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Advanced Techniques for Estimating State of Charge (SoC) in Lithium-Ion Batteries

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ABSTRACT

Accurate estimation of the State of Charge (SoC) of batteries is critical for the optimal performance and safety of electric vehicles and portable electronic devices. In this study, several machine learning regression models were investigated for state-of-charge (SoC) estimation, including Linear Regression, Support Vector Machines (SVM), Regression Trees, and Neural Networks. The publicly available LG 18650HG2 dataset [1] was utilized, comprising over 670,000 data points collected during charging and discharging cycles. Input features included voltage, current, temperature, average voltage, and average current. The models were implemented using MATLAB, and their performance was evaluated using standard metrics: Mean Absolute Error (MAE), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), and the coefficient of determination (R²). The best-performing model—a wide neural network—achieved an RMSE of 2%, MAE of 0.0109, and an R² of 99.5%. These results indicate that Neural Networks outperform traditional regression techniques in terms of prediction accuracy and robustness.

1. Introduction

Nowadays, transportation is one of the major contributors to environmental pollution and greenhouse gas emissions. As much of the world aspires for cleaner and sustainable alternatives, hybrid cars, electric vehicles (EVs), and other battery-operated systems have gained increasing prominence. EVs are particularly lauded for their silent operation, lower maintenance needs, and zero emissions. For example, In 2013, the annual sales of EVs reached 505,000 in the US, 904,000 in Japan, and 22,000 in Europe [2]. However, the performance of EVs on the road is largely dependent on our ability to manage the batteries that power them. The majority of electric vehicles (EVs) use lithium-ion batteries, owing to their superior energy density and lifespan, along with a favorable performance trade-off. However, these batteries remain unsafe, present challenges in thermal management, and exhibit altered behavior in the presence of large power systems. Charging stations for EVs have been growing everywhere, but this raised other issues about power quality and voltage drop for millions of EVs connecting to the grid. Hence, research is also being directed to battery control systems, integration of renewable energy, and smart charging methods.

Battery management in electric vehicles focuses on determining the available energy or the State of Charge (SoC). SoC estimation is complicated due to multi-dimensional battery dynamics and numerous operating conditions that

include temperature, self-discharge, hysteresis, and battery aging. It is not possible to estimate SoC straightforwardly, nor is it possible through primitive approaches using battery parameters. Therefore, the main difficulty and focus of electric vehicle technology is improving the real-time accuracy of SoC. Recently, research aimed at improving the accuracy of SoC estimation has become a prominent topic, focusing on fuel cell models and model calibration. However, it is important to acknowledge that limitations in SoC estimation methods are pervasive. Nonetheless, the necessity to enhance the accuracy and real-time performance of SoC estimation methods remains of vital importance [3].

Bridging the gap then comes the machine-learning (ML) era. Recently, it has been of astounding importance for SoC amelioration. Real battery data help feed an advanced algorithm such as artificial neural network (ANN), support vector machines (SVM), or long short-term memory (LSTM) networks geared towards identifying complex patterns unlike classical methods. They actually become much more adaptable to the erratic and complicated nature of real-life driving situations.

Nonetheless, existing limitations in the best intelligent models. Information an intelligent model is trained on determines how well it performs. Limited or scattered datasets make inaccurate projections. Hybrid solutions-combining a physics-based model with an ML model to develop a mitigated healthy system-have started receiving attention. As particle swarm optimization (PSO), deep neural networks, and Kalman filtering stretch the boundaries of what is possible [4].

This research investigates and compares several machine learning methods for estimating the State of Charge (SoC) of electric vehicle batteries. Contrasting prior studies, the present work emphasizes real-world applicability by incorporating variables such as temperature fluctuations, and realistic driving behavior to develop models that perform effectively both in laboratory settings and under actual operating conditions. The objective is to enhance SoC estimation accuracy, thereby improving the safety, reliability, and user appeal of electric vehicles, and contributing to the advancement of cleaner and more intelligent transportation systems.

2. State of Charge Estimation Techniques

State of Charge (SoC) is the percentage of residual energy to total energy that a battery can store

$$Soc = \frac{Qc}{Q0} = 1 - \frac{Qt}{Q0} \tag{1}$$

SoC is strongly affected by a number of operational and environmental conditions. Open-circuit voltage (OCV) and ampere-hour integration are typically traditional estimating methods associated with large estimation errors that often render them unsuitable for real-time applications. To increase the accuracy of the estimation, two mathematical ones have been developed: Electrochemical Impedance Models (EIMs) and filter-based methods like the Kalman Filter (KF) and its extensions, namely Extended Kalman Filter (EKF), sigma-point Kalman filter (SPKF), and adaptive extended Kalman filter (AEKF)[10]. Yet these methods come with certain disadvantages, especially under dynamics and nonlinearities in unpredictable real-world settings.

In order to circumvent these limitations, data-driven methods composed by machine learning (ML) and deep learning (DL) are becoming more accepted into SoC estimating methods. Six machine learning methods were evaluated in this study: artificial neural networks (ANN), support vector machines (SVM), linear regression (LR), Gaussian process regression (GPR), and ensemble techniques, including bagging and boosting. These basic models are trained on time-series data to capture trends and interrelations between battery signals and state of charge. Earlier studies proved hybrid techniques, where data-driven models combine with model-based frameworks, could enhance prediction accuracy and robustness. These include long-short-term memory recurrent neural networks (LSTM-RNNs), boosting techniques reducing overfitting and enhance generalization, and the deep multilayer perceptrons, load classification[11].

SoC estimating models are tested with real driving datasets that take into consideration environmental parameters, HVAC loads, and road conditions that change from time to time. It proposes a two-stage testing approach to estimate the resilience of the model under different conditions. The proposed SoC framework comprises three salient modules

based on short-term charging: feature extraction, application of the ML model, and selection of input parameters. Model performance is further evaluated using various evaluation metrics such as Mean Absolute Error (MAE), Mean Square Error (MSE), Root Mean Square Error (RMSE), and Mean Absolute Percentage Error (MAPE). Through such an exhaustive and comparative study, our goal is to advance the methods of SoC prediction, which would assist in the development of reliable and energy-efficient EV battery management systems[12].

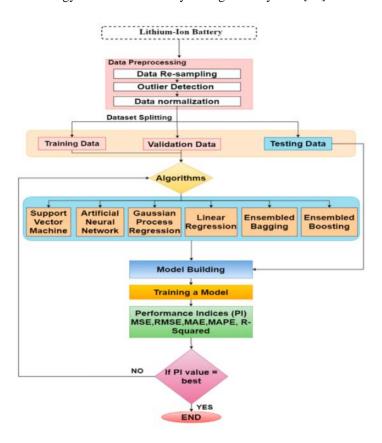


Fig1. the overall flow diagram to calculate mean square error (MSE), root mean square error (RMSE), mean absolute error (MAE), and mean absolute percentage error (MAPE) for the proposed battery using state of charge. [12]

3. Methodology

In 2020, Ariche et al. [13], researchers explored how electric vehicle (EV) energy consumption varied based on factors such as road topography and ambient temperature, particularly when the vehicle operated in comfort ride mode on Moroccan roads. While insightful, this analysis fell short of delivering accurate range estimations for battery electric vehicles in real-world conditions across both regular and comfort ride scenarios. To enhance the reliability of state of charge (SOC) estimation under such dynamic conditions, a rigorous data preprocessing stage is essential. This involves cleaning the dataset to eliminate noise and inconsistencies, transforming it to unify the format, and selecting the most relevant features that impact SOC prediction accuracy. For this purpose, the LG 18650HG2 Original Dataset from McMaster University was utilized, comprising approximately 670,000 data points collected during battery charging and discharging cycles. The dataset contains key parameters—voltage, current, temperature, average voltage, and average current—that are essential for accurate and reliable SoC estimation. Proper feature selection from this dataset not only improves model performance but also reduces computational demands. A diverse set of machine learning algorithms—linear regression (LR), support vector machine (SVM), regression tree (CART), and neural networks (NNs)—was chosen to balance interpretability and predictive power. LR serves as a baseline due to its

simplicity, while SVR is effective for capturing non-linear dependencies. RF contributes robustness and feature importance insights, and NNs offer superior accuracy in modeling complex relationships. These models are assessed using performance indices such as mean absolute error (MAE), mean squared error (MSE), root mean squared error (RMSE), and R², across both initial and secondary test sets. The second test set, composed of additional trip data with identical features but recorded under different conditions, serves to evaluate the models' generalizability and minimize overfitting. This two-stage validation approach ensures that SOC estimation models remain accurate and robust across varying real-world EV usage scenarios.

To better understand how each algorithm contributes to SOC estimation, the following section provides a numbered analysis of the selected models. Each algorithm is evaluated based on its underlying principles, suitability for the dataset, and performance in predicting SOC.

3.1 Linear Regression (LR):

Linear regression is one of the most fundamental and widely used algorithms in predictive modeling, particularly valued for its simplicity, interpretability, and computational efficiency. It is quite an easy and interpretable but at the same time quite a limited algorithm in case of nonlinear dependencies of their nature in battery dynamics[14]. It is a supervised machine learning algorithm that models a continuous output variable—in this case, the state of charge (SOC)—based on one or more input features such as voltage, current, and temperature. LR assumes a linear relationship between the dependent variable and independent variables, which it fits using the least squares method. The empirical form of the model is given by the equation:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n$$
 (2)

where y is the predicted SOC, x_1 , x_2 , ..., x_n are the input features, β_0 , β_1 , ..., β_n are the model coefficients, and ϵ is the error term. This model performs well on small- to medium-sized datasets and offers a useful baseline for comparison with more complex algorithms. However, its major limitation is its inability to capture non-linear relationships within the data, which can hinder its performance in more dynamic EV operating conditions.

3.2 Support Vector Machine (SVM):

Support Vector Machine is one of the finest and popular methods of supervised learning applied in both classification and regression problems. It is gaining popularity in many fields. This is because it assumes that there is some nonlinear mapping function that maps the input data to a higher-dimensional feature space and that finally applies to that new feature space a linear algorithm to find the best separation hyperplane of maximized margin between the classes of data

Strength of SVM is, however, that it handles the case of linear inseparability by using nonlinear mapping techniques through the kernel functions like polynomial kernel or radial basis function (RBF). Thus makes it possible for the model to capture complex patterns and predict results accurately even if the actual data structure is very nonlinear[15].

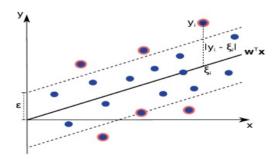


Fig. 2 The functioning of SVM can be illustrated by w * T x for regression. [15]

An equation derived from actual data

$$Yi = \sum_{i}^{N} W. K(Xi, X) + B \tag{3}$$

Yi = predicted output W = stands for weights. K = kernel technique (xi, x) = vectors of support B = bias.

3.3 Regression Tree (CART):

Decision Tree Regression is a supervised machine learning algorithm that predicts a continuous output—in this case, the state of charge (SoC)—by learning decision rules from input features such as voltage, current, and temperature. It is especially useful for capturing non-linear dependencies and variable interactions. The model works by recursively partitioning the data into regions with minimal variance, and the final prediction is the average of values in the corresponding leaf node. In the study by Wang et al. (2019), a Classification and regression tree (CART) model was applied for SoC estimation in hybrid electric vehicles, achieving simulation errors under 3.5% and experimental errors below 5%, which confirms the algorithm's effectiveness and robustness under real driving conditions. Despite its interpretability and accuracy, tree models can overfit unless pruned or regularized.

3.4 Neural Networks (NNs):

Artificial neural networks (ANNs) can achieve the State of Charge (SoC) of battery systems from the data since they can find out the hidden and non-linear relationships from the training data. Their electronic architecture is made of layers of neurons, after making a few simple calculations, passes on its result to the next layer. Weights define the strength of the connections and are updated during the training to ensure that they best fit the prediction error [16].

The design of the network structure is the first step in training the model. One of the primary methods used to match the prediction error with the information from the input data is the gradient and momentum in combination with the weight and bias adjustments to suppress the continuous growth of the error. This process is repeated, i.e., a certain number of the so-called epochs is passed until the network generates proper SoC values from the given input features. The validation data is used for this purpose since it ensures that the model will not sacrifice the level of performance even in the face of unforeseen circumstances.

Artificial neural networks (ANNs) can be trained to estimate SoC Instead of relying on accurate equivalent circuit models or detailed physical equations, ANNs learn to approximate the nonlinear relationship between input variables (such as voltage, current, and temperature) and the SoC directly from data. This data-driven approach enables ANNs to model the behavior of batteries effectively, even when the internal dynamics are complex or poorly understood. Consequently, they become the most favorable battery management system providing safe and efficient operation as long as they acquire the knowledge of patterns from the data environment in an appropriate way.

This training ANN is found to be the best method based on MSE and RMSE of (0.04%) and (2.1%), respectively.

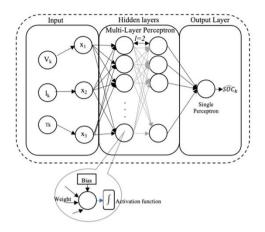


Fig.3. input and output layers of ANN [16]

Empirical equation for ANN: $s(\sum_{j=1}^{N} \{Wijxj + bi\})$ (4) Wij=weight to neuron i from neuron j bi=bias xj= input vectors

4. Training Dataset

The data set is split into validation set, testing set, and training set. In the training set, there are 669956 data values, from which the model is trained, and then the accuracy is tested using the testing set. During the lithium battary LG18650 battery test, voltage, battery current, battery temperature, average voltage, average current, and SoC values are the type of data being utilized [1], All the data are standardized to minimize training volatility and to make the training process faster.

4.1 Model Training Configuration

The The machine learning models were developed using MATLAB R2024b's Regression Learner app with the following configurations:

• Neural Networks:

Narrow Neural Network: one fully connected layer with 10 neurons; ReLU activation function; iteration limit of 1000; regularization strength (lambda) = 0; data standardized before training.

Medium Neural Network: one fully connected layer with 25 neurons; ReLU activation function; iteration limit of 1000; regularization strength (lambda) = 0; data standardized before training.

Wide Neural Network: one fully connected layer with 100 neurons; ReLU activation function; iteration limit of 1000; regularization strength (lambda) = 0; data standardized before training.

Bilayered Neural Network: two fully connected layers each with 10 neurons; ReLU activation function; iteration limit of 1000; regularization strength (lambda) = 0; data standardized before training.

Trilayered Neural Network: three fully connected layers each with 10 neurons; ReLU activation function; iteration limit of 1000; regularization strength (lambda) = 0; data standardized before training.

5. Error Metrics

An important task is to compare the anticipated SoC values with experimentally obtained SoC data to evaluate the precision of SoC prediction done by models approved. Each model is further assessed on the quantitative basis by a number of error metrics intended to reflect the different dimensions of prediction accuracy[17].

5.1 RMSE:

The Root Mean Square Error considers residuals squared: hence, the more a prediction is off, the more say it has in calculating the average size of errors. RMSE becomes better suited for those applications where large discrepancies between expected and actual outcomes are intolerable.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - \widehat{y}_i)^2}$$
 (5)

where y_i is the actual value, $\hat{y_i}$ is the predicted value, and n signifies the total number of observations.

5.2 MAE:

One way to measure the dissimilarity of two continuous variables in statistics is with the help of a mean of the absolute differences between the predicted values and the observed data.

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |y_i - \widehat{y}_i| \tag{6}$$

 $MAE = \frac{1}{n} \sum_{i=1}^{n} |y_i - \widehat{y}_i|$ (6) where y_i is the actual value, \widehat{y}_i is the predicted value, and n signifies the total number of observations.

5.3 MSE:

By calculating the average of the squared differences, the Mean Square Error (MSE) determines the divergence between the predicted and actual values. The MSE is heavily affected by outliers due to its squaring of errors in comparison with the MAE.

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$
 (7)

where y_i is the actual value, $\hat{y_i}$ is the predicted value, and n signifies the total number of observations.

$5.4 R^2$:

This statistical measure called coefficient of determination is also referred to as R2, which tells us about how much of the dependent variable's variation in a regression model can be explained with the help of independent variables. Similarly, the degree to which projected values match actual observed data is a measure of the quality fit of the model. An R2 value of 100% indicates perfect fit because both the values predicted by a model match exactly with those that were actually observed.

$$R^2 = 1 - \frac{\sum_{l=1}^{n} (y_l - \widehat{y_l})^2}{\sum_{l=1}^{n} (y_l - \overline{y})^2}$$
 (8) where yi is the actual value, $\widehat{y_l}$ is the predicted value, \overline{y} is the mean of actual values, and n is the number of

observations.

6. Experimental Result and Discussion

In order to evaluate the performance of each machine learning model in estimating the State of Charge (SoC), Linear Regression, Support Vector Machine Regression, Decision Tree Regression, and Neural Network Regression models were trained and tested on the preprocessed LG 18650HG2 dataset [1]. After training, the models were evaluated using standard performance metrics: Mean Absolute Error (MAE), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), and the coefficient of determination (R²). This section presents and compares each model's results based on its performance on the test set. The following tables and figures illustrate the respective predictive accuracies of each approach—specifically, how effectively the models captured the relationship between the input features and the actual SoC.

TABLE 1

Training Results					
Model Number	Model Type	RMSE (Validation)	MSE (Validation)	R Squared (Validation)	MAE(validation)
1.1	Neural Network(narrow)	0.0248	0.00061	0.9944	0.0152
1.2	Neural Network(medium)	0.0229	0.00052	0.9952	0.0131
1.3	Neural Network(wide)	0.0211	0.00045	0.9959	0.0109
1.4	Neural Network(bilayered)	0.0226	0.00051	0.9954	0.0127
1.5	Neural Network(trilayered)	0.0221	0.00049	0.9956	0.0119
2.1	Linear Regression	0.0442	0.00195	0.9824	0.0329
2.2	Linear Regression(interactions linear)	0.0328	0.00108	0.9903	0.0217
2.3	Linear Regression(robust linear)	0.0456	0.00208	0.9812	0.0315
2.4	Linear Regression(Stepwise)	0.0328	0.00108	0.9903	0.0217
3.1	Tree(fine)	0.0216	0.00047	0.9958	0.0098
3.2	Tree(medium)	0.0214	0.00046	0.9959	0.0099
Model Number	Model Type	RMSE (Validation)	MSE (Validation)	R Squared (Validation)	MAE(validation)
3.3	Tree(fine)	0.0216	0.00047	0.9957	0.0098
3.4	Tree(coarse)	0.0221	0.00049	0.9956	0.0104
4.1	SVM(Quadratic)	0.2462	0.0606	0.4539	0.1693
4.2	SVM(cubic)	13	194	-1750	6.6
4.3	SVM(linear)	0.1027	0.0105	0.9049	0.0775
4.4	SVM(coarse Gaussian)	0.0356	0.0013	0.9886	0.0313
4.5	SVM(Kernel)	0.1262	0.0159	0.8565	0.072
4.6	SVM(fine)	0.0378	0.0014	0.9871	0.0337
4.7	SVM(gaussian)	0.0313	0.0009	0.9912	0.0252

0For the estimation of the State of Charge (SoC), the Neural Network (wide) model was the best among all machine learning models, as seen in Table 1. Its validation errors on the important parameters were the lowest among the other models, with an RMSE of 2%, MSE of 0.4%, MAE of 1.09%, and R² value of 99.5%, revealing remarkable accuracy and predictive ability. Also, competitive results were achieved with other neural network variants and the decision tree models, such as Tree (fine) and Neural Network (tri-layered).

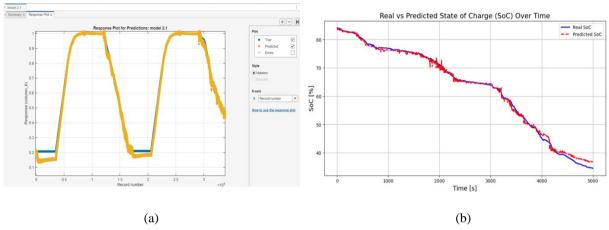


Fig.4 .a,b. NN Real vs predicted state [18]

Figures 4A and 4B illustrate the comparison between real and predicted values of the battery's state of charge (SoC) using neural networks. Figure 4B, sourced from Ariche et al. [18], serves as a benchmark visualization, while Figure 4A represents our model's performance on the LG 18650HG2 dataset [1], publicly available from McMaster University. Both figures clearly demonstrate the predictive capabilities of neural networks in capturing the dynamics of battery behavior. In our study, we applied four types of regression learning models—Linear Regression, Decision Trees, Support Vector Machines (SVM), and Neural Networks. For each model, we evaluated performance using common regression metrics: coefficient of determination (R²), Mean Squared Error (MSE), Mean Absolute Error (MAE), and Root Mean Squared Error (RMSE), enabling a comprehensive assessment of prediction accuracy across methods.

Support Vector Machine the other hand, performed the worst overall. The SVM (cubic) and SVM (quadratic) models in particular showed a total inability to adequately represent the data, with the cubic kernel achieving an R² of -1750% and extremely high error values and low, even negative, R² scores. These results demonstrate that neural networks, particularly those with broader architectures, are the most appropriate for this use case, but SVMs were not.

These findings are consistent with results reported in [Ariche et al., 2024][18], where Neural Networks also outperformed other machine learning models in predicting battery State of Charge. That study similarly concluded that wider network architectures offered improved generalization and lower prediction errors compared to models like SVM and linear regression. The alignment between our experimental outcomes and those in the literature reinforces the reliability and robustness of Neural Networks for SoC estimation.

7. Conclusion

In conclusion, this study demonstrates the effectiveness of using machine learning models, particularly neural networks, for accurate State of Charge (SoC) estimation of Li-ion 18650 batteries under real-world conditions. Among the tested models, the Neural Network (wide) outperformed all others, achieving the lowest validation errors across all performance metrics—most notably an R^2 used with error 99.5% from the real data and RMSE of 2% highlighting its strong predictive capability with MSE = 0.00045, MAE = 0.0109. Other models, such as the tri-layered NN and

decision tree approaches, also delivered competitive results, but none matched the consistency and precision of the wide NN model. By using a large, real-world dataset and incorporating a two-phase testing strategy, this work adds robustness and generalizability to the findings. The results confirm that neural networks are a reliable choice for SoC estimation, especially when trained on complex, diverse datasets reflective of actual electric vehicle usage. This contribution supports ongoing efforts to make battery management systems more accurate, efficient, and adaptive to real-life scenarios.

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