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AutoEIS: Automated equivalent circuit modeling from electrochemical impedance spectroscopy data using statistical machine learning

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Summary

AutoEIS is an innovative Python software tool designed to automate the analysis of Electrochemical Impedance Spectroscopy (EIS) data, a key technique in electrochemical materials research. By integrating evolutionary algorithms and Bayesian inference, AutoEIS automates the construction and evaluation of equivalent circuit models (ECM), providing more objective, efficient, and accurate analysis compared to traditional manual methods.

EIS data interpretation is fundamental for understanding electrochemical processes and generating mechanistic insights. However, selecting an appropriate ECM has historically been complex, time-consuming, and subjective (Wang et al., 2021). AutoEIS resolves this challenge through a systematic approach: it generates multiple candidate ECMs, evaluates their fit against experimental data, and ranks them using comprehensive statistical metrics. This methodology not only streamlines analysis but also introduces reproducibility and objectivity that manual analysis cannot consistently achieve.

The effectiveness of AutoEIS has been validated through diverse case studies, including oxygen evolution reaction electrocatalysis, corrosion of multi-principal element alloys, and CO~2 reduction in electrolyzer devices (Zhang et al., 2023). These applications demonstrate the software's versatility across different electrochemical systems and its ability to identify physically meaningful ECMs that accurately capture the underlying electrochemical phenomena.

Statement of need

EIS is widely used in electrochemistry for applications spanning battery research, fuel cell development, and corrosion studies. Accurate interpretation of EIS data is essential for understanding electrochemical reaction mechanisms and material behaviors. Traditional EIS analysis faces three significant challenges: it requires substantial expert knowledge, consumes significant time, and introduces potential researcher bias in model selection and interpretation.

AutoEIS addresses these limitations through an automated platform that reduces the expertise barrier for rigorous EIS analysis. By systematically evaluating numerous potential circuit models, the software minimizes human bias and dramatically reduces analysis time. This automation is particularly valuable for complex systems where manual trial-and-error approaches become impractical. Furthermore, this automation capability enables the application of rigorous EIS analysis within high-throughput experimental workflows, where manual approaches become intractable.

Current EIS analysis tools—including open-source options like 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 such as ZView, RelaxIS, and Echem Analyst—all require users to manually propose ECMs and iteratively refine them. This approach becomes increasingly unreliable as system complexity grows, as researchers may not explore the full model space or may unconsciously favor familiar circuit elements.

AutoEIS distinguishes itself by comprehensively exploring the model space through evolutionary algorithms, ensuring that potentially valuable circuit configurations are not overlooked. This capability aligns with the growing trend toward self-driving laboratories and autonomous research workflows in materials science and electrochemistry.

Software description

AutoEIS implements a four-stage workflow to analyze EIS data as shown in Figure 1:

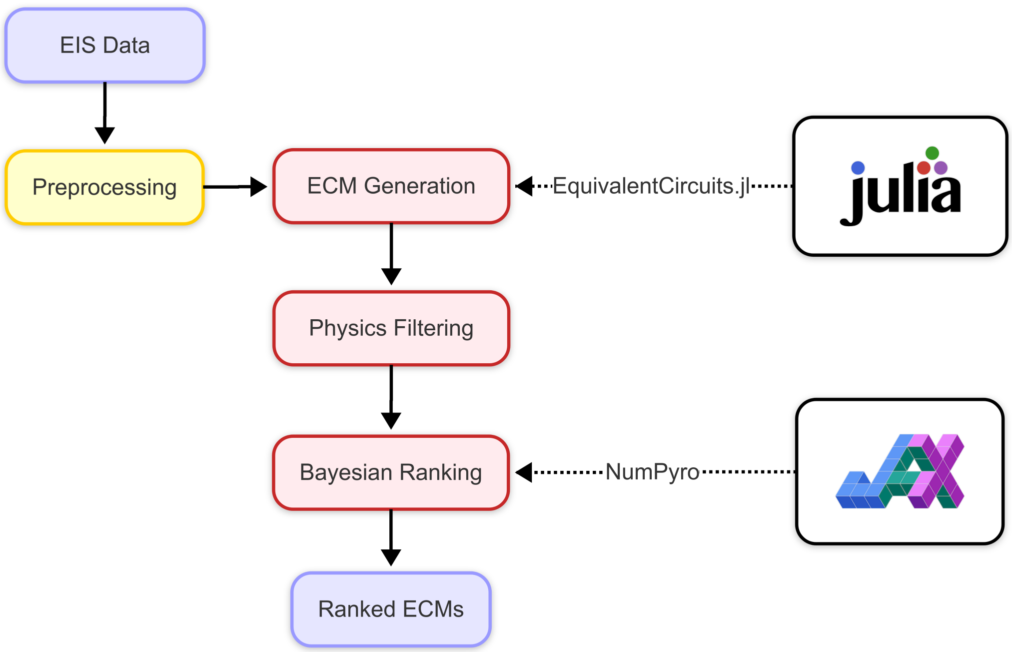

Figure 1: AutoEIS workflow. The four-stage process includes data validation via Kramers-Kronig checks, ECM generation using evolutionary algorithms, filtering based on electrochemical theory, and Bayesian parameter estimation for uncertainty-aware model ranking.

Data preprocessing and validation

Before model fitting, AutoEIS applies Kramers-Kronig transformations (Boukamp, 1995) to validate experimental data quality. This critical step identifies measurement artifacts and ensures that only reliable data proceeds to model fitting. Poor-quality data that violates Kramers-Kronig relations is flagged, allowing researchers to address experimental issues before interpretation.

ECM generation via evolutionary algorithms

AutoEIS employs evolutionary algorithms through the Julia package EquivalentCircuits.jl (Van Haeverbeke et al., 2021) to generate diverse candidate ECMs. This approach efficiently explores the vast space of possible circuit configurations, including models that might not be intuitively chosen by researchers.

Physics-based model filtering

The software then applies electrochemical theory-based filters (Zhang et al., 2023) to eliminate physically implausible models. For example, models lacking an Ohmic resistor are automatically rejected as physically unrealistic, despite potentially good mathematical fits. This step ensures that analysis results remain consistent with established electrochemical principles.

Bayesian parameter estimation

For physically plausible models, AutoEIS employs Bayesian inference to estimate circuit component values and their uncertainty distributions. Unlike point estimates from traditional least-squares fitting, this approach quantifies parameter uncertainty, providing crucial information about model reliability. The Bayesian framework also enables model comparison through metrics like the Bayesian Information Criterion, helping identify the most statistically justified model complexity.

Authorship contributions

The original AutoEIS software was developed by RZ. MS conducted a comprehensive refactoring of the codebase that improved algorithmic efficiency. MS also implemented unit testing, expanded documentation, and established automated CI/CD workflows to ensure software reliability. JHS provided project supervision and domain expertise in electrochemical theory. All authors—RZ, MS, and JHS—contributed substantively to the writing and editing of this manuscript.

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References

Boukamp, B. A. (1995). A linear Kronig-Kramers transform test for immittance data validation. *Journal of the Electrochemical Society*, *142*(6), 1885–1894. https://doi.org/10.1149/1.2044210

Knudsen, K. B. (2019). *kbknudsen/PyEIS: PyEIS: A Python-based electrochemical impedance spectroscopy simulator and analyzer*. Zenodo. https://doi.org/10.5281/zenodo.2535951

Koch, S., Graves, C., Vels Hansen, K., & DTU Energy. (2021). *Elchemea Analytical*. https://www.elchemea.com/

Murbach, M. D., Gerwe, B., Dawson-Elli, N., & Tsui, L. (2020). impedance.py: A Python package for electrochemical impedance analysis. *Journal of Open Source Software*, *5*(52), 2349. https://doi.org/10.21105/joss.02349

Van Haeverbeke, M., Stock, M., & De Baets, B. (2021). Practical equivalent electrical circuit identification for electrochemical impedance spectroscopy analysis with gene expression programming. *IEEE Transactions on Instrumentation and Measurement*, *70*, 1–12. https://doi.org/10.1109/TIM.2021.3113116

Wang, S., Zhang, J., Gharbi, O., Vivier, V., Gao, M., & Orazem, M. E. (2021). Electrochemical impedance spectroscopy. *Nature Reviews Methods Primers*, *1*(1), 41. https://doi.org/10.1038/s43586-021-00039-w

Yrjänä, V. (2022a). DearEIS-a GUI program for analyzing impedance spectra. *Journal of Open Source Software*, *7*(80), 4808. https://doi.org/10.21105/joss.04808

Yrjänä, V. (2022b). *Pyimpspec - python package for electrochemical impedance spectroscopy* (Version 3.2.4). Zenodo. https://doi.org/10.5281/zenodo.7436137

Zhang, R., Black, R., Sur, D., Karimi, P., Li, K., DeCost, B., Scully, J. R., & Hattrick-Simpers, J. (2023). AutoEIS: Automated bayesian model selection and analysis for electrochemical impedance spectroscopy. *Journal of The Electrochemical Society*, *170*(8), 086502. https://doi.org/10.1149/1945-7111/aceab2