AutoEIS: Automated Bayesian Model Selection and Analysis for Electrochemical Impedance Spectroscopy

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1. Introduction

Electrochemical impedance spectroscopy (EIS) is a cornerstone analysis technique for understanding the complex transport processes occurring in electrochemical systems. However, traditional methods of analyzing EIS data such as equivalent circuit models (ECMs) rely on experts' tacit knowledge and thus are prone to subjectivity. This can lead to inconsistent and biased analysis and physical interpretations. To mitigate these concerns, we developed AutoEIS a tool that combines evolutionary algorithms and Bayesian Inference to automatically proposing statistically plausible equivalent circuit models. AutoEIS does this without requiring curated training data and thus can be applied to any electrochemical system in a way that minimizes bias in EIS analysis.

AutoEIS firstly identifies a broad range of candidate ECMs that fit the EIS measurement via an evolutionary algorithms-based exploration. It then evaluates the appropriateness of each ECM based on the information contained in the EIS using Bayesian Inference. These processes allow AutoEIS to detect potential misalignments in EIS-ECM pairs. Such mismatches occur when a given ECM appears to fit well based on standard metrics and intuition but lacks credibility due to insufficient information contained in the EIS data.

Here we validate AutoEIS's ability to identify statistically plausible ECMs across various electrochemical scenarios, ranging from relatively simple systems like oxygen evolution reaction to more complex systems such as carbon dioxide reduction. We further demonstrate that this framework can be used to determine the minimal frequency required to be measured for maintaining the integrity of EIS analysis. It points to a pathway for expediting EIS acquisition by intelligently streamlining low-frequency EIS collection. These results highlight AutoEIS's potential in both in-situ and high-throughput EIS analysis by enabling more efficient data acquisition while preserving analysis reliability.