Gradient Boosting Decision Tree based State of Health Estimation for Lithiumion Batteries

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ABSTRACT

Accurately estimating the state of health (SOH) of the lithium-ion batteries (LIB), for battery management systems, plays an important role in an ensuring reliable system operation and reducing maintenance costs. Because of the complicated degradation mechanism and the complex internal electrochemical reactions, accurate SOH estimation remains challenging for battery energy management and applications. In this study, we proposed a new SOH estimation method. First, the data is preprocessed and multiple features are extracted to simulate the aging process of the LIB, and the battery capacity is selected as the state variable. Because of the strong capability to fit complex nonlinear problems, a regression model based on gradient boosting decision tree (GBDT) is proposed to estimate the SOH. In addition, a new hybrid optimization algorithm based on quantum particle swarm optimization (QPSO) algorithm and Nelder-Mead simplex (NMS) algorithm is proposed for parameter optimization of the GBDT model. Several lithium-ion battery test data sets from the NASA Ames Prognostics Center of Excellence were selected to validate the proposed method. Compared with other SOH estimation methods and other parameter optimization algorithms, the experimental results show that the proposed method is superior in terms of accuracy, generalization performance and reliability.

Keywords: Lithium-ion batteries, state of health, feature selection, parameters optimization, gradient boosting decision tree

1. INTRODUCTION

Globally, owing to growing concerns about energy consumption and environmental issues, new energy vehicles with energy saving and low carbon emissions, such as electric vehicles (EVs), have become the mainstream development trend of energy conversion and applications. EVs have contributed to solving

environmental problems such as global warming due to their advantages in performance and efficiency [1]. At present, lithium-ion batteries (LIB) have become the most widely used battery types in EVs because of high energy density, good stability and long cycle life [2]. However, even if the battery management system (BMS) has been widely applied to manage the control of LIB, there are some potential threats to the advantages of LIB, such as safety, service life, and the like. Accurate estimation of state of health (SOH) which is one of the key state parameters of the battery can provide a reference for BMS to rationally plan energy storage and supply, effectively avoid some potential threats [3], and avoid injuries caused by excessive use of batteries. However, in real life, the degradation of the capacity of LIB is caused by the superposition of various complicated factors [4], and they cannot be studied in isolation from each other, so the estimation of SOH is still a problem.

With the continuous exploration and research, the data-driven method has gradually become the mainstream method for SOH estimation, because it does not need to study the chemical mechanism inside the battery, and the results are more accurate than the second method. Data-driven methods are mainly machine learning methods [5]. Many popular machine learning methods are widely used in SOH estimation of the LIB, such as support vector machine (SVM) [6], Gaussian process regression (GPR), group method of data handling (GMDH), extreme learning machine (ELM), artificial neural network (ANN) and so on, although these methods have their own advantages [7], they also have some shortcomings in the estimation, such as too many parameters in SVM, will affect the prediction effect. On this basis, the estimation method is continuously improved [8]. However, these methods have similar problems such as too long training time, difficulty in adjusting parameters, and inaccurate fitting [9]. It is necessary to continue to improve the method or use a new method to predict the SOH of the LIB.

Aiming at the above problems, this paper established a new hybrid GBDT model based on QPSO-NMS to predict the SOH. Compared with other traditional machine learning methods, this hybrid method greatly shortens the modeling time, and has stronger generalization ability and more accurate SOH estimation results.

2. SOH ESTIMATION METHOD BASED ON HYBRID ALGORITHM

2.1 Experimental data processing

The lithium-ion battery data set for this article is from the National Aeronautics and Space Administration (NASA) Ames Prognostics Center of Excellence. The data set is obtained by continuous charge and discharge experiments on several types of batteries including a commercial rechargeable lithiumion battery 18650, and mainly includes two processes of charging and discharging, as shown in Fig. 1. The charging process starts with a constant current of 1.5A. As the charging process progresses, the voltage across the battery rises. When the voltage rises to 4.2V, this time starts to charge at a constant voltage of 4.2V. In the process of constant voltage charging, the current across the battery will gradually decrease. When the charging current drops to 20 mA, the charging process ends, and the voltage, current, temperature, and other information are recorded at regular intervals. The discharge process begins with a constant current of 2A until the battery voltage drops to the set value. In this paper, experiments were carried out on batteries No. 5, No. 6 and No. 7 of the NASA lithium-ion battery dataset.





Generally, the SOH is a percentage representing the decrease in battery capacity and increase in internal resistance. In this paper, the capacity ratio is chosen as the definition of the SOH, and its expression is:

$$SOH(i) = \frac{C_i}{C_0}$$

where the C_i represents the battery capacity of the i-th charge and discharge cycle, and the C_0 represents the initial capacity of the battery.

It is well known that battery degradation is mainly affected by its operating voltage, current and temperature, and its degree of degradation is also reflected in the changes in these three characteristics. Therefore, SOH is selected as the output of the model, and through data correlation analysis, five features with higher correlation with SOH are selected from the input voltage, current, temperature and time as the input of the model. The input and output of the algorithm model in this paper are shown in Table 1.

Table. 1. Input and output

Input	Average charge voltage	Average discharge voltage	Time spent charging 3.5v to 4.2v	Constant voltage charging time	Average discharge temperature
Output			SOH		

2.2 Gradient boosting decision tree for SOH estimation

Gradient boosting decision tree (GBDT) is a promising machine learning algorithm proposed by Friedman that combines a series of weak prediction models (which usually is decision trees) to generate classification or regression models. The GBDT regression model is suitable for processing low-dimensional data, can deal with complex nonlinear problems well, is robust to outliers, and has high prediction accuracy. It is suitable for estimating the physical quantity of battery SOH which is not described by a clear quantitative formula. Therefore, this paper uses the GBDT regression model to estimate the SOH. The process of the GBDT algorithm is shown in Fig. 2.

The process of GBDT is as follows:

Input: $T = \{(x_1, y_1), (x_2, y_2), ..., (x_N, y_N)\}$, loss function is L(y, f(x)).

Output: Regression tree is F(x).

Step1: Initialization: Estimate the constant value that minimizes the loss function. It is a tree with only one root node. The general squared loss function is the mean of the nodes, and the absolute loss function is the median of the node samples;

$$f_0(x) = \arg\min_c \sum_{i=1}^N L(y_i, c)$$



where, *c* represents the average of the label values of all training samples, y_i represents the SOH label value of the i-th battery, $L(y_i,c)$ represents the loss function, *N* represents the number of training samples, and $f_0(x)$ represents the initial weak learner.

Step2: For m = 1, 2, ..., M (M means the number of iterations): Calculate the negative gradient of the loss function for sample i = 1, 2, ..., N. The value of the current model is used as an estimate of the residual. For a general loss function, it is an approximation of the residual:

$$r_{mi} = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f(x_i) = f_{m-1}(x)}$$

where, m is the number of iterations, i is the sample number, r_{mi} is the residual of the i-th sample in the m-th iteration, x_i is the i-th training sample value, $f(x_i)$ is the basis function of the i-th training sample, and $f_{m-1}(x)$ is the m-1 weak learner obtained from two iterations, the negative gradient $L(y_i, f(x_i))$ is calculated using a squared loss function, as follows:

$$L(y,f(x)) = (y - f(x))^2$$

And then fit a regression tree to $\{(x_1, r_{m1}), ..., (x_N, r_{mN})\}$ to get the leaf node area $R_{mj}, j = 1, 2, ..., J$ of the m-th tree (J represents the number of leaf nodes per tree).

Using a look-ahead search for j = 1, 2, ..., J, estimating the value of the leaf node region, minimizing the loss function, and calculating:

$$C_{mj} = \arg\min_{c} \sum_{x_i \in R_{mj}} L(y_i, f_{m-1}(x_i + c))$$

Finally, update:

$$f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J} C_{mj} I \ (x \in R_{mj})$$
$$I(x \in R_{mj}) = \begin{cases} 1, x_i \in R_{mj} \\ 0, x_i \notin R_{mj} \end{cases}$$

Step3: Get the final regression tree F(x):

$$F(x) = \sum_{m=1}^{M} \sum_{j=1}^{J} C_{mj} I(x \in R_{mj})$$

Step4: Get the final learning machine H(x):

$$H(x) = f_m(x) = f_0(x) + \sum_{m=1}^{M} \sum_{j=1}^{J} C_{mj} I(x \in R_{mj})$$



2.3 Hybrid optimization algorithm

Although GBDT can obtain a more accurate fitting value for complex nonlinear problems, GBDT model has multiple parameters. Manual tuning is too cumbersome, and traditional methods have many shortcomings in terms of computational efficiency and accuracy of results. For example, grid search (GS) uses exhaustive search, which will increase the time spent by multiple parameters due to too many parameters. The PSO algorithm has many parameters and is easy to fall into local optimum, which is not optimal parameters; Differential evolution (DE) algorithm is very sensitive to parameter settings. Improper parameter settings can lead to convergence too fast and fall into local optimum. Therefore, this paper uses an improved QPSO-NMS hybrid optimization algorithm to optimize the parameters of the GBDT model.

The QPSO algorithm is a random global search algorithm that is suitable for dealing with complex and nonlinear problems that are difficult to solve with traditional search methods. However, due to the randomness of the algorithm, it is difficult to obtain an exact solution to the problem. It is an algorithm with strong global search ability and insufficient local ability. The NMS algorithm has the advantages of small calculation amount and fast calculation speed, but it is sensitive to the initial value, and the initial value selection is poor, which easily leads to the trap of local optimum. According to the characteristics of the above two algorithms, this paper combines the two and establishes a hybrid optimization algorithm of QPSO-NMS. Firstly, the QPSO algorithm searches the approximate optimal solution in the global scope, and then uses the NMS algorithm to perform local search in the approximate solution neighborhood to find the exact optimal solution. The entire hybrid algorithm flow is shown in Fig. 3.

2.4 Experimental Results

In order to verify the accuracy and versatility of the SOH estimation method proposed in this paper, this section gives the experimental results based on the NASA battery data set. In this paper, three datasets No. 5, No. 6, and No. 7 in the NASA battery data set are selected. Three batteries are charged and discharged in cycles, and the total number of cycles is 168, and 80% of the data samples were randomly selected for training the GBDT hybrid model. The remaining data was used to verify the performance of the proposed method. For the No. 5 battery, the parameters of the GBDT model are optimized by the QPSO-NMS hybrid algorithm. The optimal results of the GBDT model parameters are: "learning rate" is 0.17, "estimators" is 63, "max depth" is 6, and "min samples split" is 2.

In this part, the performance of the method was compared with the performance of SVM, MC-PKNN and PSO-BPNN. The comparison results are shown in Fig. 4 and Fig. 5. These figures give the overall prediction graph and partial details. It can be seen that compared with other methods, the error of the proposed method is smaller and most closely matches the real SOH curve. Table 2 and Table 3 show the performance comparison of the method of this paper with other methods. Compared with other methods, this method achieves



Fig. 4. Comparison of GBDT and other algorithms in the

Coll Num	Battery 5#				
Centrum	MSE	MAE	RMSE		
QPSO-NMS- GBDT	1.63E-05	1.42E-03	4.03E-01		
PKNN	3.55E-05	4.12E-03	5.96E-01		
MC-GMDH	3.39E-05	3.63E-03	5.83E-03		
SVM	2.93E-04	9.44E-03	1.71E+00		
PSO-BPNN	3.39E-04	1.13E-02	1.84E+00		

Table 2. Battery NO.5 e	experimental result
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the minimum MSE, MAE and RMSE at the same time. It can be seen from the above results that the proposed method can achieve a more accurate SOH estimation.

In order to verify the versatility of the method, three data sets were trained and predicted using this method. The data of the three data sets is different, which leads to the need to adjust the GBDT model before training. The hybrid optimization algorithm used in this paper will automatically optimize the parameters of GBDT according to the performance index, without giving the initial value, no need to manually adjust the parameters, etc. Complex operation. Table 4 gives the comparison results between the accuracy and time of the optimization algorithm and other optimization algorithms. It can be seen from Table 4 that the GS method is too many iterations and takes too much time in the face of multiple parameter optimization. It can be seen from Fig. 6 that under the same number of iterations and the same optimization goal, PSO and QPSO fall into the local optimum, and the obtained



Fig. 5. Comparison of GBDT and other algorithms in the estimation results of battery No. 6 and No. 7

J	Cell Num	Battery 6#			Battery 7#		
		MSE	MAE	RMSE	MSE	MAE	RMSE
	QPSO-NMS-GBDT	3.75E-05	2.80E-03	6.12E-01	9.57E-06	1.37E-03	3.09E-01
	PKNN	4.54E-05	5.37E-03	6.73E-03	3.38E-05	4.32E-03	5.81E-03
Q	MC-GMDH	9.13E-05	5.95E-03	9.56E-03	8.71E-05	6.28E-03	9.33E-03
Ø	SVM	4.56E-04	1.14E-02	2.14E-02	5.80E-04	9.13E-03	2.41E-02
	PSO-BPNN	1.18E-03	2.09E-02	3.43E-02	3.54E-03	1.30E-02	5.95E-02

Table 3. Battery NO.6 and NO.7 experimental result

parameters are not optimal. The QPSO-NMS hybrid optimization algorithm has better effect on the optimization of GBDT parameters. The results show that the hybrid optimization algorithm used in this paper has



better effect on the optimization of GBDT model parameters, and it can take a shorter time to get more accurate result.

Table 4. Comparison of optimization algorithm results

Algorithms	Number of iterations	The optimal value	Running time(s)
QPSO- NMS	QPSO 10 times, NMS 47 times	1.63E-05	893.7
QPSO	10 particles, iteration 100 times	1.69E-05	3009.4
PSO	10 particles, iteration 100 times	1.75E-05	3808.2
Grid Search	Grid iteration 1080 Search times		5507.9

It can be seen from the experimental data that, compared with other machine learning algorithms, the hybrid algorithm proposed in this paper has more accurate SOH estimation results. Compared with other optimization algorithms, the hybrid optimization

2.5 Discussion

algorithm proposed in this paper requires the shortest time and the least number of optimizations, resulting in more accurate estimation results and lower errors. It shows that the generalization ability of this hybrid algorithm is better than other algorithms. It can be concluded that the method proposed in this paper has higher accuracy, faster optimization speed, and powerful generalization ability, and is more suitable for estimation of battery SOH and monitoring of battery working status in real life.

3. CONCLUSIONS

The focus of this paper is to propose and validate a SOH estimation method based on the hybrid optimization algorithm for GBDT regression model. Firstly, the data was preprocessed, and five characteristics with high correlation with SOH were selected from the charge and discharge curves according to the correlation analysis. Then a new GBDT regression model was used to estimate the SOH. A new QPSO-NMS-based hybrid optimization algorithm is used to optimize the parameters of the GBDT model, which solves the problem that the GBDT model is difficult to adjust parameters. Compared with other novel the battery SOH estimation methods, the experimental results show that this method has a high accuracy for the estimation of the battery SOH with an overall error of about 1.3%. It has been verified by multiple NASA battery data sets. Compared with other parameter optimization algorithms, the results show that compared with other methods, this method does not need to give the initial values of parameters, and the overall work efficiency is improved by about 73.3%, which has strong generalization ability and versatility. In summary, the method proposed in this paper can accurately estimate the SOH, which is very suitable for the management and operation of lithium-ion batteries in BMS.

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