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Published in:
APEC 2023 - 38th Annual IEEE Applied Power Electronics Conference and Exposition

DOI (link to publication from Publisher):
10.1109/APEC43580.2023.10131132

Publication date:
2023

Document Version
Accepted author manuscript, peer reviewed version

Citation for published version (APA):
Sui, X., He, S., Vilsen, S. B., Teodorescu, R., & Stroe, D.-I. (2023). Hyperparameter optimization in bagging-based ELM algorithm for lithium-ion battery state of health estimation. In *APEC 2023 - 38th Annual IEEE Applied Power Electronics Conference and Exposition* (pp. 1797-1801). Article 10131132 IEEE. https://doi.org/10.1109/APEC43580.2023.10131132

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Hyperparameter Optimization in Bagging-Based ELM Algorithm for Lithium-Ion Battery State of Health Estimation

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Abstract— **Artificial neural networks are widely studied for the state of health (SOH) estimation of Lithium-ion batteries because they can recognize global features from the raw data and are able to cope with multi-dimensional data. But the performance of the model depends to some extent on the selection of the hyperparameters, which remain constant during model training. To improve the generalization performance as well as accuracy, an ensemble learning framework is proposed for battery SOH estimation, where multiple extreme learning machines are trained combined with bagging technology. The numbers of bags and neurons of the base model are then tuned by five commonly used hyperparameter optimization methods. Moreover, the SOH value with maximum probability density is selected as the output estimate to further improve the estimation accuracy. Finally, experimental results on both NMC and LPF batteries demonstrate that the proposed method with hyperparameter optimization can achieve stable and accurate battery SOH estimation. Regardless of which optimization method is used, the average percentage error for SOH estimation of NMC and LFP batteries can keep below 1% and 1.2%, respectively.**

Keywords— **Lithium-ion battery, state of health, robust estimation, ensemble learning.**

I. Introduction

With the emergence of global issues, such as the energy crisis, global warming, and the rapid growth of travel demand, the transportation sector is undergoing a revolutionary shift from the internal combustion engine to an electric drivetrain. Lithium-ion batteries (which serve as the main power system) have long limited the development of new energy vehicles [1-2]. The poor safety, short cruising range, long charging time, and high cost of energy vehicles are still problems that need to be solved urgently. Health management plays an important role in avoiding thermal runaway, optimizing fast charging, and extending the cruising range [3]. Generally, the battery's state of health (SOH) is a figure of merit that indicates the condition of the battery throughout its service life. SOH is defined as the ratio between the current available capacity and the initial capacity. Usually, 20% or 30% capacity fade is adopted as the end-of-life criteria [4]. Machine learning (ML) technologies possess immense potential in inferring battery SOH since they do not rely on specific battery models. Many algorithms have been successfully applied such as support vector machine, gaussian process regression (GPR), artificial neural network, deep learning, etc. [5]. Ensemble learning (EL) is emerging because it generally produces more accurate and robust results than a single base learner [6].

EL method can be categorized into heterogeneous ensemble and homogeneous ensemble [5]. In the heterogeneous ensemble, multiple different types of base learners from above-mentioned ML algorithms will be trained [7-10]. For example, linear regression and GPR models were established based on the residuals and a series of intrinsic mode functions decomposed from the original signal [7]. In [9], eight convolutional neural networks are built based on the aging data of eight battery cells. Together with transfer learning and average aggregation, the accuracy and robustness are enhanced. It is obvious that training multiple ML models will increase the computational complexity. To guarantee the estimation accuracy, a small number of but relatively accurate models will be selected for the ensemble. In addition, overfitting is still a concern when the available dataset is small. Therefore, the homogeneous ensemble is proposed where resampling technologies such as bagging and boosting are used to create diverse subsets, and then multiple homogeneous models can be established [10]. The computationally efficient algorithm, such as the extreme learning machine (ELM), is preferred as the base model [11]. However, the performance of the EL algorithm can be greatly affected by the hyperparameters, e.g., the number or the size of the base models [12]. Therefore, a Bagging ELM-based (BaggELM) SOH estimation method with optimized hyperparameters is proposed in this work.

The rest of this paper is organized as follows. The estimation framework for SOH estimation including bagging-based data augmentation, hyperparameter optimization, and output aggregation method is introduced in Section II. Section III describes the cyclic aging tests for commonly used NMC and LFP batteries. Then the performance of the proposed Bagging-based EL methods and hyperparameter optimization are investigated. Section IV gives the conclusion of this work.

This research was funded by the "SMART BATTERY" project, granted by Villum Foundation in 2021 (project number 222860).

II. METHODOLOGY

Fig. 1 gives an illustration of the proposed EL-based framework for SOH estimation. It consists of two parts: model training and validation. Battery aging data (i.e., voltage (V), current (I), temperature (T), and time (t)) are measured and stored through various laboratory tests. Considering the real application where batteries are typically operated in a partial (between 10% and 90% SOC or even a narrower SOC range) rather than a full SOC range, a partial voltage was chosen as the input for the ML model. Through model training on known data, the relationship between input and output can be established. According to the BaggELM method [5, 6], two hyperparameters related to the structure of the model need to be optimized, i.e., the numbers of hidden neurons (N), and the numbers of the bootstrap samples (B). Five commonly used algorithms, namely pattern search, Bayesian optimization, simulated annealing, genetic algorithm, and particle swarm are applied to search for the optimal combination of N and B. The established model is then validated on the unseen dataset.

Traditionally in the EL method, based on a weighted average of the base model or through voting, the final output is given. However, because of the random parameterization of BaggELM, each base learner may show significantly different performance. It is worth noting that the estimation error for NMC battery, as shown in Fig. 2(a) and Fig. 3(a), fluctuates with the increase of B, and finally tends to be stable. Besides, when BaggELM is trained multiple times with a random N and B, the model shows unstable estimation and is even invalid.

The RMSE for NMC battery obtained from the 6th and 9th training is almost as large as 3%, indicating a significant fluctuation in the estimation from different times of training. In this case, the average-based ensemble will still bring errors caused by poor base learners. To better utilize the output of multiple base models, the probability density function (PDF) of estimated SOH from all B base models is obtained. The mode value rather than the mean value is then output as the final estimate. The PDF of the output results distribution is calculated as

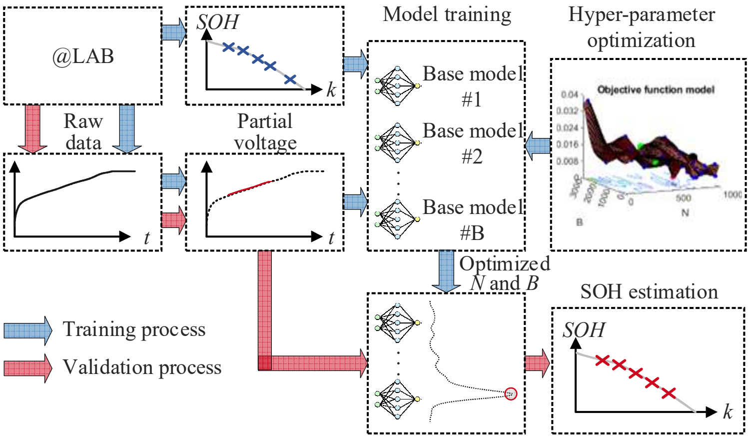

Fig. 1. Schematic diagram of the proposed SOH estimation framework.

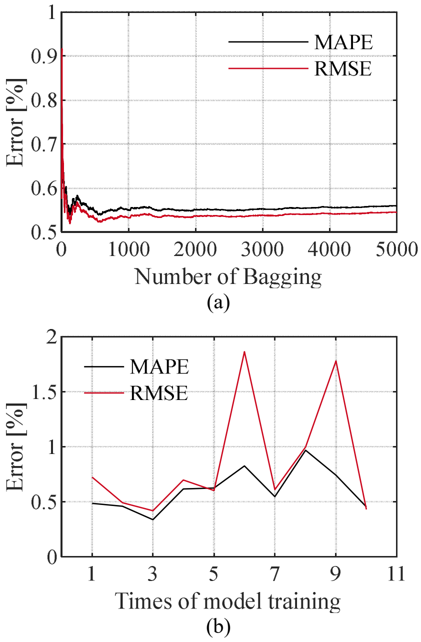

Fig. 2. Impact of the hyperparameters on SOH estimation for NMC battery. (a) N is fixed to 40, and B is varied from 1 to 5000. (b) Ten times of model training with randomly selected N and B.

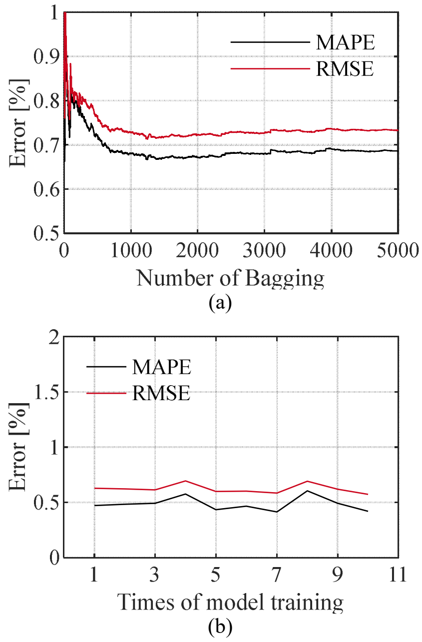

Fig. 3. Impact of the hyperparameters on SOH estimation for LFP battery. (a) N is fixed to 40, and B is varied from 1 to 5000. (b) Ten times of model training with randomly selected N and B.

$$f(x)=\frac{1}{\sqrt{2\pi\sigma^2}}e^{-x^2/(2\sigma^2)} \quad (1)$$

where σ is the scale parameter. $\sigma = 1$ and $\sigma \neq 1$ represent that variables follow the symmetrical and asymmetrical distribution. The predicted value of a new observation, $\mathbf{x}_{new}$, can be considered as the mode of the PDF.

$$\hat{Y}_{new} = \text{mode}\left[\text{PDF}(\hat{f}_b(\mathbf{x}_{new}), b=1,\ 2,\ \ldots, B)\right] \quad (2)$$

where $\hat{f}_b(\cdot)$ is the bth single ELM. Take the NMC battery as an example, the estimation results using mean and mode as output has been compared. Fig. 4(a) shows the estimation results for all 137 single ELMs, along with the corresponding probability density distribution in Fig. 4(b). The mode of distribution, i.e., the peak value in the probability density function, represents the most likely case. As shown in Fig. 4(b), the mode value is closer to the real SOH than the mean. Therefore, to better utilize the output of multiple base models and further compensate for the instability of the weak learner, the EL model outputs its mode as the estimate. The whole framework for battery SOH estimation has been implemented in MATLAB code, where Global Optimization Toolbox is used for hyperparameter optimization. The model training was performed on a PC with an Intel core i7 processor and Nvidia MX450, with 48GB RAM.

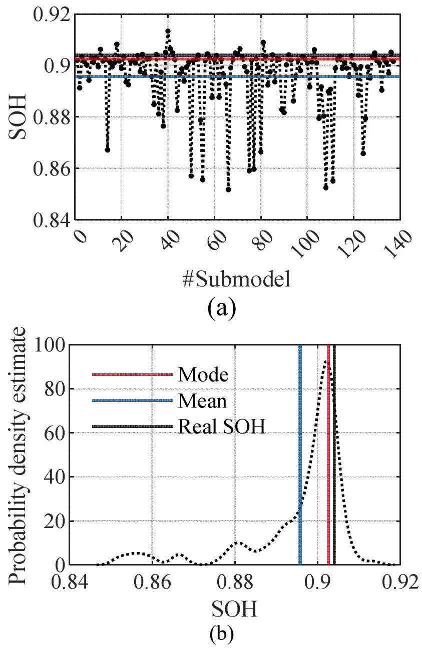

Fig. 4. Statistical plot of estimated SOH values from each base model. (a) SOH estimates. (b) Probability density function of the output results.

III. Experimental Aging Tests

To verify the effectiveness of the proposed SOH estimation method, two commonly used batteries, i.e., NMC and LFP batteries were subjected to accelerated aging tests. The main electrical parameters of the tested batteries are summarized in Table I. Respectively, the NMC battery was aged at 35°C using the standardized WLTC driving cycle for class B vehicles; at the end of the test (i.e., after 580 full equivalent cycles, FECs), the cells reached a capacity fade of 13%. The capacity of the NMC battery was measured at 25°C with CC-CV charging and CC discharging. It was conducted initially after every week of cycling (corresponding to 20 FECs). Since it was found that the battery capacity fades slowly, the capacity test was changed to every 3 weeks after 14 weeks of cycling. The LFP battery was aged with a one-week frequency regulation mission profile, and the battery state of charge varies from 10% and 90%. The CC-CV charging was also conducted for measuring the capacity of the LFP battery. Particularly, it was first charged with a 1C-rate constant current until the voltage reaches 3.6 V. Then the voltage was held to be 3.6 V until the current equals 0.1 A where batteries are considered fully charged (CC-CV charging). After 15 minutes of relaxation for achieving electrochemical stability, the current battery capacity was measured following a 1C-rate constant current discharging procedure (CC discharging). During both charging and discharging, the battery data is sampled with one second. The above two experiments were carried out in a loop until the tested battery reached 18% capacity fade. As a result, the obtained voltage and the corresponding SOH curves during the capacity test can be seen in Fig. 5 and Fig. 6.

TABLE I. The Datasheet of the Tested NMC and LFP Batteries

Item	NMC	LFP
Nominal capacity	3.4 Ah	2.5 Ah
Nominal voltage	3.6 V	3.3 V
Maximum voltage	4.2 V	3.6 V
Cut-off voltage	2.65 V	2.0 V
Maximum continuous charge current	2 A	10 A
Maximum continuous discharge current	8 A	50 A

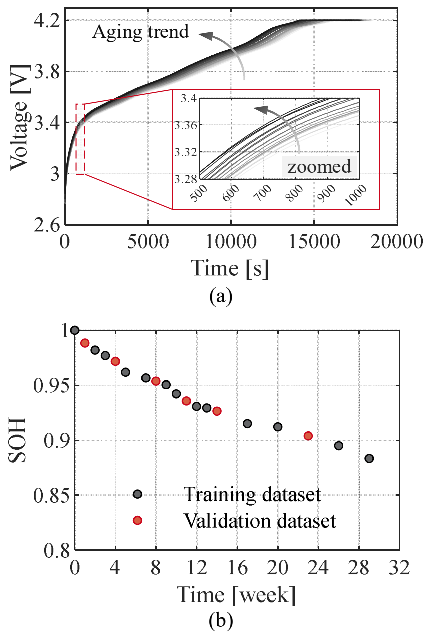

Fig. 5. Data obtained from cyclic aging of the NMC battery. (a) Voltage responses under CC-CV charging. (b) SOH curve.

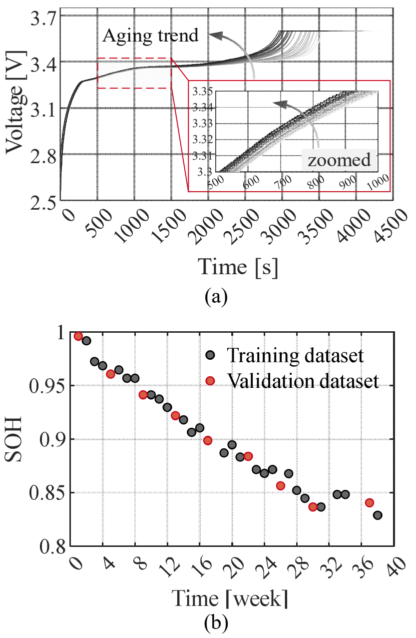

Fig. 6. Data obtained from cyclic aging of the LFP battery. (a) Voltage responses under CC-CV charging. (b) SOH curve.

IV. SOH Estimation Results

The root-mean-squared error (RMSE), mean absolute percentage error (MAPE), and absolute percentage error (APE) are the metrics used to evaluate the effectiveness of the proposed method. They are defined as:

$$RMSE = \sqrt{\frac{1}{N_T}\sum_{i=1}^{N_T}\left(\hat{SOH}_i - SOH_i\right)^2} \tag{3}$$

$$MAPE = \frac{1}{N_T}\sum_{i=1}^{N_T}\left(\frac{\left|\hat{SOH}_i - SOH_i\right|}{SOH_i}\times 100\%\right) \tag{4}$$

$$APE = \frac{\left|\hat{SOH}_i - SOH_i\right|}{SOH_i}\times 100\% \tag{5}$$

where N_T is the total number of validation data, $\hat{SOH}_i$ and SOH_i is the estimated SOH and the real SOH of the ith validation data point, respectively. The self-validation approach is used, where the aging datasets of the tested batteries are divided into a training group (65% of the dataset, i.e., the black points in Fig. 5(b) and Fig. 6(b)) and a validation group (35% of the dataset, i.e., the red points in Fig. 5(b) and Fig. 6(b)).

A. Effectiveness of ensemble learning

As shown in Fig. 7 and Fig. 8, the effectiveness of bootstrap aggregating technology has been investigated. For both NMC and LFP batteries. An ELM (N=40) and a BaggELM model (with N=40, B=10) are established, respectively. The hyperparameters are randomly selected without optimization. As can be observed, BaggELM provides a good generalization performance and the APE for NMC and LFP remains under 1% and 2%, respectively, throughout the battery's lifetime, while ELM shows a relatively large fluctuation in the estimation.

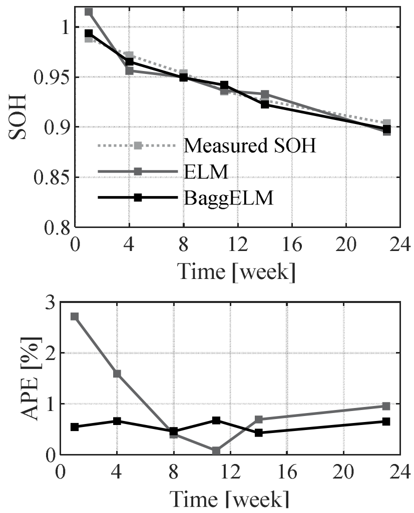

Fig. 7. SOH estimation results with ELM and BaggELM methods for NMC battery.

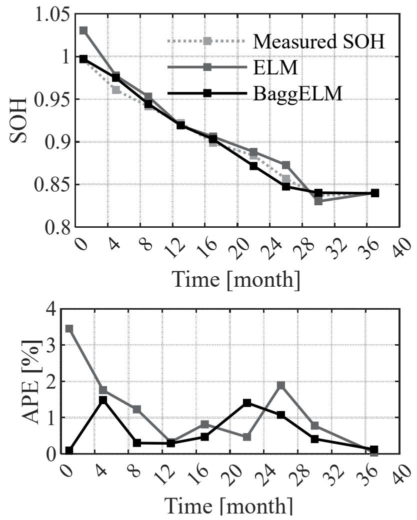

Fig. 8. SOH estimation results with ELM and BaggELM methods for LPF battery.

B. Effectiveness of hyperparameter optimization

By using optimized parameters N and B, the estimation results are summarized in Fig. 9, Fig. 10, and Table II. It can be seen that the model can fail to converge if the hyperparameters are not chosen properly. In addition, using hyperparameters optimization, no matter what the algorithm, is effective in improving the stability and accuracy of estimation. Specifically, for the NMC battery and the model built on optimal parameters, its APE keeps below 1%, and both RMSE and MAPE are less than 0.5%, regardless of which optimization method is used. For the LFP battery, due to the plateau characteristic in voltage response, the SOH estimation error is slightly higher than that of the NMC battery. Similar results are obtained for the LFP battery where its APE maintains less than 1.2%, and RMSE and MAPE are less than 0.8%.

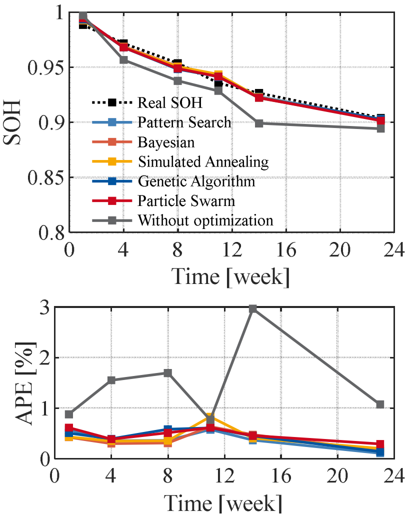

Fig. 9. SOH estimation results of BaggELM using different hyperparameter optimization methods for LFP battery.

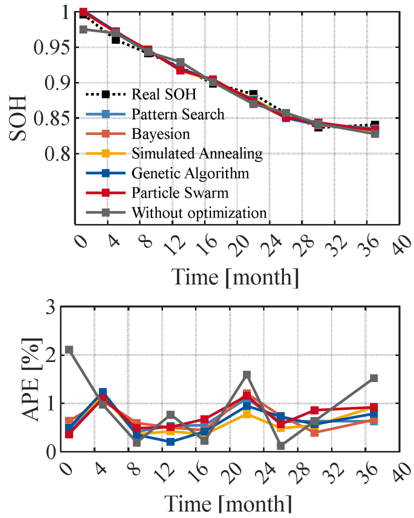

Fig. 10.SOH estimation results of BaggELM using different hyperparameter optimization methods for NMC battery.

TABLE II. SUMMARY OF THE SELECTED HYPERPARAMETERS (I.E., N AND B) BY EACH OPTIMIZATION METHOD AND SOH ESTIMATION ERRORS OF THE CORRESPONDING MODELS

Method	NMC battery			LFP battery		
	Hyperparameter values	MAPE [%]	RMSE [%]	Hyperparameter values	MAPE [%]	RMSE [%]
Without optimization	*N=1672, B=733	1.56	1.31	*N=700, B=10	0.76	1.04
Pattern Search	N=5, B=262	0.39	0.40	N=144, B=1809	0.66	0.68
Bayesian	N=137, B=394	0.38	0.39	N=231, B=87	0.69	0.67
Simulated Annealing	N=69, B=286	0.43	0.45	N=174, B=142	0.62	0.61
Genetic Algorithm	N=47, B=406	0.45	0.45	N=163, B=129	0.64	0.64
Particle Swarm	N=5, B=54	0.48	0.47	N=159, B=30	0.70	0.74

Note*: N and B are randomly selected for BaggELM without optimization

V. CONCLUSIONS

In this paper, an EL-based battery SOH estimation framework, including partial voltage selection, BaggELM base model training, hyperparameter optimization, and output selection determined by probability density is proposed. The experimental results on both NMC and LFP batteries indicate that BaggELM performs better than the single ELM. However, the estimation accuracy is influenced by network-related hyperparameters, namely B and N, significantly. By optimally choosing these two parameters, the estimation accuracy and stability of the model are greatly improved. Moreover, due to the plateau characteristic, the aging information contained in the voltage measurements of the LFP battery is less than that of the NMC battery. This makes it challenging in SOH estimation for the LFP battery when only raw voltage is used. Hence, it can further demonstrate the significance of the proposed method in practical applications.

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