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State of health estimation of lithium-ion batteries based on incremental capacity curves

Mengyao Geng, Qiaoqiao Yang, Huixing Meng*

State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing, 100081, China. E-mail: huixing.meng@bit.edu.cn

Te Han*

Center for Energy and Environmental Policy Research, Beijing Institute of Technology, Beijing 100081, China. E-mail: hante@bit.edu.cn

State of health (SOH) is adopted as a key predictor in the battery management system to ensure the safety and reliability of electric vehicles. In this paper, based on incremental capacity (IC) curves and long short-term memory network (LSTM) with Bayesian optimization, we propose a method for SOH estimation of lithium-ion batteries. Firstly, IC curves are obtained and health features are extracted from partial IC curves. Secondly, LSTM model is established to capture the mapping relationships between health features and SOH. Thirdly, Bayesian optimization is applied to automatically select hyper-parameters of LSTM. Eventually, the effectiveness and superiority of the proposed method are validated on real lithium-ion battery aging datasets from CALCE Prognostics Data Repository.

Keywords: Lithium-ion batteries, incremental capacity curve, LSTM, Bayesian optimization.

1. Introduction

Lithium-ion batteries (LIBs) are penetrating into the field of electric vehicles (EVs) due to the advantages of high energy density, longevity, and low cost (Luo et al., 2022). In practice, the performance of LIBs degrades with increased use and improper handling, which may lead to battery system breakdown, even resulting in catastrophic disasters (Meng & Li, 2019; Xu et al., 2021). In this situation, state of health (SOH) is considered as an essential indicator in the battery management system. Accurate SOH estimation not only guarantees the safety and reliability of EV operations, but also prolongs battery service life (Meng et al., 2022).

An essential issue of SOH estimation and prognostic is health indicators (HIs) extraction and how to construct the mapping relationship between HIs and SOH (Wang et al., 2021). Geometric HIs based on voltage or current curves are also important HI types, which can be visually associated with SOH degradation (Guo et al., 2019). The mechanism of geometric HIs is not clear thus limiting their application in practice (Tang et al., 2020). Recently, incremental capacity analysis (ICA) is used as an effective HIs for offline SOH estimation. Zhou et al. (Zhou et al., 2023) took the peak value of the incremental capacity (IC) curves as HIs to enhance the adaptability to different charging regions of the degradation model. Li et al. (Li et al., 2019) used grey relational analysis and entropy weight method to evaluate the importance of IC features. Lin et al. (Lin et al., 2023) considered eight HIs extracted from IC, differential temperature, and differential thermal voltammetry curves. Considering the electricity anxiety of EV users in real life, the extraction of IC peaks encounters obstacles because it usually relies on the complete or specific charging process while users take charging process start and end randomly.

In recent years, deep learning models have received extensive attention in lithium-ion battery SOH estimation due to their powerful non-linear modeling abilities, such as deep neural network (DNN) (Obregon et al., 2023), deep belief network (DBN) (Niu et al., 2022), convolutional neural network (CNN) (Shen et al., 2020), and recurrent neural network (RNN) (Zhang et al., 2021). Long short-term memory network (LSTM) has been applied in many fields with excellent performance in time series prediction and nonlinear mapping (Ardeshiri et al., 2022).

Despite their success, the selection of hyper-parameter remains a challenge to improve the accuracy of the deep learning model.

To cope with the above problems, this paper proposes an improved SOH estimation approach for lithium-ion batteries based on Bayesian optimization and partial IC curves. Firstly, the IC curve is calculated with historical monitoring data, and partial IC curve is selected considering the real charging behavior. Then, LSTM model is built to construct the mapping relationship between IC and SOH. Meanwhile, Bayesian optimization algorithm is incorporated to select optimal parameters automatically.

The remainder of this paper is structured as follows. Section 2 presents the proposed LSTM model with Bayesian optimization. Section 3 shows the experimental results of the proposed method based on the CALCE battery dataset. Eventually, Section 5 concludes the paper.

2. Methodology

In this section, we present the methodology of the proposed model, including IC curve acquisition, LSTM model, and Bayesian optimization.

2.1. *IC curve acquisition*

ICA has been widely used in feature extraction for lithium-ion battery SOH estimation. It can establish the relationship between the external characteristics and the internal electrochemical characteristics. Based on the constant current–constant voltage (CC–CV) charging mode, IC curve can be acquired by differentiating the voltage relative to the charged capacity as follows (She et al., 2020).

$$IC = \frac{dQ}{dV} = \frac{I \cdot dt}{dV} = I \cdot \frac{dt}{dV} \quad (1)$$

where Q indicates charged capacity during the charging process, V denotes the voltage of the battery, I represents the charging current of the battery, and t stands for the charging time of the battery.

2.2. *LSTM model*

Gradient vanish and gradient explosion are domain challenges in traditional recurrent neural network. LSTM is proposed to solve the problem (Shi & Chehade, 2021). The architecture of LSTM is composed of three control gates called input gate (i_t), forget gate (f_t), and output gate (o_t) to process the long-term dependence of time series as shown in Fig. 1. Information can be stored in, written to, or read from the cell by operating these gates.

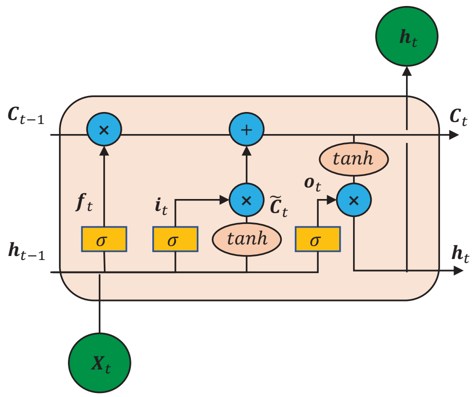

Fig. 1. The architecture of LSTM model.

For the input sequence consisting of partial IC data X_t and the previous hidden state h_{t-1}, the current hidden state h_t can be obtained by the following chain of equations (Gong et al., 2020).

$$f_t = \sigma\left(W_f[h_{t-1}, X_t] + b_f\right) \quad (2)$$

$$C_t' = tanh(W_c[h_{t-1}, X_t] + b_c) \quad (3)$$

$$i_t = \sigma(W_i[h_{t-1}, X_t] + b_i) \quad (4)$$

$$C_t = f_t * C_{t-1} + i_t * C_t' \quad (5)$$

$$o_t = \sigma(W_o[h_{t-1}, X_t] + b_o) \quad (6)$$

$$h_t = o_t * tanh(C_t) \quad (7)$$

Where (W_x, b_x) , $x \in (f, c, i, o)$ denotes the weights and deviations of forget gate, control gate and input gate, and output gate. C_t and C_{t-1} stand for the previous and current cell state, respectively. σ indicates the sigmoid activation function, $\sigma(z) = \frac{1}{1+e^{-z}}$. $tanh$ represents the tanh activation function, $\tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$. $*$ is the element level multiplication.

2.3. *Bayesian optimization*

Traditionally, hyper-parameters of deep learning models are tuned by experience (Remadna et al., 2023). Manual adjustment not only is timeconsuming, but also leads to low accuracy and efficiency. To improve the estimation accuracy and obtain the optimal solution, Bayesian optimization algorithm is proposed to optimize the hyper-parameters of the LSTM model. We adopt Tree-structured Parzen estimator (TPE) to reduce the burden of hyper-parameter computation, which is a type of sequential model-based Bayesian optimization algorithm.

Assume that K represents a combination of hyper-parameters in LSTM model, Expected Improvement (EI) is employed to obtain the best set of hyper-parameters can be expressed as:

$$EI_{y^*}(x) = \int_{-\infty}^{\infty} \max(y^* - y, 0)\, p_M(y \mid K)\, dy \quad (8)$$

where $p_M(y \mid x)$ refers probability model representing the probability distribution of the objective function.

TPE defines $p(K \mid y)$ using two such densities:

$$p(K \mid y) = \begin{cases} l(K), & y < y^* \\ g(K), & y \geq y^* \end{cases} \quad (9)$$

where, $l(x)$ repents the probability density formed by the value of objective function less than y^*, and $g(x)$ is the probability density consisting of the remaining objective function values.

TPE sets hyper-parameter γ to be quantile of the observed y, so that we can obtain:

$$\begin{aligned} p(x) &= \int_R p(x \mid y) p(y) dy \\ &= \gamma l(x) + (1-\gamma) g(x) \end{aligned} \quad (10)$$

The EI formula can be derived as follows:

$$\begin{aligned} EI_{y^*}(x) &= \frac{\gamma y^* l(\theta) - l(\theta) \int_{-\infty}^{y^*} p(y) dy}{\gamma^{l(\theta)} + (1-\gamma) g(x)} \\ &\propto \left(\gamma + \frac{g(x)}{l(x)}(1-\gamma)\right)^{-1} \end{aligned} \quad (11)$$

According to Equation (11), it can be seen that maximizing the EI means making hyper-parameter x has high probability under $l(x)$ and low probability under $g(x)$ (Shen et al., 2022). Therefore, TPE obtains the maximum EI of the hyper-parameter set x for each iteration.

3. Experimental Study

In this section, we introduce the battery dataset used in this paper. Based on the experimental data, IC curves are acquired and partial is extracted. And the configurations of the proposed model are presented.

3.1. *Experiment Data*

The experimental data used in this paper is from the Center for Advanced Life Cycle Engineering (CALCE) at the University of Maryland. A set of batteries (denoted as CS35, CS36, CS37, and CS38) with 1.1A/hr was selected for the analysis. Their cathode material is lithium cobalt oxide ($LiCoO_2$). The four batteries were cycled in the Arbin Battery Tester 2000 under the same experimental condition to obtain the full-life-cycle data. The experiment was conducted under CC-CV protocol. The batteries are charged with a constant current rate of 0.5C until the voltage reached 4.2 V. The charging stage continues with constant voltage and stops when the current drops to 20 mA. The batteries are discharged with a constant current rate of 1C until the voltage decreases to 2.7 V.

3.2. *Partial IC curve*

Fig. 2 shows IC curves at different cycles of CS35. It is found that IC curves tend to decrease as the number of cycles increases, with the most obvious pronounced change in peak. Considering the extraction of the peak relies on the complete IC curve, which is difficult to obtain in practice, we developed a deep learning model based on partial IC curve. It can be noticed that IC peak around 3.9V exhibits a significant change. To improve the applicability in practical applications, we choose the IC curve within 3.85V-4.00V as the input of deep learning model.

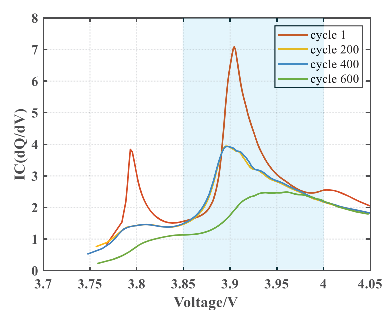

Fig. 2. IC curves at different cycles of CS35.

3.3. *Configurations of the proposed models*

This study utilized Hyperopt package in the Python programming language to implement TPE Bayesian optimization. Table 1 presents the hyper-parameters involved in the proposed LSTM model. The hyper-parameters to be optimized include *lstm units*, *dense units*, and *learning rate*.

Table 1. Hyper-parameters involved in the proposed LSTM model.

Hyper-parameters	Selection range
lstm_units	(2, 400)
dense_units	(2, 200)
learning_rate	(1e-3, 0.1)
Optimizer	Adam
Activation function	ReLu
Loss function	MSE

To quantify the estimation performance, the root mean square error (RMSE), mean absolute error (MAE), and mean absolute percentage error (MAPE) are applied as evaluation metrics.

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\tilde{y}_i - y_i)^2} \tag{12}$$

$$MAE = \frac{1}{N}\sum_{i=1}^{N}|\tilde{y}_i - y_i| \tag{13}$$

$$MAPE = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{\tilde{y}_i - y_i}{y_i}\right| \tag{14}$$

where $\tilde{y}_i$ represents the SOH prediction results, y_i denotes the actual SOH, and N stands for the number of testing samples.

4. Results and Discussions

In this section, we take the four batteries of CALCE battery dataset as an example to evaluate the performance of the proposed model. Meanwhile, to demonstrate the effectiveness and superiority of the proposed model, we introduced other state-of-the-art deep learning models for comparison, that is LSTM, RNN, and gated recurrent unit (GRU). The training set is set to 40% of the total cycle. The remaining data is treated as the test set. For a fair comparison, LSTM, RNN, and GRU keep the same configuration with the proposed model without Bayesian optimization. Specifically, *lstm_unit*, *dense_units*, and *learning_rate* are set as 32, 10, 1e-3, respectively.

Fig. 3-Fig. 6 presents the prediction results of different deep learning models on CS35, CS36, CS37, and CS38, respectively. It can be seen that the estimation curve of RNN deviates from the actual curve. We attribute this phenomenon to the limitation of the RNN model cannot store long-term memory, resulting in a large error in the estimation curve. The curve fluctuation caused by the capacity regeneration phenomenon is especially obvious in the late stage of RNN prediction. LSTM and GRU obtained smoother estimation results and were closer to the actual degradation curve compared to RNN. However, the dependence on manual adjustment of the parameters makes their estimation performance on different batteries widely different. With the embedding of Bayesian, the prediction curves of the proposed model are more consistent with the actual degradation curve.

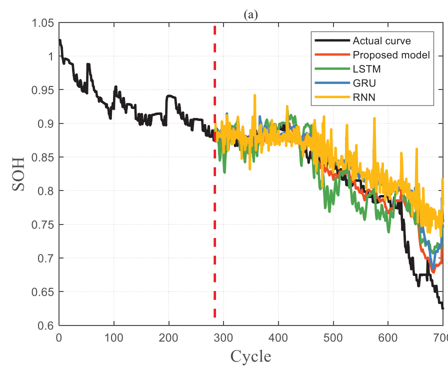

Fig. 3. SOH estimation results of the different models for CS35.

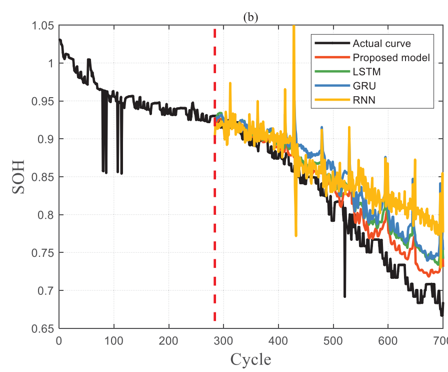

Fig. 4. SOH estimation results of the different models for CS36.

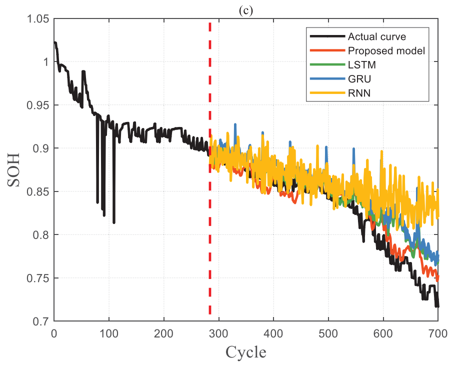

Fig. 5. SOH estimation results of the different models for CS37.

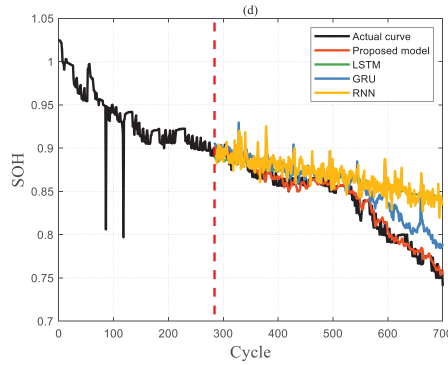

Fig. 6. SOH estimation results of the different models for CS38.

Table 2 exhibits the three evaluation metrics results for the four batteries based on different deep learning methods. The proposed method shows better applicability to all four batteries with the incorporation of Bayesian optimization. This also can be proved in Table 2, where the RMSE of the proposed method does not exceed 3.00 for all four batteries.

Table 2. Three metrics results of different methods for the four batteries

Battery No.	LSTM			GRU			RNN			**Proposed model**		
	RMSE	MAE	MAPE	RMSE	MAE	MAPE	RMSE	MAE	MAPE	**RMSE**	**MAE**	**MAPE**
CS35	3.42	2.69	3.83	3.55	2.38	3.51	4.49	3.07	4.54	**2.45**	**1.66**	**2.44**
CS36	3.59	2.93	4.20	4.44	3.70	5.26	5.77	4.46	6.49	**2.57**	**2.02**	**2.88**
CS37	2.27	1.67	2.30	2.81	2.66	3.10	4.30	3.09	4.30	**1.65**	**1.31**	**1.78**
CS38	3.58	2.62	3.56	2.09	1.70	2.27	3.67	2.81	3.81	**0.73**	**0.56**	**0.74**

5. Conclusion

In this paper, an LSTM model with Bayesian optimization based on partial IC curve is proposed to estimate SOH of lithium-ion batteries. We selected IC curve with a reasonable voltage range, avoiding the identification of specific features like IC peak. Bayesian optimization is incorporated into LSTM to automatically select hyper-parameters. Experiments based on CALCE dataset show that the proposed LSTM framework outperforms the other neural network models, such as RNN, LSTM, and GRU.

This paper focuses on dealing with historical data without considering the impact of future operating conditions on SOH estimation. As discussed by (Chang et al., 2022), batteries operating under different conditions can lead to dissimilar degradation patterns. Accordingly, it is worth to consider the dynamics of operating conditions in future work. Furthermore, the combination of deep learning models and self-attentive mechanisms can be integrated into the proposed methodology to improve the estimation performance.

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