using cftool and then the estimation of the filtering method is performed to show the final results. In addition, long and short-term memory is introduced and a model based on it is constructed, while the results of the model runs are shown.

## Design of equivalent circuit model

In fact, there are better electrochemical models for the determination of the internal mechanism of Li-ion batteries, such as the Shepherd model and the Unnewehr unified model. However, in order to increase the speed of computation for large-scale applications in practical scenarios, while still providing a comprehensive description of the system state and maintaining a certain degree of reducibility, many studies have opted for equivalent circuit. Similar to the principle of conventional battery power generation, There is a certain point difference between the two poles of a lithium-ion battery and this potential difference is expressed as the electric potential of the battery, which can be modelled in an equivalent circuit using capacitance. Research has shown that there is a certain functional relationship between the electric potential of the battery and the SoC of the battery, and this functional relationship is tentatively expressed by . Secondly, the principle of internal current generation mentioned above is the embedding, de-embedding and movement of lithium ions between anode and Cathodes. During this electrochemical reaction and ion movement, a certain resistance is inevitably generated, so the equivalent circuit uses a resistance to simulate resistance.

Research has shown that the internal resistance of a battery can be further divided into ohmic internal resistance and polarised internal resistance due to the different mechanisms of formation when the battery is operating. Ohmic internal resistance is the inherent resistance of the system and depends on the nature of materials used in two poles, which is related to period of use, temperature and other factor. The polarisation resistance is to measure the movement of Li-ions between two poles. It can be further subdivided into the polarisation resistance and another resistance caused by concentration difference. Electrochemical polarisation, also known as activation polarisation, is a polarisation caused by the rate of electrochemical reaction occurring at the positive and negative electrode active substances being less than the rate of electron movement, with a response time of microseconds. Concentration polarisation is caused by unequal rates of reactant consumption, with some reactants on the electrode surface being consumed too quickly and not replenished, and some reactants being consumed too slowly and accumulating on the electrode surface. An example of this is the accumulation of lithium ions at the positive electrode of a battery, resulting in a concentration deviation from the calculated concentration before the start, with a response time in the order of seconds.

图表, 折线图

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Figure 4. different contributions of three type of polarisation

Figure 4 above describes the different contributions of three polarisation reactions. Ohmic internal resistance almost remains unchanged because it does not have relationship with the voltage. Concentration polarisation increases faster with time and is a concave function, whereas electrochemical polarisation, on the contrary, increases slowly with time and is a convex function. Therefore, the reaction efficiency of concentration polarisation is slower than electrochemical polarisation at the beginning but quicker than that in the end.

In the equivalent circuit, the two polarised internal resistances are simulated by combining two series of RC combination (resistance and capacitance), and the current and terminal voltage of this combination are measured to simulate the real state of the battery during operation. The reason for the large deviations in the first-order equivalent circuit is the lack of the simulation of one polarised internal resistance, while circuits of more than fourth-order produce other errors, so second-order and third-order are more ideal models. Figure 5 describes a two-order model.

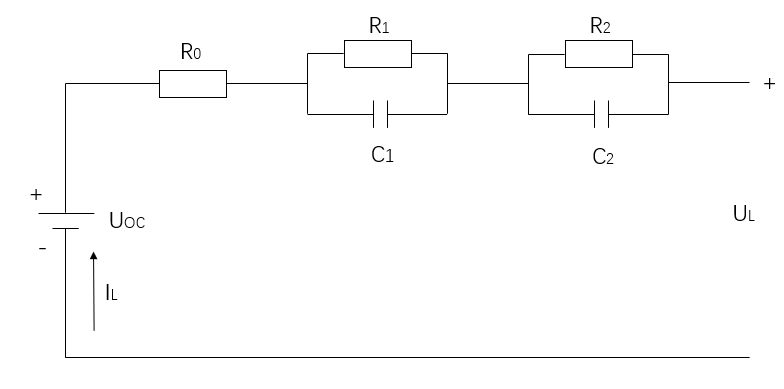


Figure 5. two-order equivalent circuit model

There is still room for improvement in this model. When taking into account the different internal resistance of the system during charge and discharge, the ohmic internal resistance can also be divided, the circuit can be made by connecting two ohmic internal resistances in parallel and designing the diode so that the circuit flows through different resistances during charging and discharging state.

Adding time as a metric factor, the electric potential of the entire circuit is , which can be fitted to a function on SoC, has four components, open-circuit voltage and other three voltage on different resistances, is the open-circuit voltage, is the ohmic internal resistance, and are polarised internal resistances, and is the polarisation capacitance. In a series circuit, the voltage is the sum of the voltages across the components, and current is equal everywhere, in a partial parallel circuit (RC model), the current is the sum of the currents on each component and voltage is equal everywhere, therefore, according to Kirchhoff's law, the following electric model can be generated.

(6)

(7)

## Design of experiment and result

US Department of Energy (2003) specified a kind of Hybrid Pulse Power Characterisation (HPPC) testing to test the pulse charge and discharge performance of power batteries. This testing have been widely used in battery system in hybrid electric vehicle (HEV) and module and single battery. The aim is to demonstrate the power-assisted target's ability to discharge pulses and regenerate charging pulse power at different depths of discharge (DOD). For instance, the battery is filled to capacity and then left to stand and pulsed for a long period of time after every 10% DOD discharge to bring the internal electrochemical and thermal reactions into equilibrium, record the voltage change in this stage, try to fit the relationship with voltage and DOD percentage. the current remains unchanged in discharging stage and after that it returns to 0 in following graph.

In the real equivalent circuit, here is HPPC experiment plan:

The experiment was conducted by the University of Maryland, USA in 2015, using an INR 18650-20R battery with a capacity of 2000mA and LNMC/Graphite battery material.

The experimental protocol is to first fully charge the battery at room temperature of 25 degrees so that the voltage of the battery reached its rated voltage, then discharge it for 12 minutes and leave it for 120 minutes, discharging it 10 times, each time at 10% of the total charge. When the minimum voltage is reached, the battery is recharged and left to stand for 120 minutes every 12 minutes, cycling 10 times. Physical parameters such as voltage, current, charge and discharge capacity, transient voltage are recorded every second during both the charging and discharging phases, and every 10 seconds at the very beginning, when the battery is fully charged. Ideally, the data set should have 142560 entries, which should not include the preparation time period, however, due to some problem, some discharging stages are less than 12 minutes, so the final collection is 142119. All voltage, current and charge data are measured for the entire period. The following graph shows the result of HPPC experiment.

When pre-processing the data, those in the preparation phase were first removed, marking the amount of SoC at each second, which was an estimate to be used as a data annotation for supervised learning. The physical quantities such as voltage before and after the state change were then obtained and taken out separately for subsequent model processing, based on the positive and negative currents and the time elapsed in the phase to determine when to start moving to the next state.

The following figure represents the result of HPPC test, the terminal voltage starts over than 4 volt when SoC is equal to 100%, after 10 times discharge, it reaches nearly 2.5 volt. Then, after charging, it recovers to over 4 volt. During the whole process, current remains nearly consistent. It is clear from figure 6 that whether charging or discharging, the voltage has a definite rebound after the end because the internal chemical reactions have not yet finished simultaneously at the end stage. The individual charging and discharging phases will be dissected in detail below.

图表, 直方图

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Figure 6. charge and discharge graph of the whole process

## Analysis of single process after experiment

图表

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Figure 7. voltage changes on charging/discharging stage

This two graphs show the increase and decrease of voltage in single charging and discharging process between two resting time, the sudden change in voltage in BC segmentation of the diagram is due to the ohmic internal resistance within the circuit. According to the Ohm’s law, it is not difficult to get the specific value.

(8)

CD segmentation is caused by two polarised internal resistance, at this stage, the capacitor has a slow discharge process, so the voltage across the capacitor shows a relatively smooth downward trend, this relationship can be fitted with an exponential function. The time constant (Tao) is the time elapsed when the capacitor voltage decays to 1/e of its value and is determined by the resistance of the capacitor component and the properties of the capacitor, independent of time, resistors and are connected in series with and respectively, according to the formula for the time constant

(9)

remaining total voltage on two capacitors is equal to:

(10)

So the terminal voltage after E point can be described as the following function:

(11)

The function is therefore modeled as y = f(t), parameters are shown:

(12)

(13)

## Parameter identification

Battery electromotive force (EMF) is a very important physical indicator, and the relationship between SoC and EMF varies from stage to stage. EMF cannot be measured directly, so the open circuit voltage (OCV) in the data is used instead. In order to combine the different characteristic values of the two stages of charging and discharging, it is necessary to introduce the concept of an equilibrium voltage in the equivalent circuit. This equilibrium voltage can be replaced by simply using the average value of the charge/discharge EMF at the same SoC. The average value of the difference between the two is described as the hysteresis voltage.

The voltage under different situations:

Table 1. voltage in different SoC

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| SoC | 10% | 20% | 30% | 40% | 50% | 60% | 70% | 80% | 90% | 100% |
|  | 3.468 | 3.556 | 3.599 | 3.626 | 3.665 | 3.754 | 3.840 | 3.940 | 4.050 | 4.176 |
|  | 3.264 | 3.483 | 3.577 | 3.611 | 3.637 | 3.674 | 3.763 | 3.849 | 3.980 | 4.176 |
|  | 3.366 | 3.519 | 3.588 | 3.618 | 3.651 | 3.714 | 3.801 | 3.894 | 4.015 | 4.176 |
|  | 0.102 | 0.036 | 0.011 | 0.008 | 0.014 | 0.040 | 0.038 | 0.046 | 0.035 | 0.000 |

As the graph shows, the voltage changes significantly when the SoC is below 20% or above 60% in both charging and discharging phases, and the voltage changes faster the closer when getting to the ends, while between 20% and 60% the voltage changes slowly. The difference in voltage variation between charge and discharge shows that between 0% and 40%, the difference decreases rapidly and the voltage values converge, while after 50% there is a rebound, which reaches its maximum at around 80% and then decreases rapidly until it narrows to 0%.

图形用户界面, 图表, 折线图

描述已自动生成

Figure 8. voltage and SoC relationship

The average voltage was selected and a polynomial was fitted to the relationship between voltage and SOC. The polynomial was chosen for ease of calculation and as many papers in previous studies have set the order at 7th order, a 7th order fit was used. According to Taylor expansions, a complex function can be expanded to a sum of nth order polynomials after nth order derivations, and the error gets smaller as the order increases.

(14)

Pybamm is a python library for implementing an ideal battery experiment. By calling it and designing a set of parameters for the experiment, it is easy to get the following graph. Pybamm contains a generator for differential equations, which transforms the manually entered parameters into equations and solves them:

图表, 折线图

描述已自动生成

Figure 9. a simulated HPPC test process

This is a graph of the end of a discharge process lasting one hour, from which it can be seen that the current remains at around 0.7A and the voltage drops slowly at the beginning of the discharge, when the SoC value is high, and rapidly when the SoC is low, in line with the performance of the voltage under the real test. As the test ended, the concentration of negative particles (mainly electrons and negatively charged electrolyte ions) decreases, but the distribution is slightly unbalanced. The two vertical lines in the second column of the diagram can be regard as the diaphragm of a Li-ion battery, the left side is negative electrode and the right side is positive electrode, at the end of discharge, a large number of positively charged lithium ions enter the positive electrode, so the concentration of positive charge near the positive electrode is higher, while the potential near the negative electrode is higher the closer it is to the negative material, and the more towards the middle the lower the potential. The concentration of negatively charged electrolyte ions is higher on the negative side than on the positive side, and the potential is higher than on the positive side.

The ohmic internal resistance under different situations:

Table 2. ohmic resistance in different SoC

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| SoC | 10% | 20% | 30% | 40% | 50% | 60% | 70% | 80% | 90% | 100% |
|  | 0.230 | 0.224 | 0.222 | 0.221 | 0.221 | 0.222 | 0.221 | 0.220 | 0.220 | 0.219 |
|  | 0.237 | 0.221 | 0.217 | 0.236 | 0.239 | 0.237 | 0.234 | 0.232 | 0.230 | 0.220 |

It can be seen from the table that ohmic internal resistance is between 0.22 and 0.23 during the charging and discharging phases, indicating that the change in SOC is independent of the ohmic internal resistance, there is an overall higher charging phase than discharging phase.

图表, 折线图

描述已自动生成

Figure 10. relationship between ohmic resistance and SoC

(15)

The cftool tool in Matlab is used to fit a function for the voltage rebound part of each discharge stage, the function is modelled using the double exponential equation mentioned above, the following is an example for one stage:

(16)

Result of goodness of fit: R square = 0.8677, SSE = 0.01346, adjusted R square = 0.856, Confidence interval is 95%, these indicators indicate that with 95% probability more than 85% of the data can be explained by fitting this expression. Therefore, the resistance and capacitor can be calculated:

(17)

The other stages follows the same algorithm and table 3 can be obtained:

Table 3. relationship of polarised resistance and capacitor

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| SoC | 10% | 20% | 30% | 40% | 50% | 60% | 70% | 80% | 90% |
|  | 0.041 | 0.042 | 0.042 | 0.0413 | 0.040 | 0.037 | 0.041 | 0.042 | 0.045 |
|  | 4.552 | 4.543 | 4.545 | 4.549 | 4.554 | 4.533 | 4.518 | 4.476 | 4.355 |
|  | 0.261 | 0.366 | 0.646 | 0.399 | 0.264 | 0.321 | 0.46 | 0.442 | 0.298 |
|  | 68.12 | 51.60 | 38.07 | 59.56 | 75.19 | 68.07 | 57.84 | 58.207 | 57.603 |

图表, 折线图

描述已自动生成

Figure 11. relationship between SoC and resistance and capacitor

The fitting functions show in the figure 12:

图形用户界面, 文本, 应用程序

描述已自动生成

Figure 12. polynomial fittings of four parameters

It is clear from the experiment that the ohmic internal resistance is almost uncorrelated with the change in SoC, it does not change as SoC grows or decreases. For the relationship between voltage and SoC, polarised internal resistance and SoC, and capacitance and SoC, approximate results can be obtained by polynomial fitting. The reason why a polynomial fit is used is that the principle of Taylor expansion approximates an arbitrary function as a polynomial summation of nth order derivatives, calling the error the Peyano cosine, and this can be ignored by mathematical means, so that the fit of this relationship can be made by a polynomial instead.

## Kalman Filter and its extension

The basic idea of Kalman filtering holds the view that the observed value obtained from experiment and the predicted value obtained by the inner pattern are both inaccurate, in order to obtain a more accurate estimate, it is necessary to weight these two values, the current state of a system is from weighted calculation between these two values from the former states, which is so called dynamic update. After several steps, the difference between the obtained estimate and the true value will decrease dramatically. Assuming the relationship between the observed and true values, the relationship between the predicted and true values are in accordance with the Gaussian distribution, the position with the highest probability in the distribution represents the true value, and the standard variance of the observed value’s distribution is significantly smaller than that in predicted value’s distribution, which is reflected in the weight assignment, and the observed value gets a larger weight.

Suppose the true value of each state of a linear system is xk, then the state equation of the system can be written with a control matrix and the previous period jointly determined by the equation, the control matrix determines what law the whole system will follow, for example, in a system of uniformly accelerated linear motion, the displacement of the object s =1/2\*vt^2, in a battery system, the control matrix means that the capacitance of the battery after time k:

(16)

A denotes a state transfer matrix, B denotes a control matrix, u denotes the control vector, and w denotes the noise present in the real system, this equation shows that the estimate in period k depends on the estimate in the previous period, the control situation provided by the previous period to the next period and the system noise.

The observed value can be measured by the instrument, based on the measured value, the transformation matrix can be calculated from the following equation:

(17)

For the predicted value, this logic is consistent with the true value, which can be obtained from the predicted value of the previous period and the control vector, the noise could be taken into consideration in this equation.

(18)

Therefore, estimated value is generated by the weighted calculation from observed value and predicted value:

(19)

Kalman gain matrix is introduced to redefine the calculation of the estimated values:

(20)

The cleverness of this equation is that the relationship between the predicted and observed values is portrayed by a Kalman gain matrix that iterates over time. represents the residuals between predicted value and estimated value, which could be large at the beginning of the system state. A large residual indicates that there is a large gap between the true and predicted values . When the system is updated after several steps, the residual decreases, the gap between the predicted and estimated values decreases, and the influence of the observed values is gradually reduced. At this point, the predicted values inferred from the internal laws of the system can already better reflect the true value and observed value.

To determine several variables mentioned above, the covariance matrix is introduced for matrix transformation. Assuming the presence of noise matrix Q of the system operation in the current period and the true value of the previous period, the presence of observation noise matrix R in the observations, the covariance matrix between the predicted and true values is (residual value), and the covariance matrix between the estimated value and true values is (remaining value).

Assume that the state and observation equations can be expressed by the following equation:

Based on the state and observation equations within the linear Kalman filter model, the equations on SoC prediction can be established:

(21)

In this system of equations, the control matrix is the ratio of the accumulated capacitance to the rated capacitance at the capacitor charging and discharging efficiency η, in other word, the descriptive formula for capacitance, where the ampere-time integration method is used as the calculation of SoC. The observation matrix H is the residual voltage obtained by removing the second-order equivalent circuit, the battery internal resistance, and the voltage consumed by the two polarized internal resistances from the open-circuit voltage. and represent two noise from system operation and observation noise.

(22)

According to the formula of voltage decay and time, and can be figured out:

(23)

Therefore, it can be found that under the second-order equivalent circuit method, the Kalman linear equation is a function with respect to the natural base (e), and this equation is no longer linear, so mathematically, the exponential function is approximated by the Taylor expansion. Suppose that the state function and the observation function both satisfy that in a closed interval [a, b] has nth order derivatives, there exists a point (x0, k0) belongs to [a, b] and the function has (n+1) th order derivatives in the open interval (a, b), one order Taylor expansion is:

(24)

is the cosine term of the formula, it can be ignored. To simplify the formula:

(25)

So the formular can be transferred into linear relationship:

(26)

Initialise the variables and , and combine them as matrix , set the covariance matrix between and as :

(27)

(28)

Set the two weight matrix as A and B:

(29)

All the matrix will be updated based on the Kalman Filter:

Step parameter is k=1, the initial estimated value is , the initial covariance matrix is . the process of algorithm is described as follow:

For (int k = 1; k <= step.length; k++) {

(30)

update the predicted value

(31)

update covariance matrix between predicted value and true value (state covariance matrix)

(32)

update Kalman gain matrix

(33)

update estimated value

(34)

update covariance matrix between estimated value and predicted value

}

if the predicted and estimated values after each cycle are stored separately and displayed as images, it can be seen that the estimated and predicted values are getting closer and closer after the cycle.

### Application of algorithm:

Need a result of algorithm

Figure 13

14

15

## Neural network algorithm

A major advantage of neural networks over equivalent circuit and electrochemical models is that they do not need to understand the complex internal mechanisms and reactions of the cell, but only fit from the measured results. The RNN model will follow the time series to replicate the information within the current layer, but as the number of layers deepens, those further away from the current layer take up less and less weight, while those closer to the current layer take up an increasing number of weight, and the current layer may in reality be more closely related to the more distant layers, so the problem of long-term dependence of information needs to be considered. In addition, RNN faces the problem of gradient disappearance, resulting in sufficient training rounds but still failing to converge.

图示

描述已自动生成

Figure 16. RNN neuron structure

To solve the vulnerability of RNN, long-short term memory has been created. One of the most critical factors to the LSTM algorithm is two parameters, one of which is the output state of every cell and the other is the output value of each cell , these two parameters depend on a three-gate structure. First is the forget gate, shown in the figure 17, which contains a small two layers neural network with two types of input information, the output information from the same hidden layer at last period () and the output from the previous hidden layer at current period (). They concatenate together and become input of this small neural networks with activation function like sigmoid. The output , known as forgetting factor, represents a kind of short-term memory and multiple with the previous cell state , which represents long-term memory, the result indicates which elements of short-term memory will be considered for the next step in the calculation, two vectors have the same dimensions. Therefore, in this way, the results of the forget gate influence the update of long-term memory .

(35)

图示

描述已自动生成

Figure 17. forget gate graph

The second step is called memory gate, it has the opposite function compared with forget gate. The memory gate contains two small neural networks, both of which have the same input, but different activation functions between them. As shown in the figure 18, takes value between 0 and 1 because of the sigmoid function while takes value between -1 and 1 because of the tanh function, the product of two vectors has the significant influence in the update of long-term memory , it forms another part of the output of cell state .

(36)

(37)

图示

描述已自动生成

Figure 18. memory gate graph

To sum up, the update of long-term memory depends on the result of forget gate and memory gate, the function will be:

(38)

At this point, the forget gate and the memory gate together determine which information will be retained for the next cell state and which information will be deleted, will be used as an input source for the next cell to continue the update in the same way.

In addition, the third gate, output gate, shown in the figure 19 is determined by the results of memory gate and forget gate, and another simple layer neural network, . It is worth mentioning that does not need to undergo a neural network transformation, just needs to be substituted into the activation function like tanh, while the original two input information and need to undergo a layer of neural network transformation. Final result of the whole cell is for next cell’s calculation. Function as follow:

(39)

图示

描述已自动生成

Figure 19. output gate graph

### Application of algorithm

1. Constructing dataset

In most cases machine learning models cannot learn from completely arbitrary data, so feature engineering becomes particularly important to determine which feature values need to be input before the model is fed. The open-circuit voltage method determines the open-circuit voltage and is used as an important indicator of SoC, while the ampere-time integration method determines the effect of charge and discharge current on soc. Therefore, it is reasonable to choose voltage and current as feature parameters. The experimental data is divided into two parts, train set is to train model while use test set to get the effectiveness of model.

1. Data pre-processing

Combine all discharge data together and remove the resting process between each two discharging processes. As each feature in the input data carries a magnitude, the magnitude needs to be normalised so that different input dimensions take smaller values in a similar range. In general, if the input data takes larger values, it will result in larger gradient updates, which will prevent the network from converging. Therefore, the input data needs to satisfy two requirements: 1. be small, with most values in the range [0,1], and 2. be homogeneous, with all features taking values in approximately the same range. The voltage, current and time are processed using normalisation methods and the formula for processing is shown below:

(40)

Once the network architecture has been determined, the loss function needs to be chosen, and the loss function is a concrete measure of prediction accuracy. In this experiment, the mean square error (MSE) is used as the loss function to detect the deviation between the predicted and true values. The specific formula is here, means the predicted value, means true value, therefore, using neural network is to find the minimum solution of this loss function:

(41)

1. Hyperparameter and optimiser choice

The optimiser chose Adam because it can dynamically adjust the learning rate for each parameter and determine the range of learning rates to make the parameters more stable. In addition, The Adam optimiser has the following advantages: the algorithm has low space complexity and consumes few computational resources; the update of parameters is not affected by the gradient scaling transformation; the hyperparameters are well interpreted and a more suitable range of hyperparameters can be found; the step size of the update can be limited to an approximate range (initial learning rate); it is well suited to situations with large amounts of data and parameters.

In order to find the appropriate hyperparameters, for instance, the number of layers in the LSTM network, the number of neurons in each layer, 3, 4, 5 and 6 layers were chosen as the range of layers and 15-35 as the number of neurons per layer to obtain the error profile under each parameter specification. It is clear that the performance of the model is at its best with 3-4 hidden layers and decreases significantly as the number of neurons per layer and the number of layers increases.

Need a figure

1. Training and testing result

Chart, histogram

Description automatically generated

Figure 20. MSE changes in each epoch

This figure 20 shows the training error after 150 epochs. It is obvious to see that the error is large at the beginning, but after several rounds of training, the error drops to 0.07%, reaching a good result.

Need the performance of testing set

# Conclusion

This article shows that in a research and experimental bias, the results of neural network models based on large amounts of real-world data are more accurate, however, in industrial application scenarios, the EKF provides a faster and more convenient prediction mechanism. In terms of accuracy, the difference between the LSTM-based test set and the actual results performs significantly better than the EKF-based test results

## Inadequacies and limitations

Although the article uses a number of papers that are well researched in this cutting-edge field, there are still a number of shortcomings. Firstly, the data set tested is a real life measurement of a single Li-ion battery and the tests were conducted at a constant temperature of 25 degrees Celsius, where Li-ion batteries perform best, and not a good simulation of a Li-ion battery pack in an electric vehicle. In a real world scenario, the current distributed to each Li-ion battery is uneven, which can result in a high concentration of current in one battery, causing high temperatures and thus irreversible damage to the electrolyte chemistry of the Li-ion battery, where the current cannot be shared out and the other locations are not fully charged.

Secondly, the data set chosen for the article is the commonly used lithium iron phosphate battery, which is currently widely used in battery systems, but with the development of battery technology, it may one day be possible to overcome the shortcomings of liquid electrolytes and allow solid electrolyte batteries to become popular, then the chemical properties of Li-ion batteries will be more stable and the incidence of burn-out accidents will be greatly reduced.

For the future research, firstly, it is important to note that temperature should be considered as an input feature and if it is possible to set up a constant current charge/discharge case at different temperatures as a control group to test the effect of temperature on the variation of the internal resistance of the Li-ion battery. Secondly, the battery type can also be set as a control group in subsequent experiments; ternary lithium, lithium iron phosphate, lithium cobaltate, or even Li-ion batteries with solid state electrolytes, different Li-ion batteries have different chemical properties and therefore there may be models that are suitable for certain types of Li-ion batteries. Finally, the choice of the most suitable model is always changing depending on the scenario and conditions, so adjustments need to be made in time to suit the situation.

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# Appendix 1 data subset example

Title information

图形用户界面, 应用程序, 表格, Excel

描述已自动生成

Sheet 1

图形用户界面, 应用程序, 表格, Excel

描述已自动生成

Sheet 2

电脑萤幕画面

描述已自动生成

Sheet 3

表格, Excel

描述已自动生成

# Appendix 2 code example

图片包含 日历

描述已自动生成

图形用户界面, 文本, 应用程序

描述已自动生成

文本

描述已自动生成

文本

描述已自动生成

文本

中度可信度描述已自动生成

图形用户界面, 文本, 应用程序

描述已自动生成

# Appendix 3 ethical approval form