AI-Guided Optimization of EIS Measurements: Minimizing Low-Frequency Sampling for Data-Efficient Electrochemical Characterization

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1. Introduction

Electrochemical Impedance Spectroscopy (EIS) is a valuable technique that has been widely used in diagnosing a system's underlying reactions or extracting key properties like charge-transfer and kinetic parameters in batteries, electrocatalysis, and energy conversion devices[1]. However, acquiring high-quality EIS data, especially in the low-frequency region, could be quite time-consuming and challenging[2]. The high noise-to-signal ratio exacerbates the challenge of selecting the circuit model mostly aligned with the data[3,4].

In this study, we present a physics-informed framework to enhance the efficiency of EIS measurements by reducing reliance on low-frequency sampling and strategically increasing point density in cleaner, high-frequency regions. Leveraging the AutoEIS software package, we apply Bayesian Inference to fit extra sampled data to a library of known ECMs, estimating both parameters and their uncertainties[5]. By adding extra data points in the high-frequency region, we successfully shift the minimum frequency needed for accurate full-spectrum reconstruction to higher values, thus improving data acquisition efficiency without sacrificing model fidelity and minimizing the engagement with noisy low-frequency data.

We validate our method on both synthetic and experimental datasets, including a single Randles circuit modelling the oxygen evolution reaction (OER) and a more complex two-Randles configuration derived from CO_2 reduction systems. In all cases, the framework preserves or improves reconstruction quality while reducing dependence on noisy, instrument-limited low-frequency data. Notably, in the two-Randles scenario, we identify a threshold, which is related to the relative ratio of the two semicircles, beyond which accurate inference is no longer feasible without direct low-frequency sampling. This finding highlights the importance of understanding when partial measurement becomes insufficient.

2. Methodology

We developed a systematic framework to determine the minimum frequency required to reconstruct full EIS spectra while maintaining model fidelity, noted as critical frequency (f_c)[6].

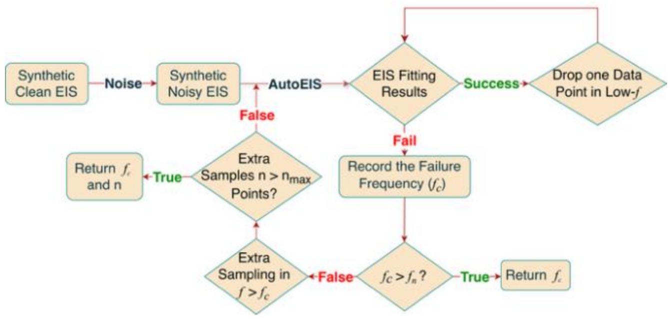

Fig. 1: The overall process for f_c determination in synthetic noisy EIS using iterative Bayesian Inference and data densification

2.1 Data Synthesis and Noise Modeling

Clean synthetic EIS data were generated from simplified experimental ECMs. We then introduced composite noise to simulate instrument-limited distortions, establishing a ground truth for evaluating parameter identifiability under noisy conditions.

2.2 Iterative Identification of f_c

Using the AutoEIS package, we apply Bayesian Inference (BI) to the spectra and iteratively reduce the frequency range:

- Fitting: The spectrum is fitted via BI to obtain parameter posteriors and fitting quality metrics.
- Truncation: If the fit meets the quality criteria, the lowest frequency point is removed, and the fit is reperformed.

- Thresholding: The process terminates when the fitting fails, defining the last successful frequency as f_c.

2.3 High-Frequency Data Augmentation

If f_c exceeds the noisy frequency boundary (f_n), the framework strategically adds extra sampling points in the cleaner, high-frequency region. The iterative fitting is repeated with this augmented data until the model reaches stability or the number of extra points reaches n_{max}.

3. Results and Discussion

3.1 Proof of Concept: Critical Frequency Shifts

We first validated the hypothesis that high-frequency data augmentation can compensate for missing low-frequency information. As shown in the two-Randles circuit example (Fig. 2), a fitting that initially failed at 9.1 Hz was successfully rectified after adding 15 extra data points in the high-frequency region. This confirms that increasing high-frequency density shifts the critical frequency (f_c) to higher values, reducing the need for noisy low-frequency data.

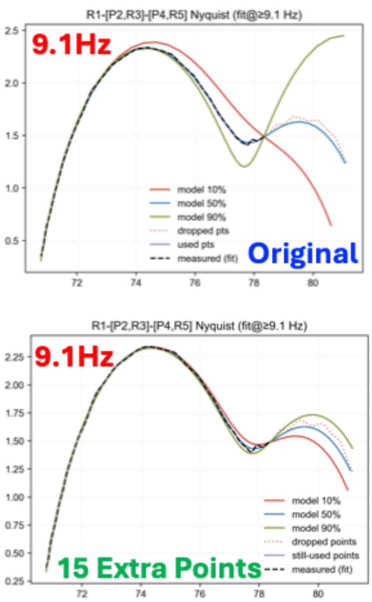

Fig. 2: Example of critical frequency shifts in a two-Randle-Circuit ECM: adding 15 extra data points in the high-frequency region enables successful reconstruction at 9.1 Hz.

3.2 Impact of Noise and Sampling Density

A systematic study across five noise levels (1%–5%) and varying sampling densities (1, 3, 7, 15 points) revealed several key trends:

- Noise Sensitivity: Higher noise levels lead to a smaller f_c, as increased signal distortion makes it significantly more difficult for the Bayesian framework to infer the full spectrum from limited data.

- Non-linear Gains: The shift in f_c does not follow a linear relationship with the number of added points.

- Diminishing Returns: The rate of improvement in f_c slows significantly after adding more than 7 points, particularly in low-noise scenarios. This indicates an upper limit where additional sampling no longer yields meaningful shifts in the critical frequency.

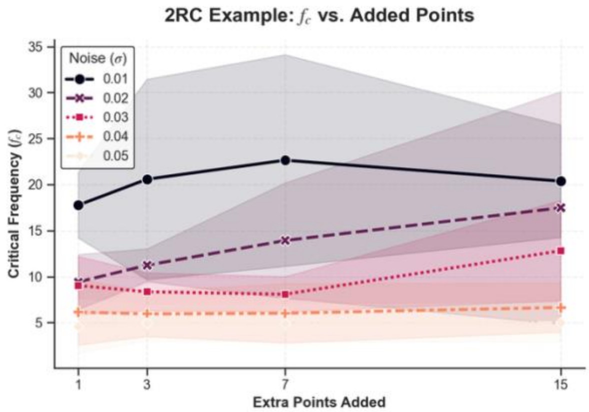

Fig. 3: Comparative analysis of critical frequency shifts across varying noise levels (1%–5%) and sampling densities (n = 1, 3, 7, 15).

4. Conclusion

This study introduces a physics-informed framework that optimizes EIS characterization by leveraging Bayesian Inference and strategic high-frequency sampling. By quantitatively defining the critical frequency f_c, we provide a method to minimize engagement with noisy low-frequency data without sacrificing model fidelity. Our findings offer a scalable blueprint for accelerating electrochemical diagnostics in batteries and energy conversion systems.

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