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AutoEIS: An automated tool for analysis of electrochemical impedance spectroscopy using evolutionary algorithms and Bayesian inference

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Software

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Summary

AutoEIS is an innovative software tool designed to automate the analysis of Electrochemical Impedance Spectroscopy (EIS) data, a key technique in electrochemical materials research. AutoEIS leverages advanced computational methods, including evolutionary algorithms and Bayesian Inference, to automate the process of constructing and evaluating equivalent circuit models (ECM). This automation provides a significant advancement in the field, allowing for more objective, efficient, and accurate analysis of EIS data compared to traditional manual methods.

In EIS, interpreting the impedance data is required to understand the underlying electrochemical processes, a crucial step in generating mechanistic understanding . However, this interpretation involves selecting an appropriate ECM, a task that can be complex and subjective (Wang et al., 2021). AutoEIS addresses this challenge by providing a systematic approach to ECM selection. It generates a wide array of potential ECMs, evaluates their fit to the EIS data, and ranks them based on a variety of statistical metrics. This process not only streamlines EIS data analysis but also introduces a level of precision and repeatability that manual methods struggle to achieve.

AutoEIS's capabilities have been demonstrated through several case studies, including the analysis of oxygen evolution reaction electrocatalysis, corrosion of multi-principal element alloys, and CO2 reduction in electrolyzer devices (Zhang et al., 2023). These studies highlighted the tool's versatility in handling different electrochemical systems and its effectiveness in identifying ECMs that accurately reflect the electrochemical processes under study.

Statement of need

EIS is a critical technique in various areas of electrochemistry, including battery research, fuel cell development, and corrosion studies. The interpretation of EIS data is pivotal for understanding the mechanisms of electrochemical reactions and material behaviors. However, this interpretation is often challenging due to the complexity of the data and the requirement of expert knowledge in constructing and evaluating ECMs. This complexity can lead to significant time investment and potential bias in EIS analysis.

AutoEIS addresses this gap by providing an automated, user-friendly platform for EIS analysis that does not require extensive prior knowledge of the underlying electrochemical processes. This makes EIS analysis more accessible to a broader range of researchers and professionals in the field. By automating the ECM construction and evaluation process, AutoEIS significantly

reduces the time and effort required for EIS data analysis. It also minimizes the subjectivity inherent in manual ECM selection, leading to more reliable and reproducible results.

There are many open-source tools for EIS data analysis, such as DearEIS (Yrjänä, 2022a), Elchemea Analytical (Koch et al., 2021), impedance.py (Murbach et al., 2020), PyEIS (Knudsen, 2019), and pyimpspec (Yrjänä, 2022b), as well as commercial software like ZView (AMETEK Scientific Instruments), RelaxIS (rhd instruments), and Echem Analyst (Gamry Instruments). However, these tools require the user to feed in an ECM, evaluate its fit to the data, and repeat this process until a satisfactory model is found. This process can be time-consuming and subjective, especially for complex EIS data. AutoEIS addresses this challenge by automating the ECM construction and evaluation process, providing a more objective and efficient approach to EIS data analysis. With the growing interest in developing self-driving laboratories, AutoEIS is a step towards automating the analysis of EIS data, a key technique in electrochemical materials research.

Software Description

AutoEIS comprises four main components:

1. **Data Preprocessing**: It applies techniques like Kramer-Kronig transformations for initial data assessment, ensuring the reliability of EIS data for further analysis.
2. **ECM Generation via Evolutionary Algorithms** : AutoEIS generates a range of ECMs, exploring various configurations to fit the given EIS data. This part is done using the Julia package `EquivalentCircuits.jl` (Van Haeverbeke et al., 2021) via a thin Python wrapper.
3. **Post-filtering of ECMs**: Once candidate ECMs are generated, AutoEIS applies filters based on electrochemical theory to refine the ECM pool, focusing on models that are physically plausible. For instance, models without an ohmic resistor are discarded, as they are not physically realistic.
4. **Bayesian Inference for Model Evaluation**: This step focuses on accurately estimating the most probable values and determining the likely statistical distributions for each individual element within the remaining candidate ECMs using Bayesian inference. The Bayesian approach provides a robust and objective method for evaluating the fit of the models to the data. It also allows for the quantification of uncertainty in the model parameters, providing a more comprehensive understanding of the model's performance.

Authorship Contributions

The original AutoEIS software was developed by RZ. MS conducted a significant refactor of the code base, which improved performance, resulting in a tenfold speed increase compared to the original version. Additionally, MS implemented unit tests, added documentation, and established automated test and deployment workflows. Supervision of the project was provided by JHS. All authors, including RZ, MS, and JHS, contributed to the writing or editing of the manuscript.

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