



Article

State of Health Prediction of Lithium-Ion Batteries Based on Multi-Kernel Relevance Vector Machine and Error Compensation

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Abstract: Though lithium-ion batteries are extensively applied in electric vehicles as a power source due to their excellent advantages in recent years, the security risk has inarguably always existed. The state of health (SOH) of lithium-ion batteries is one of the most important indicators related to security, the prediction of SOH is paid close attention spontaneously. To improve the prediction accuracy of SOH, this paper constructs an SOH prediction model based on a multi-kernel relevance vector machine and error compensation (EC-MKRVM). The provided model comprises a pre-estimation model and an error compensation model, both of which use the multi-kernel relevance vector machine (MKRVM) algorithm. The pre-estimation model takes the feature factors extracted in the charging segment as the input variable and the SOH pre-estimation value as the output. The error compensation model takes the pre-estimation error sequence as the input variable and the SOH prediction error as the output. Finally, the SOH prediction error is used to compensate for the SOH pre-estimation value of the pre-estimation model, and the final SOH prediction value is obtained. To verify the effectiveness and advancement of the model, the CACLE dataset is used for comparative experimental analysis. The results show that the proposed prediction model in this paper has higher prediction accuracy.



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Keywords: lithium-ion batteries; state of health; multi-kernel relevance vector machine; error compensation

1. Introduction

Due to their high energy density, long cycle lifetime, low self-discharge rate, low cost, and many other advantages, lithium-ion batteries are increasingly used in electric vehicles (EVs) [1,2]. However, with the number of charging-discharging cycles increasing, electrochemical constituents in lithium-ion batteries will degrade, and the capacity of the batteries will decline irreversibly. Generally, a capacity fade over 20% means the end-of-life of lithium-ion batteries for driving EVs [3], and the batteries that exceed this threshold are more likely to cause malfunction, instability, serious economic losses, and security risks. Therefore, to ensure the security and other performance factors of the batteries in the case of aging in practical applications, accurate prediction of state of health (SOH) has vital engineering significance [4,5]. In recent years, various SOH prediction methods have been presented, but most of them cannot work well unfortunately due to the interactions inside lithium-ion batteries being complex and uncertain.

Generally, the methods for predicting the SOH of lithium-ion batteries include model-based methods and data-driven methods [6,7]. With respect to the model-based methods, the equivalent circuit models or electrochemical models for the dynamics of the batteries need to be established first, and the relative parameters of the model must be identified accurately, otherwise, the prediction accuracy of the battery SOH will be significantly

affected [8]. To achieve this purpose, adaptive filtering algorithms are usually implemented for the identification of the model parameters [9]. For example, a sequential extended Kalman filter (EKF) integrated with the third-order EKF and an improved discrete Arrhenius aging model to estimate the capacity of lithium-ion batteries was proposed [10], and an improved multiscale extended Kalman filtering joint estimation algorithm [11] was presented on the basis of reference [12], which not only improved the estimation accuracy but also simplified the complexity of the calculation. However, the inherent property of model-based methods is that the prediction accuracy is highly susceptible to the accuracy of the models and training data quality, and the robustness is usually poor [13].

For data-driven approaches, suitable input–output mapping relations need to be established by constructing regression prediction models based on various data analysis methods. Compared with model-based methods, it is unnecessary to study the internal mechanism of lithium-ion batteries and establish complex equivalent circuit models. These methods include autoregressive integrated moving average (ARIMA) [14], artificial neural networks (ANNs) [15,16], relevance vector machines (RVMs) [17], support vector machines (SVMs) [18,19], and extreme learning machines (ELMs) [20,21]. In [22], an improved empirical mode decomposition method was used to decompose the capacity degradation curve of lithium-ion batteries into an aging trend item and interference items, a weighted least squares support vector machine and a long short-term memory neural network were used to predict the aging trend item and interference items, respectively, and a multistage support vector machine algorithm to estimate the SOH of lithium-ion batteries was proposed in [23]. Reference [24] noted that the RVM has the advantages of better model generalizability and shorter calculation time than other data-driven models. However, a single kernel function will lead to poor accuracy and low model applicability of the RVM in long-term prediction applications [25].

Moreover, due to the intrinsic disadvantages of various data-driven models and the limited quantity of training data, prediction errors are often present. To increase the prediction accuracy, the idea of error compensation was proposed [26,27]. In the current literature, the original feature factors that are the same as the pre-estimation models or part of them are selected as the inputs of the error compensation models, and the random errors generated by the pre-estimated models during training are usually ignored. However, reference [28] noted that the random prediction error sequence also follows the internal logic relationship of the prediction models, so using the error sequence as the input of the compensation model may improve the accuracy to some extent.

In this paper, an SOH prediction model based on a multi-kernel relevance vector machine algorithm and error compensation strategy (EC-MKRVM) is proposed. The model comprises a pre-estimation model and an error compensation model, both of which use the multi-kernel relevance vector machine (MKRVM) algorithm. It should be noted that the input feature factors of the pre-estimation model are extracted from partial charging segment data, and the output error sequence of the pre-estimation model is taken as the input variables of the error compensation model to improve the prediction accuracy by a large margin. To verify the effectiveness and advancement of the proposed model, the dataset from the Center for Advanced Life Cycle Engineering (CACLE) at the University of Maryland is used for comparative experimental analysis.

The rest of this article is organized as follows. Section 2 presents the methodology for constructing the prediction model. In Section 3, the experimental results of the prediction model are analyzed in detail. Finally, in Section 4, the conclusions of this paper are given.

2. Methodology

2.1. Overview of the Proposed SOH Prediction Framework

As mentioned above, the SOH prediction model for lithium-ion batteries based on the EC-MKRVM constructed in this paper comprises a pre-estimation model and an error compensation model, both of which use the MKRVM algorithm. The framework of the

proposed methodology is illustrated in Figure 1, and the main procedure includes four steps in detail.

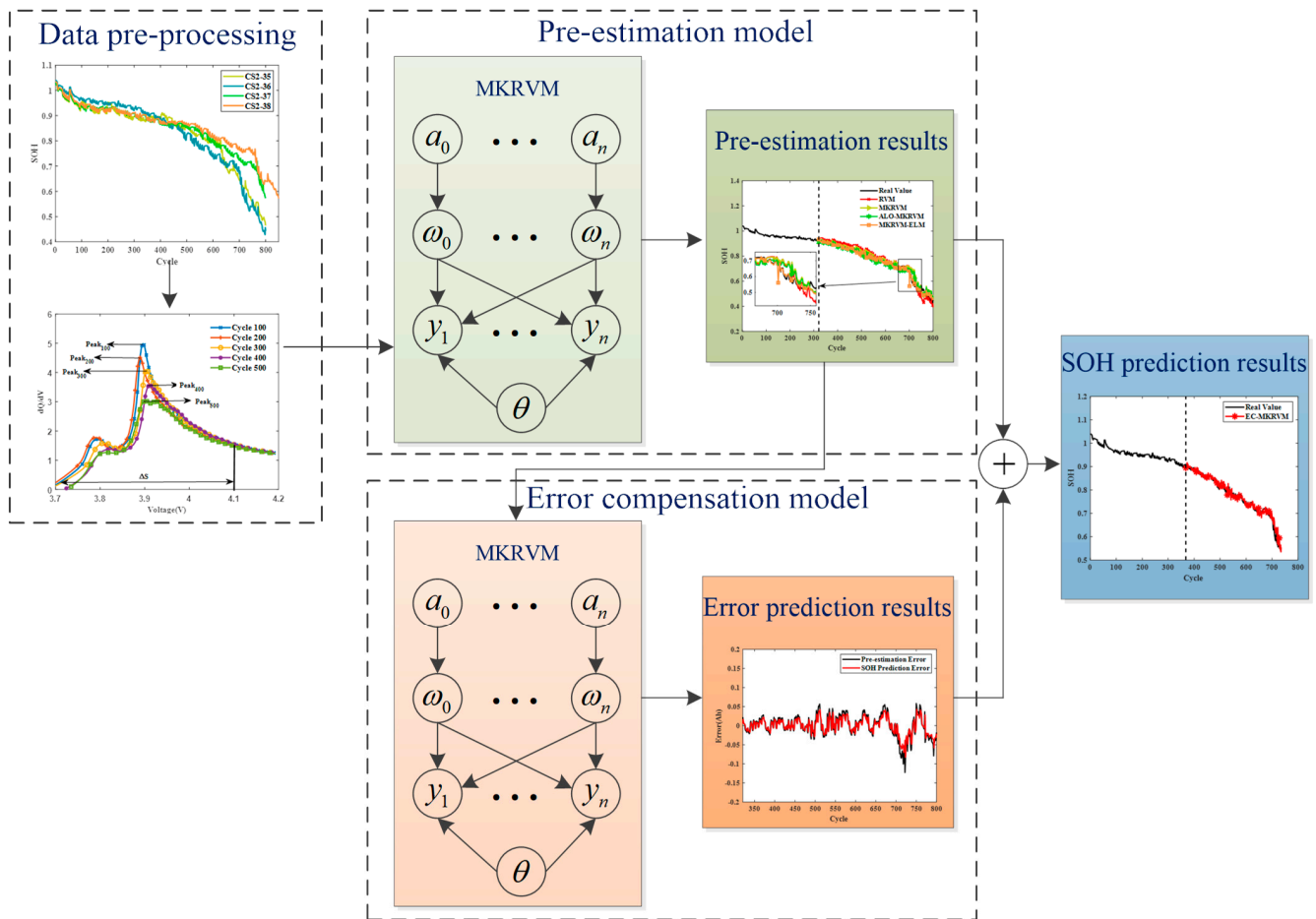


Figure 1. Framework of the proposed prediction model based on the EC-MKRVM.

(1) Data preprocessing and feature factors extracting. As we know, the raw aging datasets from CACLE just include the data of voltage and current of the tested batteries, and there are noises inside them, so these data need to be culled, and then the feature factors that can map the SOH of batteries strongly need to be extracted. In this paper, the feature factors, such as isobaric rise charge time, peak value of increment capacity curve, isobaric rise charge capacity, and cycle times, which are highly correlated with the SOH [29,30], are calculated from the datasets, and they are taken as the input variables of the pre-estimation model. Meanwhile, the obtained dataset of feature factors is divided into a training set and a test set, which are used for model training and performance testing, respectively.

(2) SOH pre-estimation model construction. Considering the nonlinear mapping relationship between the feature factors and SOH, an MKRVM with three Gaussian kernel functions is proposed to establish the pre-estimation model for lithium-ion batteries. In the model, the feature factors extracted by step (1) are taken as the inputs, and the output is the pre-estimation result of SOH.

(3) Error compensation model construction. The error compensation model is also based on MKRVM, which is trained to compensate for the pre-estimation results of SOH to further improve the prediction accuracy. In this model, the pre-estimation error sequence of previous times, which is obtained by comparing the pre-estimation results of SOH produced in step (2) with the actual values, and the corresponding mean value and variance value are used as the inputs together, and the SOH prediction error of the current time is used as the output.

(4) Model training. Considering that the performance of the proposed method can be conveniently compared with that of other methods, the extracted feature factors within the training set of four lithium-ion batteries in the CACLE datasets, namely, CS2_35, CS2_36, CS2_37, and CS2_38, are used for model training.

By the above four steps, the SOH prediction model is constructed, and the final SOH prediction value is obtained by accumulating the SOH pre-estimation value of the pre-estimation model and the prediction error of error compensation model. Finally, the extracted feature factors within the test set of the same four batteries are applied as performance evaluation.

2.2. Multi-Kernel Relevance Vector Machine

The RVM is a sparse probability prediction model based on the Bayesian framework. After setting the prior parameters, some irrelevant points are eliminated through the uncorrelated theory. Thus, a sparse probability model can be obtained.

In the multi-input and single-output regression prediction model of the RVM, the input variable is assumed to be $\{x_i\}_{i=1}^N$, the output variable is set to $\{y_i\}_{i=1}^N$, where N is the total number of samples, and the relationship between the input and the output needs to meet the following equation.

$$y_i = \sum_{i=1}^N w_i k(x, x_i) + \theta_i \quad (1)$$

where $k(x, x_i)$ is the kernel function, w_i is the weight of $k(x, x_i)$, and θ_i is the Gaussian noise with a mean of zero and a variance of σ^2 . When w and σ^2 are known, the probability distribution of the output can be obtained, as follows:

$$p(y|w, \sigma^2) = (2\pi\sigma^2)^{-\frac{N}{2}} \exp\left(-\frac{\|y - \Phi w\|^2}{2\sigma^2}\right) \quad (2)$$

where $w = [w_1, w_2, L, w_N]$, and φ is the kernel function matrix, which is defined as

$$\Phi = [\varphi(x_1), \varphi(x_2), \dots, \varphi(x_N)]^T \quad (3)$$

$$\varphi(x_i) = [1, k(x_i, x_1), k(x_i, x_2), \dots, k(x_i, x_N)] \quad (4)$$

To avoid overlearning in the solution process, that is, the overfitting phenomenon, w is defined as a Gaussian prior distribution with zero mean, which is defined as

$$p(w|\alpha) = \prod_{i=0}^N N(w_i | 0, \alpha_i^{-1}) \quad (5)$$

where α is an $N + 1$ dimensional hyperparameter vector, defined as $\alpha = (\alpha_0, \alpha_1, L, \alpha_N)$.

When the output y is given, the posterior probability distribution formula of all other parameters is shown as

$$p(w, \alpha, \sigma^2 | y) = p(w | y, \alpha, \sigma^2) p(\alpha, \sigma^2 | y) \quad (6)$$

According to Equations (2) and (5), combined with the Bayes theorem, the posterior probability distribution of w can be derived, as shown in Equation (7):

$$p(w | y, \alpha, \sigma^2) = \frac{p(y | w, \sigma^2) p(w | \alpha)}{p(y | \alpha, \sigma^2)} = (2\pi)^{-\frac{N}{2}} |\Sigma|^{-\frac{1}{2}} \times \exp\left\{-\frac{1}{2}(w - u)^T |\Sigma|^{-1} (w - u)\right\} \quad (7)$$

where Σ and u are the covariance and mean of w , respectively, that is $\Sigma = (\sigma^{-2}\Phi^T\Phi + A)^{-1}$ and $u = \sigma^{-2}\Sigma\Phi^T y$, where A is the diagonal matrix composed of hyperparameters α_0 to α_N .

The process of RVM model training involves calculating the posterior probability $p^{(w, \alpha, \sigma^2 | y)}$ and finding the hyperparameter α and noise variance σ^2 when Equation (7) obtains the maximum value. The solution of hyperparameter α and noise variance σ^2 are obtained by continuous iterative operation to complete the RVM regression prediction model training.

In the RVM regression prediction model, the Gaussian kernel function is usually used. Nevertheless, the Gaussian kernel function has difficulty accurately describing the complex nonlinear degradation trend of the SOH of lithium-ion batteries and provides high long-term prediction accuracy. In the RVM model, common kernel functions include the Gauss kernel function, Laplace kernel function, linear kernel function, and sigmoid kernel function. However, because it is difficult for the linear kernel function to describe the strong nonlinear degradation trend of the SOH of lithium-ion batteries, this paper constructs a compound kernel function based on three different common single-kernel functions to define a multi-kernel relevance vector machine model. The compound kernel function consists of a weighted combination of Gaussian, Laplace, and sigmoid kernel functions. The three single-kernel functions are described as follows:

$$K_1(x_i, x_j) = \exp\left(-\|x_i - x_j\|^2 / 2T_G^2\right) \quad (8)$$

$$K_2(x_i, x_j) = \exp\left(-\|x_i - x_j\| / T_L\right) \quad (9)$$

$$K_3(x_i, x_j) = \tanh\left(T_S * x_i^T * x_j\right) \quad (10)$$

where $K_1(x_i, x_j)$, $K_2(x_i, x_j)$, $K_3(x_i, x_j)$ are the Gaussian kernel function, Laplacian kernel function, and sigmoid kernel function, respectively, and T_G , T_L , T_S are the relative kernel parameters. Thus, the expression of the compound kernel function is obtained as follows:

$$Kenel = \lambda_1 K_1 + \lambda_2 K_2 + \lambda_3 K_3 \quad (11)$$

where λ_1 , λ_2 , λ_3 are the weight parameters of the three kernel functions, their value ranges are $[0, 1]$, and they need to meet the following requirements:

$$\lambda_1 + \lambda_2 + \lambda_3 = 1 \quad (12)$$

The weight parameters in the composite kernel function are usually selected by trial and error, and they can impact the prediction accuracy to a certain extent.

2.3. Error Compensation Model

As described earlier, the error compensation model is also based on the MKRVM. To fully exploit the regularity of the error sequence, in addition to taking the five pre-estimation errors before the i th cycle as inputs, the mean and variance of the error sequence, which can reflect the performance of the pre-estimation model, are also taken as part of the input variables of the error compensation model. The definitions of the mean and variance of the error sequence are shown as

$$\begin{cases} r_i = \frac{1}{l} \sum_{j=i-l}^{i-1} e_j \\ P_i = \frac{1}{l} \sum_{j=i-l}^{i-1} e_j e_j^T \end{cases} \quad (13)$$

where e_j is the pre-estimation error of the j th cycle; $e_j = y_j^{real} - y_j^{pre}$, y_j^{real} and y_j^{pre} are the actual and pre-estimation values of the j th cycle, respectively; and r_i and P_i represent the mean and variance of the error sequence with length l , respectively, where $l = 5$.

In summary, the error compensation model constructed in this paper has an input of $x_i = \{e_{i-5}, e_{i-4}, e_{i-3}, e_{i-2}, e_{i-1}, r_i, P_i\}$ and an output of $y_i = e_i$ at the i th cycle.

3. Materials and Experiments

3.1. Data Description

The batteries marked CS2_35, CS2_36, CS2_37, and CS2_38 in CALCE are all CS2-type batteries, which are made of LiCoO₂ cathode material, and their nominal capacity is 1.1 Ah. The specifications of the batteries are shown in Table 1. All the data for four batteries were tested under a constant current–constant voltage charging protocol independently. Firstly, the battery was charged at a constant current rate of 0.5 C until its voltage reached 4.2 V, and then the battery was sustained at a constant voltage of 4.2 V until the current declined below 50 mA. Subsequently, the discharge procedure was carried out, and the battery was discharged with a constant current rate of 1 C until the voltage decreased to 2.7 V. The SOH degradation tendency of the batteries with the increasing cycle numbers is shown in Figure 2.

Table 1. Specifications of the CS2-type batteries in CALCE.

Battery Characteristics	Value
Rated capacity	1.1 Ah
Cell chemistry	LiCoO ₂ cathode and graphite anode
Dimensions	5.4 mm × 33.6 mm × 50.6 mm
Weight	21.1 g

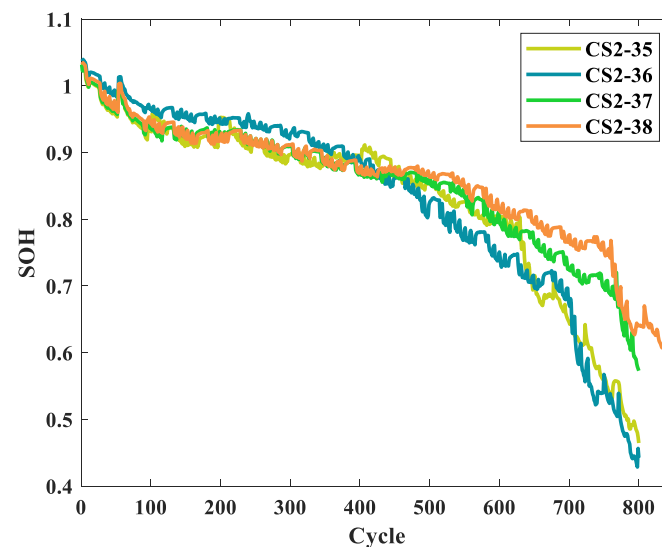


Figure 2. SOH degradation tendency curves of the tested batteries.

3.2. Performance Evaluation Criterion

To evaluate the performance of the SOH prediction models for lithium-ion batteries, three evaluation indexes, mean absolute error (MAE), root mean square error (RMSE), and coefficient of determination (R^2), are introduced. The specific formulas of the three evaluation indexes are defined as

$$MAE = \frac{\sum_{i=1}^N |y_i - y_i^{real}|}{N} \quad (14)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (y_i - y_i^{real})^2}{N}} \quad (15)$$

$$R^2 = 1 - \frac{\sum_{i=1}^N (y_i - y_i^{real})^2}{\sum_{i=1}^N (y_{average} - y_i^{real})^2} \quad (16)$$

where N is the total number of samples in the test set, y_i and y_i^{real} are the predicted and actual values of the SOH of the i cycle, respectively, and $y_{average}$ is the average of the SOH of the test set. For the three evaluation indices, smaller MAE and $RMSE$ values indicate that the performance of the prediction model is better, while a value of R^2 closer to 1 indicates that the predicted curve fits the actual degradation curve better.

3.3. Case 1: Performance Test of the Error Compensation Model

In order to verify the effectivity of the error compensation model, the proposed EC-MKRVM model and the MKRVM without error compensation are used to predict the SOH of the four batteries. For each battery, the former 40% of the historical aging data in the CALCE dataset are used as the training set, and the remaining 60% of the data are used as the test set. Firstly, the feature factors, defined as isobaric rise charge time, the peak value of increment capacity curve, isobaric rise charge capacity, cycle times, and the battery capacity are calculated according to the datasets. Then, the proposed EC-MKRVM model and the MKRVM without error compensation are trained, respectively, using the feature factors and capacity calculated from the training set. Finally, the performances of the two different models are evaluated by using data calculated from the test set, and three main evaluation indexes of different batteries are shown in Table 2. According to the evaluation results, the performances of the proposed prediction model are all improved to different degrees.

Table 2. Prediction evaluation indexes of EC-MKRVM and MKRVM.

Battery	Evaluation Indexes	MKRVM	EC-MKRVM
CS2_35	MAE (%)	2.02	0.83
	RMSE (%)	2.63	1.15
	R2	0.964	0.993
CS2_36	MAE (%)	2.28	0.99
	RMSE (%)	3.08	1.36
	R2	0.955	0.991
CS2_37	MAE (%)	1.95	0.86
	RMSE (%)	2.46	1.26
	R2	0.918	0.978
CS2_38	MAE (%)	2.09	0.83
	RMSE (%)	2.76	1.12
	R2	0.850	0.972

At the same time, to directly evaluate the performances of the proposed error compensation model, the prediction errors of the pre-estimation model are compared with the prediction errors, which are named the pre-estimation error and SOH prediction error in Figure 3. As shown intuitively in Figure 3, the prediction error curve produced by the presented error compensation model is close enough to the prediction error curve calculated by using the output of the pre-estimation model. That is, the pre-estimation error can be effectively tracked by the error compensation model, as a result, the prediction accuracy of the proposed model can be improved by introducing the error compensation model.

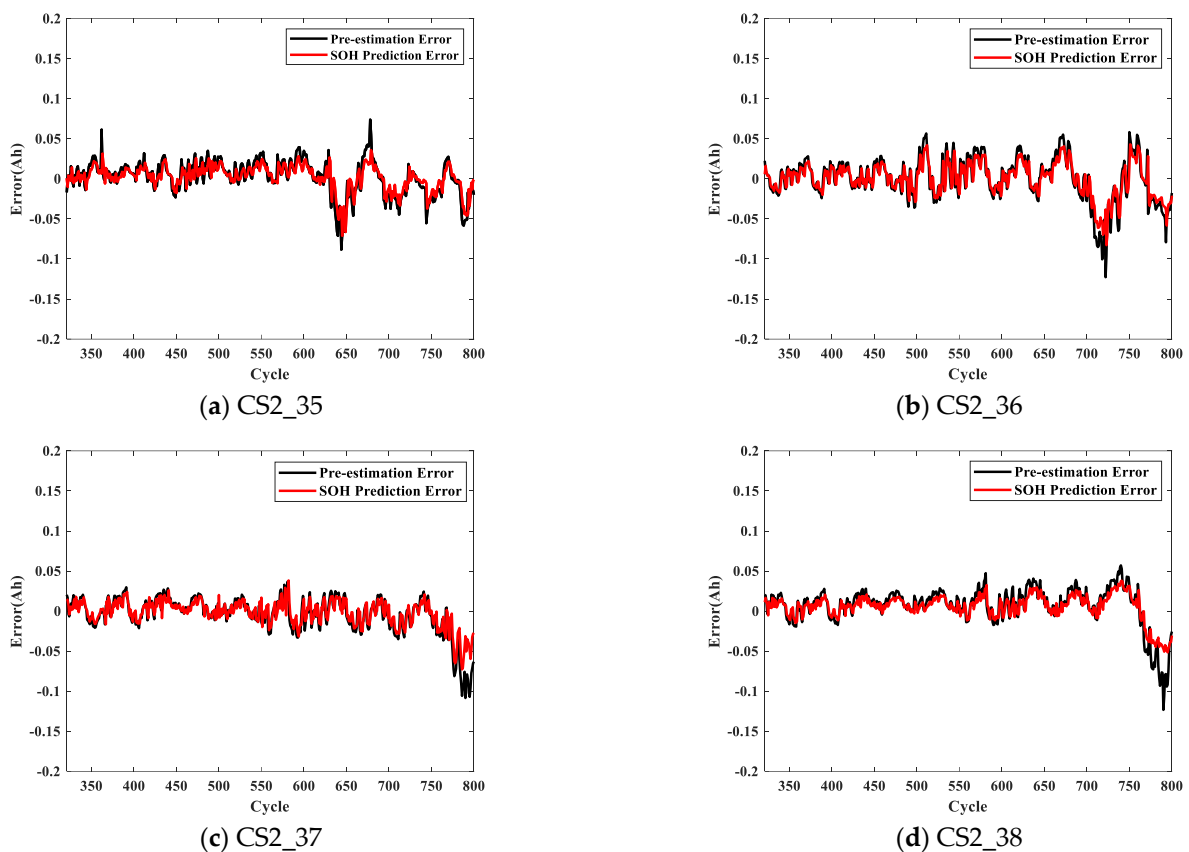


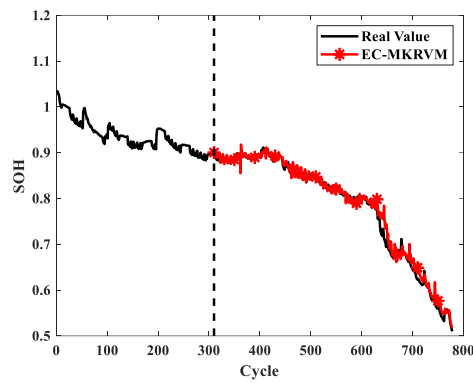
Figure 3. Error prediction results obtained by the error compensation model.

3.4. Case 2: Comparison with Other Methods

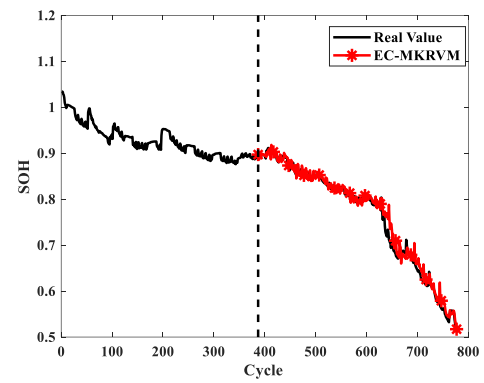
To further verify the superiority of the proposed model, the prediction results obtained by using EC-MKRVM are compared with the existing results obtained by using the models presented in the literature [6,31], which adopted the long short-term memory (LSTM) model optimized by Bayesian optimization and the SVR model optimized by ant lion optimization (ALO), respectively. To ensure the objectivity of the comparison results, we set the starting point (SP) and endpoint (END) to be the same as those presented in the literature. That is, the data before the starting point are set as the training set, while the data between the starting point and the endpoint are taken as the test set.

Figures 4 and 5 show the prediction results of batteries CS2-35 and CS2-36 under the same conditions presented in the literature [31], and Figures 6 and 7 show the prediction results of batteries CS2-37 and CS2-38 under the same conditions presented in the literature [6], respectively. Table 3 shows the detailed evaluation indexes obtained by using the models proposed in the literature [6,31] and this paper.

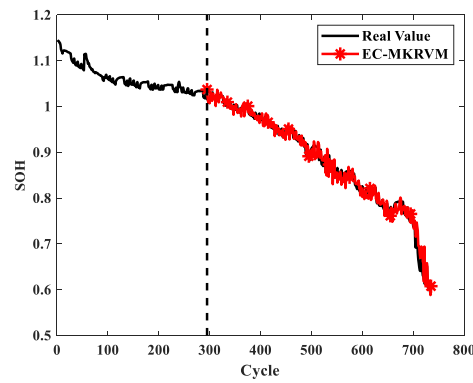
As shown in Table 3, the prediction accuracy of the proposed EC-MKRVM model is improved to a certain extent compared with that of the ALO-SVR and optimized LSTM models under the same conditions. Taking the CS2-35 lithium-ion battery as an example, under the condition of SP = 309, the MAE and RMSE of the ALO-SVR model are 1.60% and 2.64%, respectively. In comparison, the MAE and RMSE of the EC-MKRVM-based model are 0.90% and 1.31%, respectively, which are decreases of 43.75% and 50.38%, respectively. Similarly, under the condition of SP = 386, the MAE and RMSE of the EC-MKRVM-based model also decreased by 37.97% and 40.93%, respectively. For batteries CS2-36, CS2-37, and CS2-38, similar results can be obtained. In conclusion, the prediction accuracy of the proposed EC-MKRVM model is apparently higher than that of the models presented in the literature [6,31].



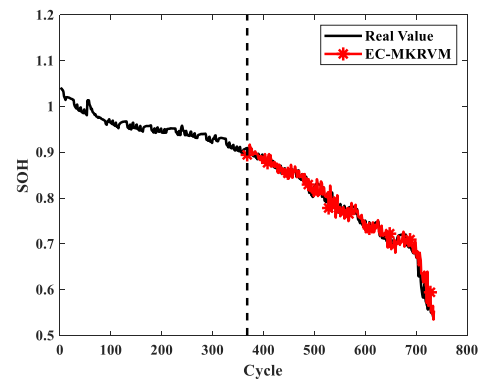
(a) SP = 309



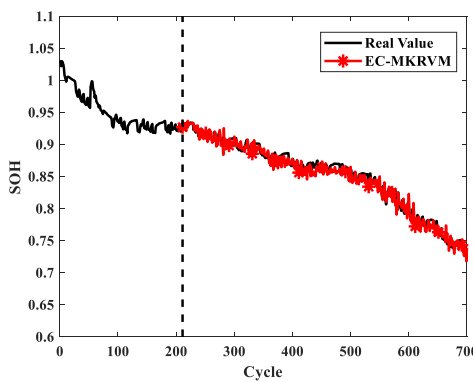
(b) SP = 386

Figure 4. Prediction results of CS2_35 with different prediction starting points.

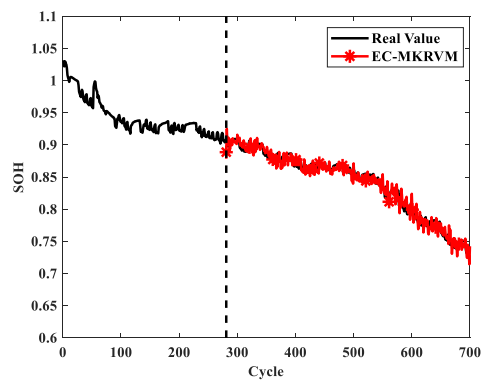
(a) SP = 294



(b) SP = 387

Figure 5. Prediction results of CS2_36 with different prediction starting points.

(a) SP = 210



(b) SP = 280

Figure 6. Prediction results of CS2_37 with different prediction starting points.

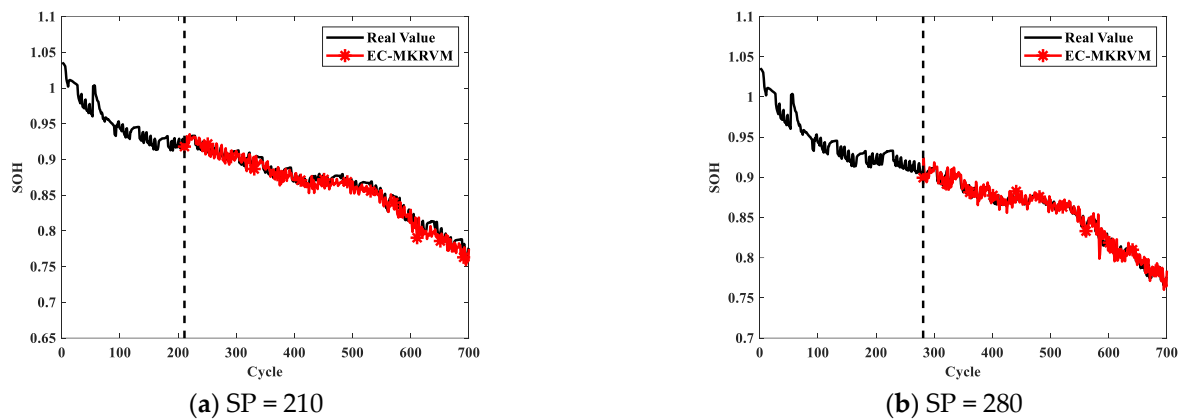


Figure 7. Prediction results of CS2_38 with different prediction starting points.

Table 3. Evaluation indexes of different models.

Battery	Prediction Model	SP	END	MAE (%)	RMSE (%)
CS2_35	ALO-SVR [31]	309	778	1.60	2.64
	EC-MKRVM			0.90	1.31
	ALO-SVR [31]	386	778	1.58	2.37
	EC-MKRVM			0.98	1.40
CS2_36	ALO-SVR [31]	294	735	1.96	3.37
	EC-MKRVM			0.97	1.33
	ALO-SVR [31]	367	735	1.32	2.17
	EC-MKRVM			1.06	1.47
CS2_37	Optimize-LSTM [6]	210	700	1.58	2.02
	EC-MKRVM			0.75	0.93
	Optimize-LSTM [6]	280	700	1.31	1.64
	EC-MKRVM			0.70	0.88
CS2_38	Optimize-LSTM [6]	210	700	0.87	1.13
	EC-MKRVM			0.77	0.94
	Optimize-LSTM [6]	280	700	0.56	0.73
	EC-MKRVM			0.55	0.71

4. Conclusions

In this paper, an EC-MKRVM model is proposed by combining two MKRVM algorithms organically to improve the SOH prediction performances of lithium-ion batteries. The proposed algorithm is experimentally validated through the CALCE dataset with different batteries. The study results show that the proposed EC-MKRVM-based prediction model has greater prediction accuracy than the single MKRVM-based prediction model and similar models presented in other studies.

However, the work in this paper only verified the feasibility of the proposed prediction model using the CALCE dataset, while the effectiveness under the practical conditions or other established datasets has not been verified yet, so more experiments can be carried out in future study work. Meanwhile, the weight parameters in the composite kernel function and other related parameters in the proposed model are selected by trial and error, which is tedious and skilled work, how to optimize the parameters of the proposed model needs to be studied, so as to further improve the performances.

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Conflicts of Interest: Shilin Liu is an employee of Anhui Polytechnic University Industrial Innovation Technology Co., Ltd. The paper reflects the views of the scientists and not the company.

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