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A novel method for SOC estimation of Li-ion batteries using a hybrid machine learning technique

Eymen İPEK, Murat YILMAZ*

Electrical Engineering Department, Electrical and Electronics Faculty, İstanbul Technical University, İstanbul, Turkey

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Abstract: The battery system is one of the key components of electric vehicles (EV) which has brought groundbreaking technologies. Since modern EVs have mostly Li-ion batteries, they need to be monitored and controlled to achieve safe and high-performance operation. Particularly, the battery management system (BMS) uses complex processing systems that perform measurements, estimation of the battery states, and protection of the system. State of charge (SOC) estimation is a major part of these processes which defines remaining capacity in the battery until the next charging operation as a proportion to the total battery capacity. Since SOC is not a parameter that can be measured, the fundamental challenge is an accurate estimation. There are different SOC estimation methods in the literature that promises high accuracy such as model-based estimations, adaptive filter based estimations, and a combination of these systems. Recently, artificial intelligence (AI) and particularly machine learning (ML) based systems are included in the battery state estimation both as a part of adaptive systems and standalone. Data-driven methods are promising approaches to battery state estimation which provide high accuracy. The purpose of this study is to present a novel and highly accurate way of SOC estimation of the Li-ion battery (LIB) cell with a considerably low parameterization and modeling effort. Therefore, a new approach is proposed to estimate SOC with reduced modeling and without performing parametrization. Based on discharge test data, XGBoost is used to estimate SOC under dynamic operating conditions and the estimation is reached 98.81% coefficient of determination. As a novel approach, exponential smoothing is performed in combination with XGBoost SOC estimation to improve the estimation performance of the model. The estimation accuracy is improved as approximately 0.62%.

Key words: Electric vehicles, Li-ion, state of charge estimation, artificial intelligence, machine learning, XGBoost

1. Introduction

Electric propulsion is not new for the industry considering the number of electric vehicles at the beginning of the 20th century [1]. Due to the restricted usage of the EVs caused by higher cost and lower performance of batteries, it was not possible to use electrical energy directly for the traction. By developing technology, electric energy has brought efficiency and CO_2-free operation to the automotive industry with tremendously lower maintenance. This change was inevitable considering the increasing demand for electrical equipment in the car. In fact, the huge difference between 20th century and now is the energy storage system of EVs. For sure, there is a significant development in the other systems. However, battery systems are the key factor in the electrification of mobility. Today, there are a lot of different energy storage systems that exist and have been developed [2].

*Correspondence: myilmaz@itu.edu.tr

A control function may be required for every electrical equipment whether it is analog or digital. Electrical equipment supplied by energy storage systems will also require a management system that controls activation, deactivation, charging, and discharging. However, Li-based batteries require more complex management systems that monitor temperature and voltage. Battery management systems that are used in LIB applications are useful to ensure safety, maximum performance, and lifetime. There could be LIB systems without BMS in special applications; however, this approach would be risky and lack of the best performance. BMS takes care of different functions such as monitoring cell voltages, cell temperatures, pack voltage, thermal management, safe operation, contactor control, state estimations, cell balancing and charge or discharge control as shown in Figure 1 [2].

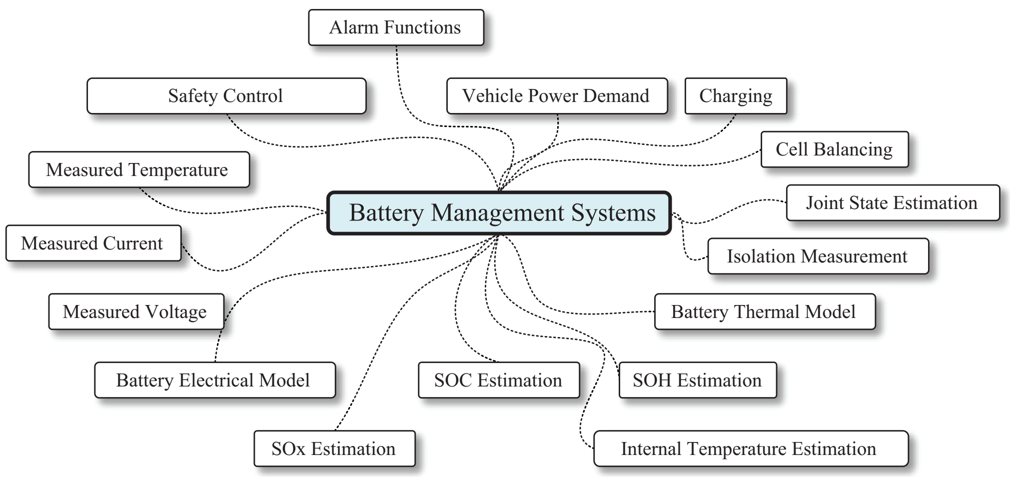

Figure 1. Key functions for BMS.

State estimation is crucial for LIB applications in terms of safety and performance. Especially, automotive applications require high accuracy state estimation of the LIB. Literature shows that there are numerous studies that focus on state estimation of LIB. Considering SOC estimation, scientists have been working since decades. A voltage and temperature measurement based method is proposed by Peled in 1984 to exhibit SOC of LIB [3]. A simple and useful method is used by Aylor which was implemented to lead-acid battery [4] as is often known as Ah or coulomb counting. Then, neural network based methods are proposed to improve [5] estimation performance. Kalman filters (KF) usage is introduced by Garche et al. in 2000 to optimize battery performance and lifetime by upgrading safety management as well [6]. SOC estimation methods are improved by developing technology and processors. It may be done based on conventional methods as OCV method [3], Coulomb counting [4], impedance measurement based methods, electrochemical method, model-based methods [7]; based on adaptive filters [8] like Kalman filter [6], extended Kalman filter (EKF) [9], adaptive extended Kalman filter [10], fading Kalman filter [11], unscented Kalman filter [12], sigma-point Kalman filter [13], adaptive sigma-point Kalman filter [14], particle filter (PF) [15], H-infinite filter [16]; and based on artificial intelligence as artificial neural network (ANN) [17], support vector machine (SVM) [18], extreme learning machine (ELM) [19], genetic algorithm (GA) [20], fuzzy logic [21]; also based on observers like nonlinear observers [22], proportional-integral observer [23], sliding mode observer [24]; and also based on hybrid models of above [25].

Currently, scientists have been included more artificial intelligence algorithms into SOC estimation areas such as deep learning, neuro-dynamic programming, and deep neural networks [26, 27]. XGBoost recently introduced to the battery systems world. In 2018, Donato et al. presented an aging model of satellite LIB by using XGBoost [28]. Then, Jiang et al. presented a capacity degradation perception by using XGBoost in 2019 [29]. The literature review shows that there are numerous studies in the LIB field as well as BMS. Recently, the data-driven models have been a research focus thanks to increasing data pool over the cloud-connected EVs. This study contributes to the data-driven approaches by bringing XGBoost capabilities in a combination of exponential smoothing to SOC estimation. It is shown that SOC estimation can be performed against dynamic operating conditions by using XGBoost with a proper dataset.

A SOC estimation method is presented that is independent of the battery model. As a data-driven approach, XGBoost is employed for estimation by using the dynamic discharge test data. By applying only the XGBoost algorithm to the test data, 98.81% R^2 and 0.05% Mean Squared Error (MSE) are obtained. The results are improved by applying a hybrid model that consists of XGBoost and exponential smoothing methods. This novel approach brings 0.62% R^2 score improvement and 0.03% MSE reduction. Thanks to the applied method, 99.43% R^2 and 0.02% MSE reached.

The following chapters introduce the appraisal criteria of this approach by presenting ML applications in SOC estimation particularly gradient boosting and XGBoost. Then, the utilized battery test data is analyzed. Furthermore, the employed method is explained in the following chapters by demonstrating application steps. Finally, the proposed hybrid method and its superiorities are compared against the existing methods.

The organization of this paper is structured as follows: In Section 2, the SOC estimation methods are explained to compare with XGBoost, the assessment criteria are explained. In Section 3, the utilized data is presented as well as explaining assumptions. In Section 4, SOC estimation by using XGBoost is presented. Finally, a conclusion is presented in Section 5.

2. SOC estimation methods

In general, there are two major methods for SOC estimation. Direct methods are measurement-based methods that promise ease of implementation and lower complexity. However, these methods have a lack of adaptiveness and neglectful of the initial state and cell aging. Electrochemical impedance spectroscopy (EIS), open circuit voltage (OCV) estimation, and Ah/coulomb counting are the basic direct methods. On the other hand, indirect methods are not easy to implement. Despite their complexities, indirect methods provide an adaptive system that can react according to the initial states and remaining useful life. Indirect methods can be model-based methods, adaptive filter based methods, adaptive artificial intelligence based methods, and other methods like a combination of these methods. Figure 2 shows the overview of fundamental SOC estimation methods [26].

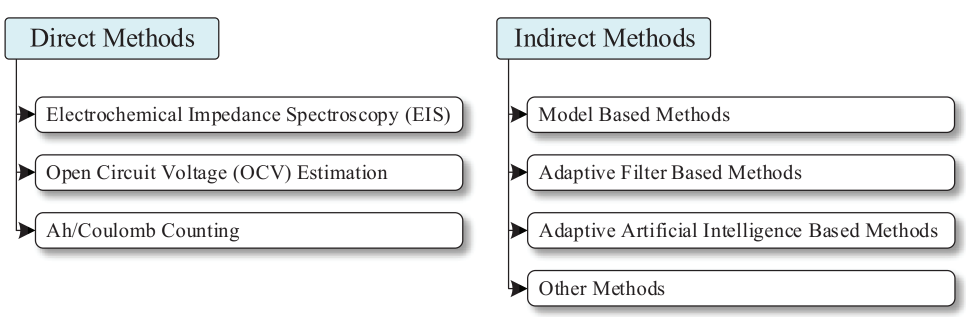

Figure 2. Fundamental methods for SOC estimation.

Even though current models promise good accuracy and adaptive structure, they need an optimized model creation, parameterization, and calibration. During these long term efforts, a small failure can cause extremely high estimation errors. Therefore, future BMS software requires more robust systems which collect also fleet information and make decisions based on a huge amount of data. Thus, numerous studies have been focused on data-driven methods considering developing cloud computing systems and data science.

2.1. ML applications in SOC estimation

Today, different ML algorithms are introduced to SOC estimation applications. Besides, different regression techniques are studied to estimate both SOC and state of health (SOH). A dataset with a relation of different parameters can be implemented into an ML algorithm to estimate SOC and SOH. Figure 3 shows an illustration of the ML application for SOC estimation.

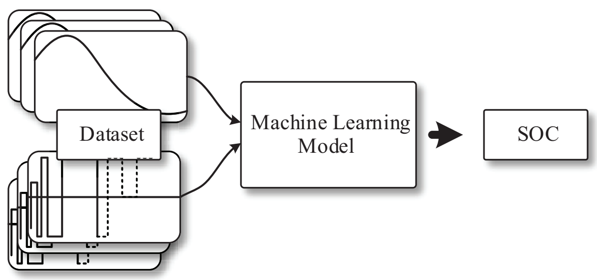

Figure 3. Block diagram of ML for SOC estimation.

The most important advantage of the data-driven models is the lack of parameter identification necessity considering that parameter identification requires exhaustive tests which can last even months. This is a huge benefit for battery management system applications. Especially, for different cell chemistries, different models must be created due to their different time constants. Data-driven models can eliminate this drawback. However, data-driven models require also a huge amount of data. By developing technology, increasing EV fleets, and improving technology in cloud systems this data can be collected from sold cars remotely. Like the autonomous cars, the performance of the data-driven model would be improved day by day by each driver.

Several studies can be shown as example applications of ML in battery systems in addition to previously mentioned methods such as fuzzy logic [30], neural networks [31], support vector machine [32–34], Markov chain [35], Gaussian process regression [36, 37] and Monte Carlo [38]. Day by day new ML algorithms have been introduced to the literature.

2.2. Gradient boosting algorithm: XGBoost

A decision tree is used to identify the optimum output by using an if-else algorithm. It can be presented as a flowchart that includes yes or no answers or particular evaluations such as win or loss. Decision trees have been used to solve regression and classification problems since the 1980s. Although decision trees can be unstable and relatively inaccurate in case of an error in the data, many advantages can be counted. First, they are quite simple and easy to interpret. Besides, comparing other machine learning algorithms, they need a small amount of data to make an outcome. Last but not least, they can be combined with different algorithms or machine learning models.

In 2001, Friedman introduced a quite efficient approach of decision trees which is called gradient boosting. Friedman proposed a linear model solver that uses a tree learning algorithm and allows randomly selected training data [39]. Gradient boosting creates an optimization algorithm for a given cost function and it is used for both classification and regression problems. It is evolved to different algorithms for several years. Figure 4 shows the evolution of decision trees from basic decision algorithms to gradient boosting. As shown in Figure 4, a basic decision tree uses a dataset for deciding output by iterating as an if-else format. To improve its performance, different datasets are used as a parallel operation which is called bagging. The gradient boosting uses different datasets sequentially by increasing importance of efficient models to decrease error rate.

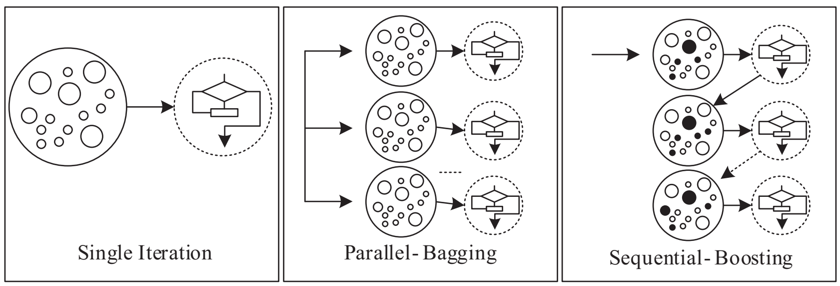

Figure 4. Evolution of decision trees from basic decision algorithms to gradient boosting (single iteration: represents a simple if-else based algorithm; bagging: parallel structured decision trees to increase prediction speed; boosting: creating sequential models and the increasing importance of efficient models to decrease error rate).

A scalable algorithm is developed by Chen and He in 2015 which is called XGBoost as a derivation of gradient boosting. XGBoost is also known as 'eXtreme gradient boosting' thanks to its automatic scalability and speed as 10 times of gradient boosting [40]. XGBoost creates a combination of different models that are similar to bagging operation. To minimize the error, convenient model dominancy is increased or in other words, boosted. Besides, regularization is done for preventing overfitting. During these operations, parallel processing is performed to decrease computational time.

2.3. Assessment criteria

Two different assessment criteria are employed during the study. R-squared or R^2 score is used to investigate the correspondence between the test and the predicted values as the coefficient of determination [41]. R^2 is calculated by using sample size, mean of test values, test, and prediction values as specified in (1).

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_\mathrm{i} - \hat{y}_\mathrm{i})^2}{\sum_{i=1}^{n}(y_\mathrm{i} - \bar{y}_\mathrm{i})^2} \tag{1}$$

where; R^2: the coefficient of determination, n: sample size, y_i: value at i^{th} data point, $\bar{y}_i$: mean of y, $\hat{y}_i$: estimated value at i^{th} point.

The second assessment criterion is mean squared error (MSE) which is frequently used in estimation problems. This value is also used to investigate the performance of the SOC estimation by indicating the deviation from the real value to the estimated value. MSE is calculated by using test and prediction values as specified in (2).

$$MSE = E(X_\mathrm{i} - d_\mathrm{i})^2 \tag{2}$$

where; MSE: the mean squared error, X_i: value at i^{th} data point, d_i: estimated value at i^{th} data point.

Using the given assessment criteria, the performed methods are compared in terms of the determination coefficient and the error rate between test values and the predicted values. Results are interpreted to achieve better estimation approaches.

3. Utilized data

The utilized cell data is chosen from the database of the University of Maryland CALCE Battery Research Group[1]. The cell test data is also used in several publications for online SOC estimation studies [42–44]. The actual SOC is assumed by calculating Ah throughout the test. Provided data includes also low current test profile to extract the voltage-SOC curve. Also, since the data is limited, only single training and test dataset used for this study. Dataset description and preprocessing steps are specified in the following sections.

3.1. Dataset description

The dataset consists of different types of tests such as initial capacity test, low current discharge test, low current charge test, dynamic stress test at 0°C, 23°C, and 45°C for 50% and 80% SOC window. Within this dataset, researchers have shared a lot of contents like test time, sampling time, current, voltage, charge capacity, discharge capacity, charge energy, discharge energy, and voltage difference. In this study, the dynamic stress test is used for the training of ML model. Both test and training data is performed at 23°C.

3.2. Preprocessing steps

The fundamental step is to adjust and clear the training data before application. Since the provided test data has also preconditioning values, all irrelevant data rows are cleared. Clear arrays are created to avoid confusing information for ML algorithm. Figure 5 shows the employed data for training the XGBoost model. As shown in the figure, the provided data includes 2 main input parameters which are voltage and current. By using Ah count, the SOC is defined with respect to given voltage and current profiles. Since the limited data is provided, the dynamic discharge data from 95% SOC to approximately 45% SOC with a 50% SOC window is employed as a training data. The training data starts from 100% SOC value by discharging the cell to 95% SOC level. Then, resting time is given to the cell to achieve a certain voltage level. Finally, a dynamic sequence starts by discharging and charging the cell with the same profile until the cell is reached to 45% SOC. The matrix consisting of the current and voltage values is used as an input for the model.

Similarly, Figure 6 illustrates the used data for testing the XGBoost model. Again, the data which is used for testing starts from 100% SOC. However, the initial static discharge is applied only for 2% SOC level. As it can be seen, the dynamic discharge continues from approximately 98% to approximately 28% SOC with a 70% SOC window. Correspondingly, the matrix consisting of the current and voltage values is used as an input for the model to compare test SOC values with the predicted values by XGBoost.

4. SOC estimation by using XGBoost

The model is created by using Python which is a frequently preferred platform for ML applications. The training and test data are separated properly in order to clear the data and prevent the mismatch during the computation. Then, the XGBoost library is trained and tested to estimate SOC. Finally, exponential smoothing is employed to increase model accuracy as a novel approach. Figure 7 shows a flowchart during the novel SOC

[1]CALCE and The University of Maryland (2017). CALCE Battery Research Group [online]. Website https://web.calce.umd.edu/batteries/data.htm [accessed 11 July 2019].

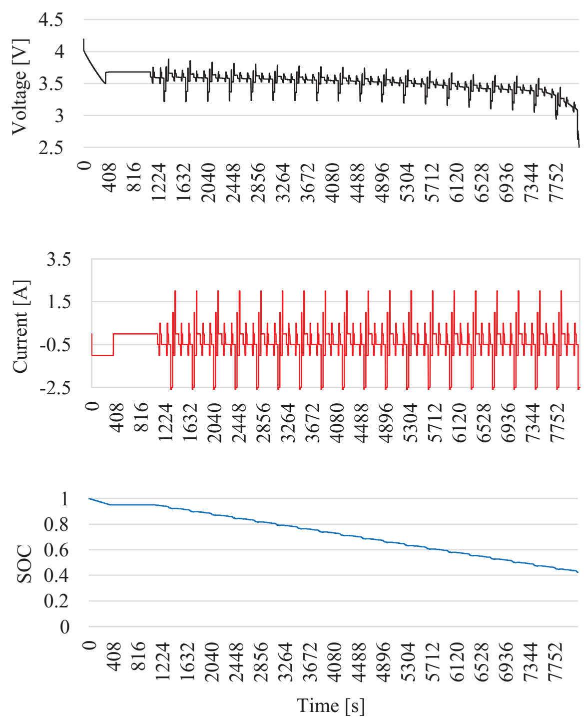

Figure 5. The utilized data for training the XGBoost model; voltage and current signals as input, SOC as the desired output.

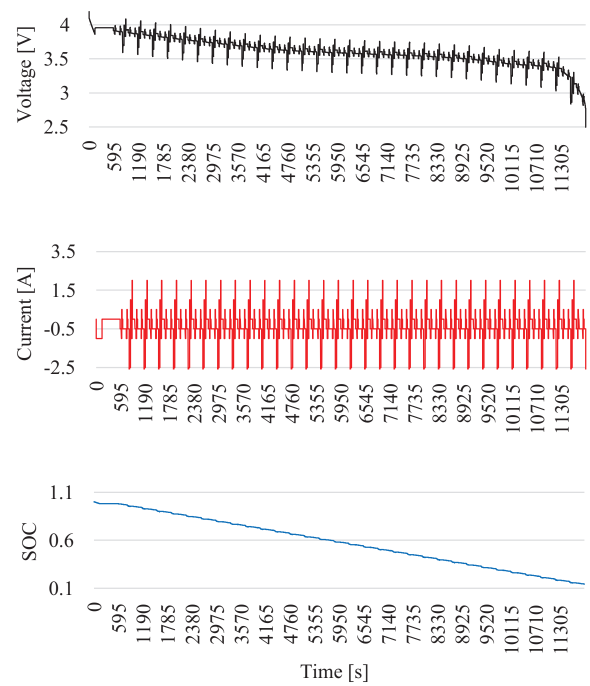

Figure 6. The utilized data for testing the XGBoost model; voltage and current signals as input, SOC as the desired output.

estimation application by using XGBoost. As mentioned above, initially XGBoost is trained first by using the XGBRegressor function. Since it is supervised learning, training data is given to the model as an input as given in Figure 7. Next, similar data is used to test the regression performance of the XGBoost. Results are exhibited in Figure 6 with respect to time and compared with the given assessment criteria by using Python. Table 1 shows the results of XGBoost performance in terms of MSE and R^2.

Results show that despite a low amount of data for training, XGBoost prediction has quite a high coefficient of determination and relatively low MSE. Even though the model performances are high, XGBoost shows a noisy profile over the test time as given in Figure 8. To solve this noisy estimation, exponential smoothing is proposed in the following section as a novel approach.

Table 1. The results of XGBoost performance in terms of MSE and R^2.

Parameter	XGBoost SOC estimation
Mean squared error [%]	0.05
R^2 Score [%]	98.81

4.1. Exponential smoothing in combination with XGBoost

Especially for forecasting and discrete systems, exponential smoothing is a useful operation [45]. By using (3), smoothing is applied to the XGBoost estimation values. Since the main focus of this study is not optimizing

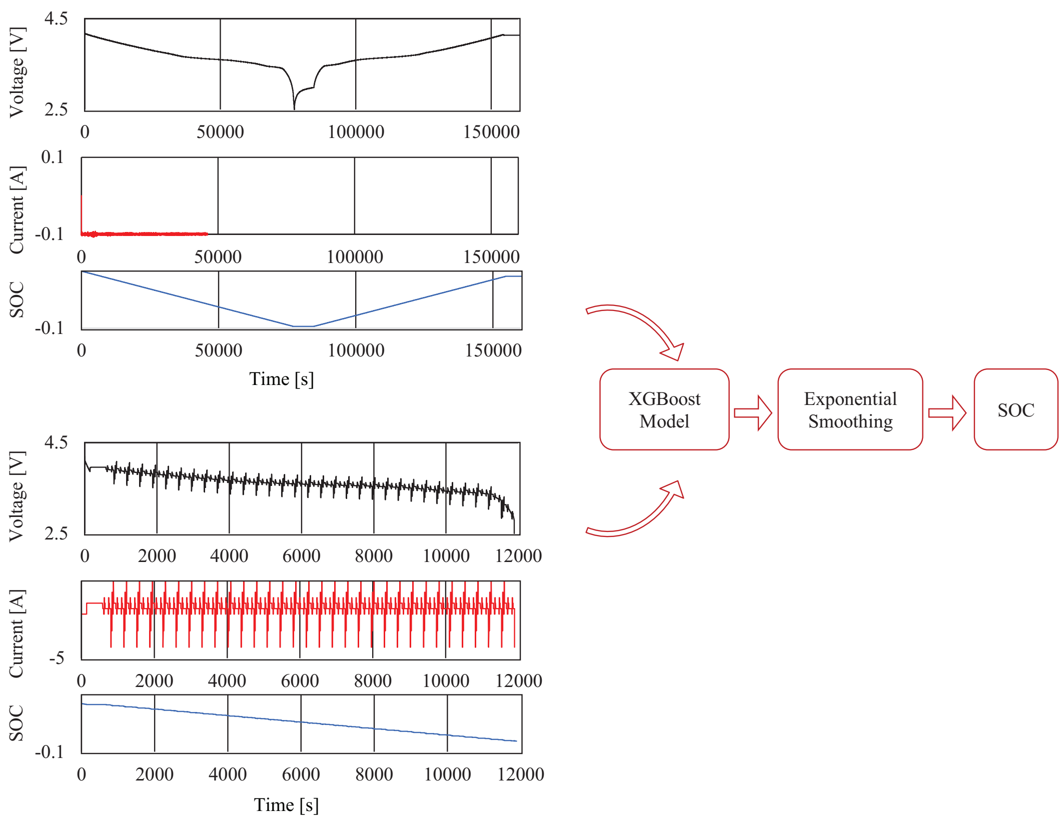

Figure 7. Block diagram for the proposed method (The most left block is used dataset for training and test).

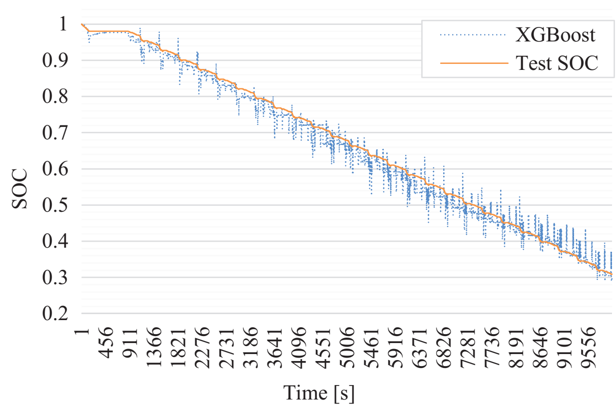

Figure 8. The results of XGBoost estimation in comparison with reference test SOC.

the smoothing factor, the smoothing parameter is selected arbitrarily to see the effects. The smoothing factor is selected arbitrarily as 0.03 to keep the smoothing rate low.

$$s(k) = \alpha * x(k) + (1 - \alpha) * s(k - 1) \tag{3}$$

where; α: smoothing factor which is between 0 and 1, *s(k-1)*: previous smoothed estimation, *x(k)*: actual SOC estimation by XGBoost, *s(k)*: smoothed SOC estimation value.

As a final step, exponential smoothing is applied to the XGBoost prediction for filtering disturbances in the data. The results are compared in terms of the same assessment criteria which is mentioned above. Figure 9 illustrates the exponential smoothing results in comparison with the pure XGBoost and the test SOC.

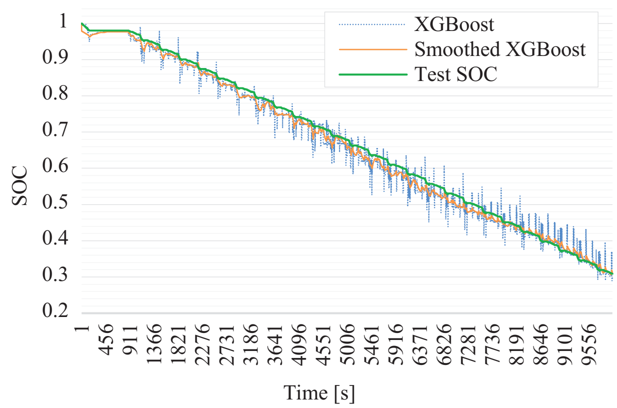

Figure 9. Comparison of estimation results between XGBoost, smoothed XGBoost and test SOC.

Since highly deviated results are observed as approximately 15%, exponential smoothing is proposed to apply to XGBoost for a combined algorithm as defined in (3). It filters the estimation and sorted out the disturbances. A significant improvement achieved by applying exponential smoothing. The comparison shows how exponential smoothing filters abrupt estimation values. The highest error for a single estimation point has reached approximately 15% throughout XGBoost estimation. By applying exponential smoothing, the individual error is kept below 5%. Figure 10 illustrates the error differences over the testing drive cycle.

It can be seen that a significant improvement is achieved by applying exponential smoothing. As a hybrid model, smoothed XGBoost performed better estimation than a pure XGBoost algorithm. Table 2 shows that the R^2 score is increased by applying the smoothing to the XGBoost algorithm. Besides, MSE is lower than the pure model.

Table 2. Performance comparison of pure XGBoost and smoothed XGBoost model for SOC estimation.

Method	R^2 Score [%]	MSE [%]
XGBoost - test SOC	98.81	0.05
Smoothed XGBoost - test SOC	99.43	0.02

Considering the real application, this hybrid model would provide better results for SOC estimation by filtering the noisy estimation data and sorting out the irrelevant points.

4.2. Comparison of performed estimation methods

Electrical circuit model (ECM) based method with EKF is also performed to compare their performances in terms of development effort, accuracy, and robustness. For model-based estimation, parameterization is done according to the two time constant (TTC) model. Figure 11 shows the TTC model illustration.

The internal series resistance values are extracted from the test dataset by observing SOC and immediate voltage changes. By using LMFIT library in Python, RC branch values R_1, τ_1, R_2 and τ_2 are estimated.

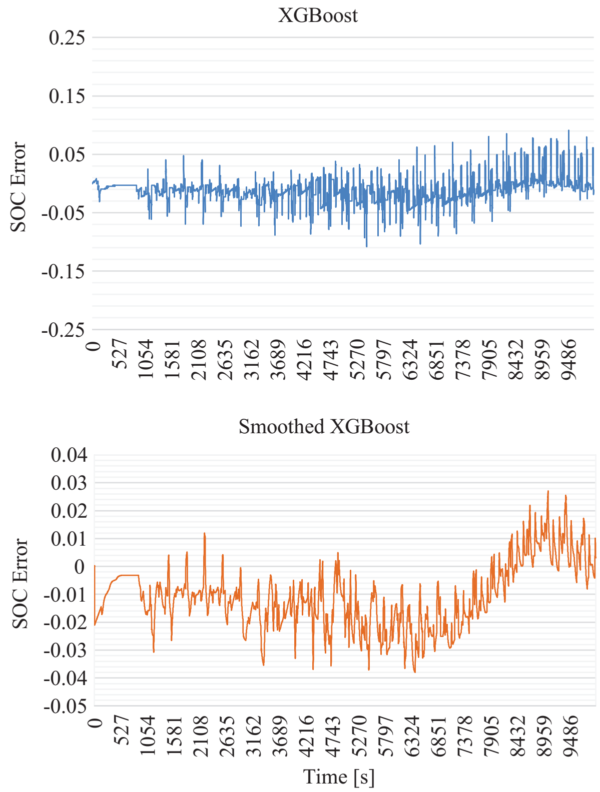

Figure 10. Error comparison of estimation results as the difference between actual and estimated SOC: XGBoost and Smoothed XGBoost with respect to time.

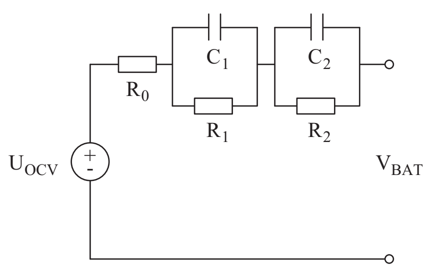

Figure 11. TTC model illustration.

After TTC model parameters are estimated with respect to different temperatures, the model parameters are implemented to look-up tables in the MATLAB-Simulink environment. When the model creation is done, the TTC model is tested against the provided test values. As mentioned above, SOC is a parameter that cannot be measured directly. That is why estimation is done by using EKF which is a type of non-linear adaptive filter. EKF matrices are implemented to create a SOC estimator block in MATLAB-Simulink. Figure 12 shows the comparison of performed estimation methods against the dynamic operation.

When the different models are compared with each other, they represent quite matching profiles against the dynamic tests. However, there are differences after the estimation data is analyzed. Table 3 shows the performance comparison of performed estimation methods against the dynamic operation in terms of R^2 and MSE.

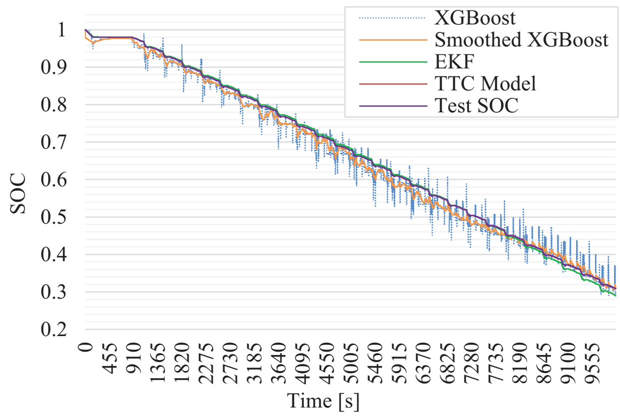

Figure 12. Comparison of performed estimation methods against dynamic operation.

Table 3. Performance comparison of performed estimation methods against dynamic operation.

Method	R^2 Score [%]	MSE [%]
TTC model - test SOC	99.99	0.000003
EKF - test SOC	99.93	0.00327
XGBoost - test SOC	98.81	0.05
Smoothed XGBoost - test SOC	99.43	0.02

Table 3 exhibits that the TTC model is properly parametrized with significantly lower errors. Besides, the estimation model with EKF is also consistent with the test results as 99.93 %. If the results are interpreted, the outcome will be that model-based methods are more accurate than the data-driven methods. However, the important point is that model-based methods require a lot of parameterization and calibration effort which are done as a scope of this application. As a matter of fact, data-driven methods do not require parameterization or calibration when a proper dataset is provided.

Indeed, the XGBoost algorithm uses quite a low amount of data to predict the results with relatively high accuracy. Besides, the estimation can be improved by applying useful filters such as exponential smoothing. Even though the algorithm has worse performance if it is compared to the other similar studies in the literature, the importance of decision trees may be adjusted to have better results. As shown in [17] deep feedforward neural networks (DNN) can achieve 0.81% RMS (root mean squared) error while the maximum error is kept below 10%. Also, by using GPR for SOC estimation, 0.81% RMS error may be achieved even the error is kept below 2% as studied in [36]. In spite of literature shows better examples in terms of maximum error, XGBoost with exponential smoothing provides lower MSE. Last but not least, the same training and test data must be used to compare directly.

5. Conclusion

The SOC estimation is performed by using different approaches in this study. The data is adjusted to create different models. First, the data is analyzed and different arrays are created to use the data easily. Preconditioning values are removed from the dataset. XGBoost is applied to the provided data for SOC estimation with a dynamic load. Between test data and XGBoost SOC estimation, 98.81% R^2 score and

0.05% MSE are achieved. After XGBoost implementation, a hybrid model is proposed in this study which is a combination of XGBoost and exponential smoothing as a contribution to the literature. Smoothed XGBoost achieved 99.43% R^2 score and 0.02% MSE as a novel approach for estimation.

In spite of insufficient data, this study has contributed to show that machine learning-based models can be used for SOC estimation if proper training data is provided. Especially, XGBoost is a fast and highly accurate algorithm for battery state estimation considering its advantages as stated before. When this method is utilized in an application that has a well-known operation profile, the results would be quite impressive even a small amount of data is used for training.

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