Software Impacts 14 (2022) 100447

Contents lists available at ScienceDirect

Software Impacts

journal homepage: www.journals.elsevier.com/software-impacts

Original software publication

LiBEIS : A software tool for broadband electrochemical impedance spectroscopy of lithium-ion batteries

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ARTICLE INFO

Keywords:
Electrochemical impedance spectroscopy
Lithium-ion batteries
Equivalent circuit models
Exploratory data analysis
Machine learning
State of charge

ABSTRACT

Electrochemical impedance spectroscopy (EIS) is a fundamental tool used in numerous research fields and applications. In particular, EIS is commonly employed for studying and monitoring lithium-ion batteries, to ensure their safe and efficient operation. The LiBEIS software tool computes EIS data by processing the voltage and current time series acquired from a battery under test, which is excited with a broadband current signal. Furthermore, LiBEIS performs fitting of the EIS data to an equivalent circuit model, which is often employed in practice to analyse the behaviour of the battery. Finally, LiBEIS implements exploratory data analysis tools and machine-learning methods aimed at estimating the state-of-charge (SOC) from EIS data.

Code metadata

Current code version	v1.0
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2022-202
Permanent link to Reproducible Capsule	https://codeocean.com/capsule/9473632/tree/v2
Legal Code License	GNU General Public License (GPL) v.3
Code versioning system used	git
Software code languages, tools, and services used	Matlab, Python3
Compilation requirements, operating environments & dependencies	Matlab, python3, Pandas, Numpy, Scikit-learn
If available Link to developer documentation/manual	https://electrical-and-electronic-measurement.github.io/LiBEIS
Support email for questions	emanuele.buchicchio@ieee.org

1. Introduction

Energy management in battery-powered devices requires estimating and monitoring the battery state-of-charge (SOC) to avoid irreversible damage and improve device usability. Unfortunately, there is currently no practical method for direct measurement of the amount of charge in a battery, hence the need to estimate SOC indirectly. Given the crucial role played by batteries in a wide range of products, it is no surprise that estimating SOC has attracted increasing research interest in recent years [1,2].

Electrochemical Impedance Spectroscopy (EIS) is one tool for assessing SOC as well as for estimating the state-of-health (SOH) in automotive, energy storage, and electronics applications [3]. Impedance measurement is also important for determining the battery aging status [4] and the remaining useful life (RUL). EIS is also widely used to characterise materials and systems in applications such as corrosion monitoring, analysis of biological tissues and characterisation of electrochemical systems. Although this work focuses on describing the use of LiBEIS for estimating the SOC of a lithium battery, the tool can also be employed for other applications such as SOH, RUL and battery

DOI of original article: https://doi.org/10.1016/j.dib.2022.108589.
The code (and data) in this article has been certified as Reproducible by Code Ocean: (https://codeocean.com/). More information on the Reproducibility Badge Initiative is available at https://www.elsevier.com/physical-sciences-and-engineering/computer-science/journals.
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https://doi.org/10.1016/j.simpa.2022.100447
Received 10 September 2022; Received in revised form 18 October 2022; Accepted 15 November 2022

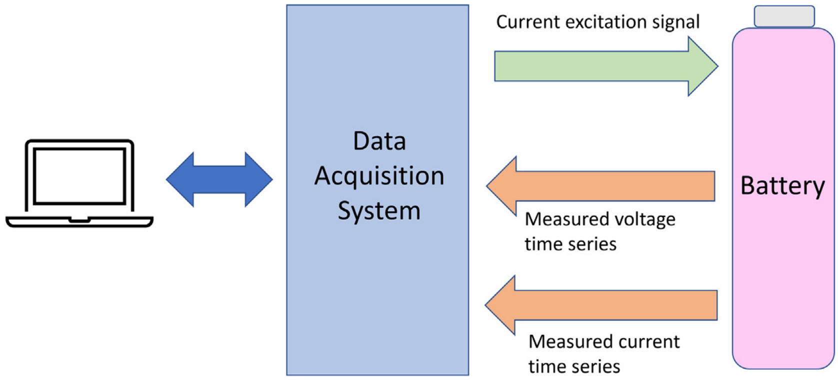

Fig. 1. Conceptual diagram of the EIS analysis system. The Data Acquisition System provides a broadband current excitation signal to the battery under test and acquires the current and voltage time series. These time series are then transferred to a PC where the software tool is employed to obtain EIS curves, perform exploratory data analysis, and estimate SOC.

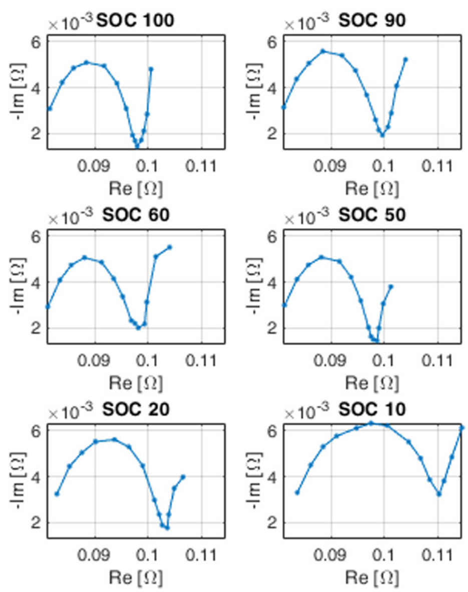

Fig. 2. A set of EIS curves obtained experimentally from a 3.7 V, 2600 mAh cylindrical lithium-ion cell for different values of the SOC, represented in a Nyquist plot.

temperature prediction [5]. These quantities are crucial for efficient, safe and reliable management of a battery-powered system [6].

LiBEIS includes the following four main functionalities, which we describe in the remainder of the paper: (1) EIS computation, (2) battery equivalent model fitting (3) EIS exploratory data analysis (4) ML SOC prediction model training and scoring.

1.1. EIS computation

As a first step, LiBEIS takes as input the voltage and current time series, each comprised of N samples, and computes the EIS values in the frequency domain. The EIS computation consists in the determination of the frequency-domain complex impedance $Z[k]$, with $k = 1 \dots N$. Such computation is performed by first calculating the discrete Fourier transform of the voltage and current time series, denoted as $V(k)$ and $I(k)$, respectively and then by dividing them, to obtain the complex impedance as $Z[k] = V[k]/I[k]$.

The voltage and current time series are acquired by an EIS analysis system, whose basic operation is illustrated in Fig. 1. This system excites the battery under test with a suitably designed broadband current signal and acquires the current and voltage time series [7]. An example of the graphical representation of the EIS curves provided by the LiBEIS software tool is shown in Fig. 2. The computed EIS data are saved in a .csv file as complex values, real part and imaginary part.

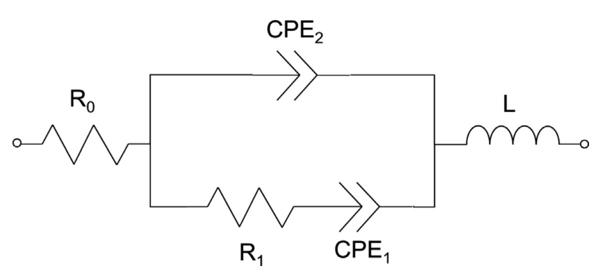

Fig. 3. Equivalent circuit model of the battery.

1.2. Battery equivalent model fitting

Equivalent circuit models are commonly used to gain insight on the battery under different operating conditions and to monitor their behaviour [8]. LiBEIS fits the EIS data that are obtained as illustrated in Section 1.1 to the equivalent circuit model shown in Fig. 3. This circuit model contains two constant-phase elements (CPEs). The CPEs are widely employed in the literature for modelling the low-frequency and mid-frequency behaviour of the battery impedance [9]. The impedance

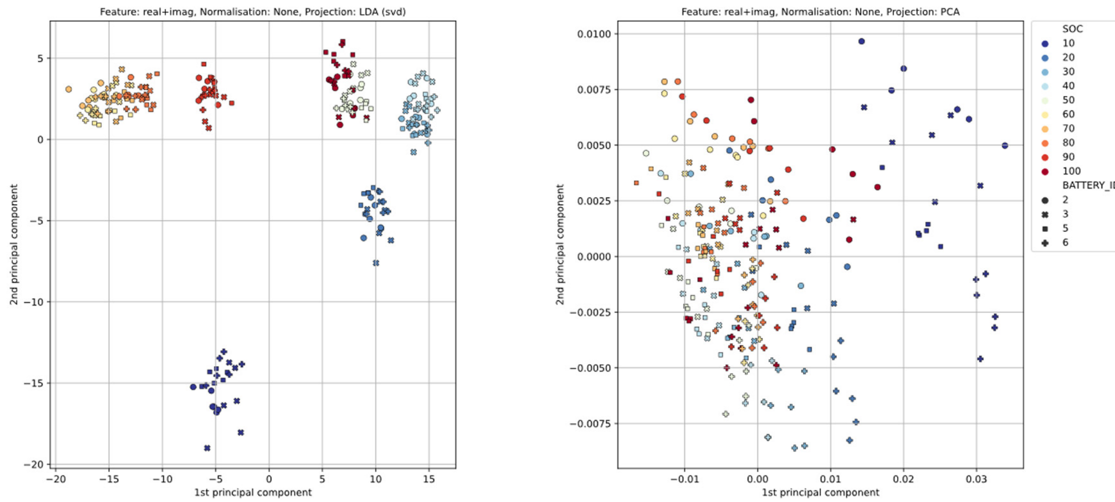

Fig. 4. An example of Linear Discriminant Analysis (LDA) and Principal Component Analysis (PCA) applied to EIS data from four different batteries in [10].

of the CPE is defined as

$$Z_{CPE}(j\omega) = \frac{1}{Q(j\omega)^p}$$

where Q and p are the parameters of the CPE, with $0 < p < 1$, and ω is the angular frequency. Since each CPE is characterised by two parameters, the equivalent circuit model of Fig. 3 has a total of 7 parameters, i.e. R_0, R_1, L, Q_1, p_1, Q_2, and p_2, where Q_1 and p_1 are the parameters of CPE$_1$ and Q_2 and p_2 are the parameters of CPE$_2$.

The fitted values of the model parameters are provided as an output and saved in a .csv file. Such parameters can be used for further analysis, processing, and to estimate SOC, as described in the following.

1.3. EIS exploratory data analysis

The LiBEIS software tool generates scatter plots of the impedance values and the circuit parameters of the equivalent model via Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA). The scatter plots were obtained by projecting the data on the first two axes resulting from PCA and LDA transformation; that is, the axes that respectively maximise the overall data variance (PCA) and the between-class variance (LDA). In both cases the calculation was based on singular value decomposition.

We used PCA and LDA projection as described above to generate scatter plots from the following seven sets of features: (1) the real part of the impedance data, (2) the imaginary part, (3) the concatenation of (1) and (2), (4) the module, (5) the phase, (6) the concatenation of (5) and (6), and (7) the circuit parameters of the equivalent model. Each set of features was pre-processed by three normalisation procedures: (1) no normalisation (features were used 'as is'), (2) min–max normalisation and (3) Z-score normalisation.

Fig. 4 shows the scatter plots of the first two PCA/LDA components computed on the concatenation of real and imaginary part of the impedance with no normalisation.

1.4. Machine learning SOC prediction model training and scoring

We tested the ability of machine learning methods to predict battery SOC from the sets of features and data normalisation methods described in Section 1.3. To this end, we considered three classification models: Gaussian Naïve Bayes (Gaussian NB), k-Nearest Neighbours (k-NN) and Linear Support Vector Classifier (lSVC). Search spaces for hyperparameter optimisation were: $k \in \{1, 2, 3\}$ (number of neighbours) for k-NN; $C = \{0.01, 0.1, 1.0, 10.0\}$ (penalty factor) and $max\_iter = 10^4$ (maximum number of iterations) for the lSVC. Accuracy estimation was based on leave-one-out validation protected for battery ID — that is, we selected one observation at a time as the single-item test set, and collected all the other observations (minus the ones associated with the same battery as the observation to test) into the train set. The process was repeated for all the observations in the dataset. The figure of merit was the fraction of observations correctly classified. The software produces as output a table (Fig. 5) in which each record respectively reports: the type of feature used (field `Feature_extraction_mode`), the data normalisation method (`Feature_normalisation_mode`), the classification model (`Classifier`), the classifier hyperparameters (`Classifier_hyperparameters`), the number of features (`num_features`) and the accuracy (`Accuracy`).

2. Impact

While researchers can perform EIS measurement using dedicated laboratory instruments or a more common source-measure unit [11], the proposed method can be implemented using a impedance measurement system such as [7], that can be embedded in the final deployed product.

LiBEIS became a fundamental piece of our laboratory toolset for measurement on batteries and is used daily by all research group members to collect and analyse impedance data and fit batteries equivalent models. We are using the LiBEIS in our current research project. The software was a fundamental aid for several recently published papers, such as [7,10–14].

LiBEIS allowed for fast data preparation for ML model training and for publication in our open access EIS data repository [10]. Using the data processed with LiBEIS, we developed several SOC estimation methods based on deep neural networks. We are currently developing a low-dimensionality model suitable for implementation in resource constrained situations.

The automatic machine learning and data transformation features of LiBEIS are powerful tools for data exploration. Moreover, the equivalent circuit fitting and feature extraction methods such as PCA and LDA allow for model dimensionality reduction and enable the usage of simple classic ML algorithms for regression and classification tasks.

3. Limitation

The current version of the software accepts input voltage and current time series measurements only as a Matlab data file. Support for other file formats (such as CSV) should be added in next versions. The model fitting feature supports the equivalent circuit model in Fig. 3 among several possible models proposed in the literature. Support for different models will be added in future versions.

	Feature_extraction_mode	Feature_normalisation_mode	Classifier	Classifier_hyperparameters	Num_features	Accuracy
95	phase	MinMax	kNN	{'n_neighbors': 1}	14	84.2
81	phase	MinMax	lSVC	{'C': 10.0, 'max_iter': 100000.0}	14	83.8
61	module+phase	MinMax	lSVC	{'C': 10.0, 'max_iter': 100000.0}	28	82.5
21	imag	MinMax	lSVC	{'C': 10.0, 'max_iter': 100000.0}	14	82.5
89	phase	MinMax	kNN	{'n_neighbors': 3}	14	82.1
96	phase	None	kNN	{'n_neighbors': 1}	14	82.1
1	real+imag	MinMax	lSVC	{'C': 10.0, 'max_iter': 100000.0}	28	80.8
92	phase	MinMax	kNN	{'n_neighbors': 2}	14	80.8
90	phase	None	kNN	{'n_neighbors': 3}	14	80.0
35	imag	MinMax	kNN	{'n_neighbors': 1}	14	80.0
82	phase	Z-score	lSVC	{'C': 1.0, 'max_iter': 100000.0}	14	79.6
83	phase	MinMax	lSVC	{'C': 1.0, 'max_iter': 100000.0}	14	79.6
36	imag	None	kNN	{'n_neighbors': 1}	14	79.6
93	phase	None	kNN	{'n_neighbors': 2}	14	79.2
29	imag	MinMax	kNN	{'n_neighbors': 3}	14	79.2
22	imag	Z-score	lSVC	{'C': 1.0, 'max_iter': 100000.0}	14	78.3
97	phase	Z-score	Gaussian NB	None	14	77.9
94	phase	Z-score	kNN	{'n_neighbors': 1}	14	77.9
99	phase	None	Gaussian NB	None	14	77.9
76	module+phase	None	kNN	{'n_neighbors': 1}	28	77.9
98	phase	MinMax	Gaussian NB	None	14	77.9
30	imag	None	kNN	{'n_neighbors': 3}	14	77.5
80	phase	Z-score	lSVC	{'C': 10.0, 'max_iter': 100000.0}	14	77.5
23	imag	MinMax	lSVC	{'C': 1.0, 'max_iter': 100000.0}	14	76.7
20	imag	Z-score	lSVC	{'C': 10.0, 'max_iter': 100000.0}	14	75.4

Fig. 5. Output of the automatic machine learning model training and score functionality of *LiBEIS*.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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