BatteryRateCap: A Python Package for Comparative Battery Rate Capability Analysis

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Software

- Review
- Repository
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Summary

We present a Python package, *BatteryRateCap*, for comparative analysis of insertion electrode batteries across different published datasets. Due to the myriad of battery chemistries and testing procedures that exist today, comparing battery performance across different cell and electrode designs is challenging. To facilitate reuse and integration of published data into new research studies, we need more standardized reporting of datasets, as recently highlighted by battery experts (Mistry et al., 2021; Stephan, 2021; Sun, 2021), and more consistent data analysis procedures along with the corresponding software infrastructure. *BatteryRateCap* is an open-source toolbox aimed at streamlining comparative analysis of different battery datasets while facilitating a more efficient data collection process for future reuse. Our goal is to help promote more rigorous and consistent comparative data analysis in the battery community through our toolbox.

BatteryRateCap analyzes battery rate capability, which focuses on how capacity (the amount of energy in a battery) responds to changing discharge and charge rates (the amount of current applied to a battery). Leveraging the empirical capacity-rate model developed by Tian et al.(Tian et al., 2019), *BatteryRateCap* is an open-source, four-component package that facilitates a systematic workflow for rate capability analysis. First, the feature extraction component uses least-square curve-fitting to tailor battery capacity-rate datasets to Tian et al.'s semi-empirical model (Tian et al., 2019) in order to extract critical fitting parameters. These fitting parameters help normalize battery rate capability across different chemistries and reveal potential rate-limiting factors (Tian et al., 2019). Next, the visualization and the correlation test components aid in discovering patterns between the extracted fitting parameters and the battery's design parameters such as electrode thickness, porosity, particle size, and other material-dependent properties. Finally, a data conversion component converts battery cycling and voltage discharge data to capacity-rate datasets. This data conversion component allows the user to collect datasets (having different formats or units) from various sources to increase a user's available datasets and improve data analysis reliability.

Statement of Need

Batteries are complex devices that are multi-scale and multi-physics in nature. Therefore, batteries are designed, characterized, and reported in various standards and formats based on the focus of each research study. When comparing different batteries, the materials, electrode composition, test conditions, and other design features must be carefully considered. The process to search, collect, and clean up datasets requires significant manual labor and effort.

As a result, reusing battery datasets across multiple publications to conduct a comparative data analysis can be challenging. To facilitate rapid data reuse and integration, the battery community has proposed standardized reporting with several checklist structures (Mistry et al., 2021; Stephan, 2021; Sun, 2021). Carrying through the resolve to foster data-intensive research in the battery community, *BatteryRateCap* is designed to lead the user through a sequential battery rate capability analysis, and *BatteryRateCap* aids in every step from data collection, to feature extraction, and to exploratory data analysis. The ingenuity of *BatteryRateCap* is the capability to organize and characterize various published battery datasets for ease of comparative analysis.

Description

BatteryRateCap has a feature extraction component that characterizes the battery's capacity-rate datasets based on the model proposed by Tian et al. (Tian et al., 2019), as shown in Equation 1:

$$Q = Q_{\max}[1 - (R\tau)^n \left(1 - e^{-(R\tau)^{-n}}\right)] \quad (3)$$

where Q is the measured capacity for an applied current rate, R, in an experiment. The coefficients of the model in Equation (1), i.e. $Q_{\max}$, τ, and n, parameterize the fitting of the model to the capacity-rate datasets. These fitting parameters, the low-rate specific capacity $Q_{\max}$, the characteristic time associated with charge/discharge τ, and the parameter associated with rate-limiting mechanism n, serve as important performance features that characterize the capacity-rate behavior of batteries (Hung et al., 2023; Tian et al., 2019). *BatteryRateCap* extracts these fitting parameters by least-square curve fitting of Equation 1 to the capacity-rate datasets, using the trust region reflective algorithm from SciPy package (Virtanen et al., 2020). Figure 1 demonstrates fitting examples of two capacity-rate datasets using *BatteryRateCap*. In Figure 1, the blue markers are the input capacity-rate data, and the red curve represents the best-fit curve. The optimized fitting parameters with the associated standard errors (SEs) are shown on the plot and tabulated in a separate Excel .csv file. In cases where there are not enough data points from the input to find a best-fit curve, a warning message is shown on the figure instead (see right panel in Figure 1).

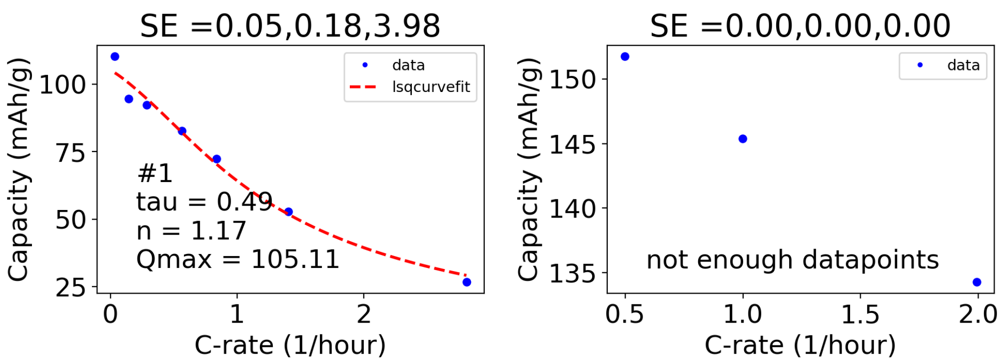

Figure 1: Examples of a successful (left) and unsuccessful (right) curve fitting results in *BatteryRateCap*.

The sparsity of datasets is a major contributor to the difficulty of comparative analysis of batteries. To assist in the collection of capacity-rate datasets, *BatteryRateCap* has a data conversion component that converts two other types of battery datasets – cycling and voltage-capacity datasets – to capacity-rate datasets. This component is built under the premise that battery datasets are often multi-dimensional and contain embedded information that can be harvested and reused on different research subjects. As shown in Figure 2, a cycling dataset demonstrates a battery's capacity values corresponding to changing current rates, where each data point represents the capacity value measured in one charge or discharge cycle at a fixed current rate. Typically, the battery is cycled at a fixed current rate repeatedly before moving on to the next current rate, resulting in the signature 'staircase' pattern. *BatteryRateCap* identifies each stairstep with a different color (see Figure 2) and calculates the average capacity of each stairstep. Then, the cycling dataset is converted to a capacity-rate dataset by pairing the corresponding current rate to each stairstep identified.

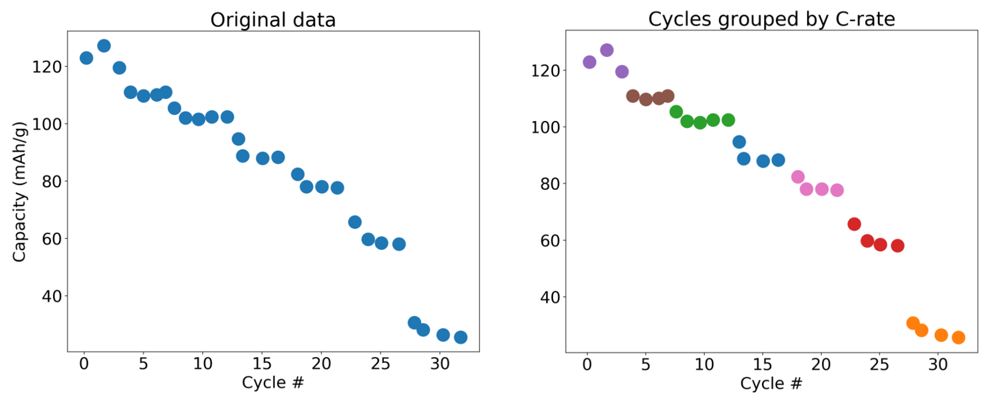

Figure 2: Battery cycling data grouped for conversion to capacity-rate data in *BatteryRateCap*

A similar feature that converts voltage-capacity data to capacity-rate data is available, and a detailed demonstration can be found on the Github repository. Additionally, to allow more integrated postprocessing of the extracted fitting parameters, *BatteryRateCap* has visualization and correlation testing components for basic exploratory data analysis. Demonstrations of these two components are also available in the repository. In summary, *BatteryRateCap* provides an open-source infrastructure and standardized workflow for battery researchers to conduct comparative rate capability analysis following Tian et al's capacity-rate model approach (Tian et al., 2019). In addition, *BatteryRateCap* can be used to collect capacity-rate data reported in voltage capacity and cycling plots. This allows access to the previously embedded and often overlooked capacity-rate datasets. We hope this package helps accelerate more data-intensive work in the community and lays the groundwork for future electrochemical analysis research.

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