pyECRtools version 0.07

User's Guide

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30 December 2024

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2 Introduction to pyECRtools

pyECRtools is a tool to analyze data obtained using electrical conductivity relaxation (ECR). It is a Python-based toolbox for:

1. Plotting and analyzing ECR data.
2. Extracting surface exchange coefficients (k) and diffusion coefficients (D) from ECR data.
3. Assessing the quality of the fit through posterior asymptotic confidence regions.
4. Establishing the sensitivity of ECR measurements.

The functionalities of pyECRtools are now accessible through Python scripts (demos), enabling a streamlined and flexible approach.

2.1 Where can you find pyECRtools?

The ECRTOOLS can be freely downloaded from https://github.com/ciuccislab/pyECRtools/

2.2 How do you get support?

Please email francesco.ciucci@uni-bayreuth.de, and I will respond as promptly as possible.

2.3 How do you cite pyECRtools?

Please cite:

1. Francesco Ciucci. Electrical conductivity relaxation measurements: Statistical investigations using sensitivity analysis, optimal experimental design and ECRTOOLS. Solid State Ionics. Volume 239, 15 May 2013, Pages 28-40 https://doi.org/10.1016/j.ssi.2013.03.020
2. Ting Hei Wan, Mattia Saccoccio, Chi Chen, and Francesco Ciucci. Assessing the identifiability of k and D in electrical conductivity relaxation via analytical results and nonlinearity estimates. Solid State Ionics. Volume 270, February 2015, Pages 18-32. https://doi.org/10.1016/j.ssi.2014.11.026
3. Mohammed B. Effat, Emanuele Quattrocchi, Ting Hei Wan, Mattia Saccoccio, Alessio Belotti, and Francesco Ciucci. *Electrical Conductivity Relaxation in the Nonlinear Regime*. Journal of The Electrochemical Society. Volume 164, Number 14, December 2017, Pages F1671. https://doi.org/10.1149/2.1241714jes

2.4 How do you install pyECRtools?

pyECRtools operates in Python. To set it up I recommend using Anaconda https://anaconda.org/ through the following steps

- clone or download the pyECRTOOLS repository from https://github.com/ciuccislab/pyECRtools/

in terminal

- conda create -n ECR matplotlib scipy spyder
- conda activate ECR
- add the pyECRTOOLS directory to your Python path or navigate to the directory when running scripts

3 Demos

3.1 Demo 1: Generating Exact and Synthetic ECR Responses

Demo 1 demonstrates how to use the Python script `demo_1.py` to generate exact and synthetic ECR responses. The synthetic response incorporates Gaussian noise, representing experimental errors.

Usage:

Run the script:

```
python -m demos.demo_1
```

Output: a plot showing the exact normalized conductivity response and the synthetic noisy data points.

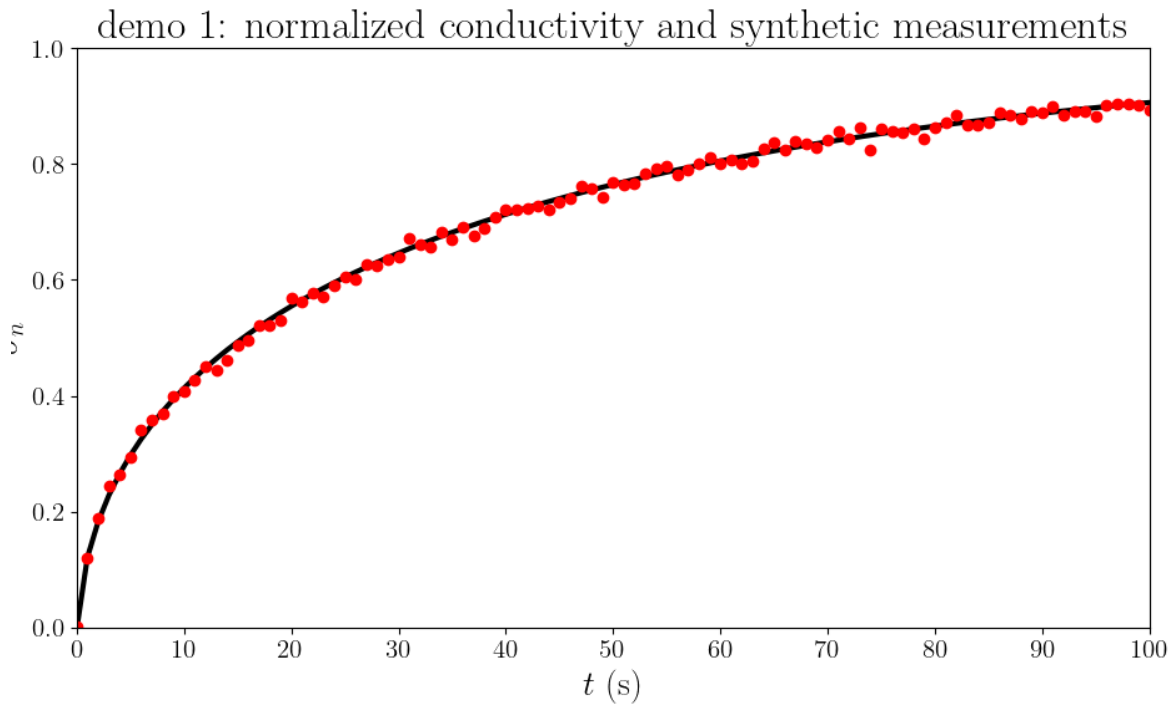

Figure 1 – Normalized conductivity plot.

3.2 Demo 2: Computing the Sensitivity of ECR

Demo 2 explores the sensitivity of the ECR response with respect to the parameters k and D. Sensitivity is crucial for evaluating experimental design quality.

Usage:

Run the script:

```
python -m demos.demo_2
```

Output: a plot showing the sensitivity curves for *k* and *D*.

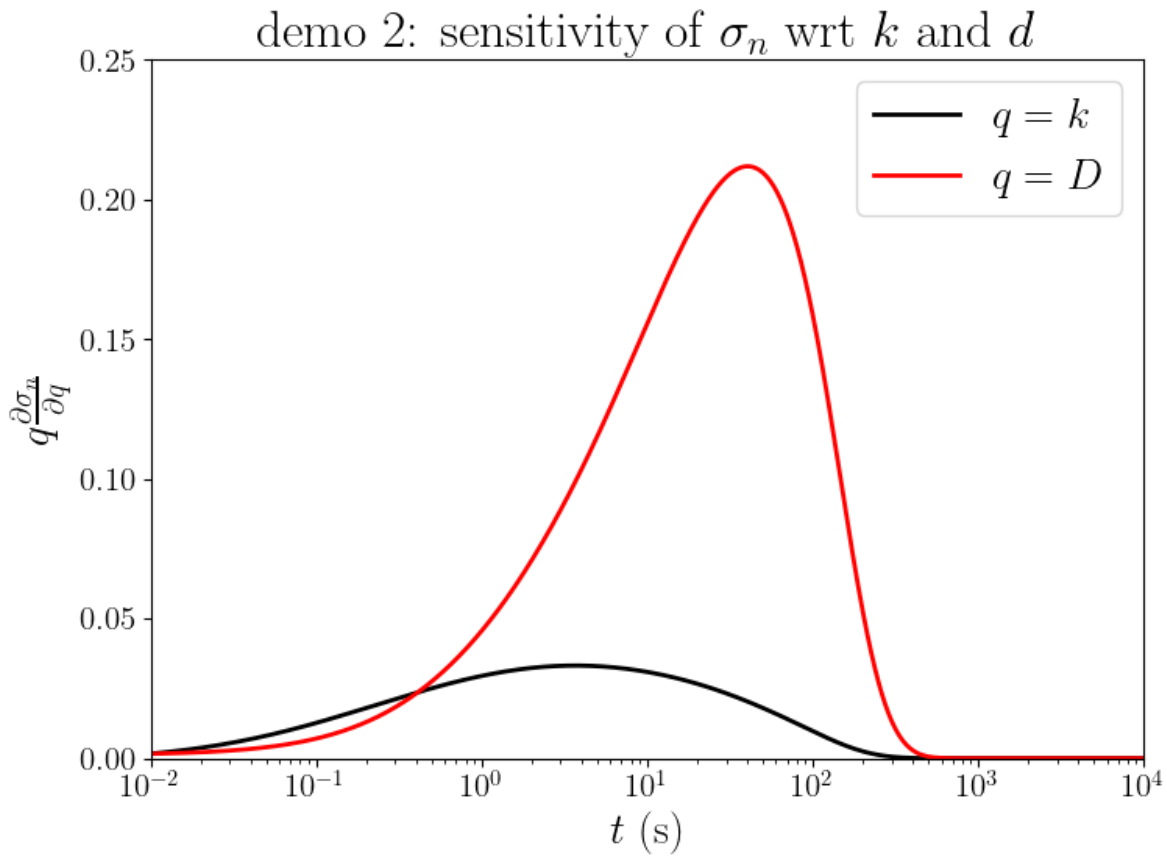

Figure 2 – Sensitivity plot.

3.3 Demo 3: Computing Asymptotic Confidence Regions and Other Parameters for Optimization

Demo 3 calculates various properties of the asymptotic covariance matrix, such as its determinant and maximum eigenvalue.

Usage:

Run the script:

```
python -m demos.demo_3
```

Output: Plots illustrating various indicators of the asymptotic confidence region characteristics.

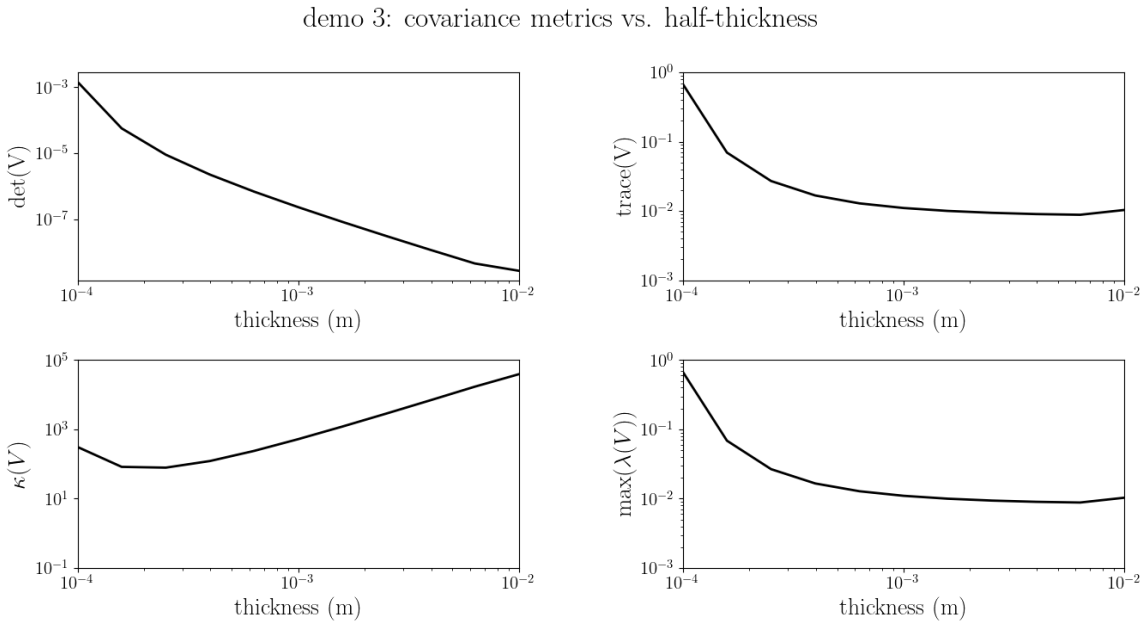

Figure 3 – Determinant, trace, condition value, and max eigenvalue of the asymptotic covariance matrix.

3.4 Demo 4: Fitting ECR Data

Demo 4 fits experimental ECR data to estimate k and D, along with confidence intervals and residuals.

Usage:

Run the script:

```
python -m demos.demo_4
```

Output: A plot comparing experimental data, fitted results, and residuals. And a pictorial view of the asymptotic covariance matrix.

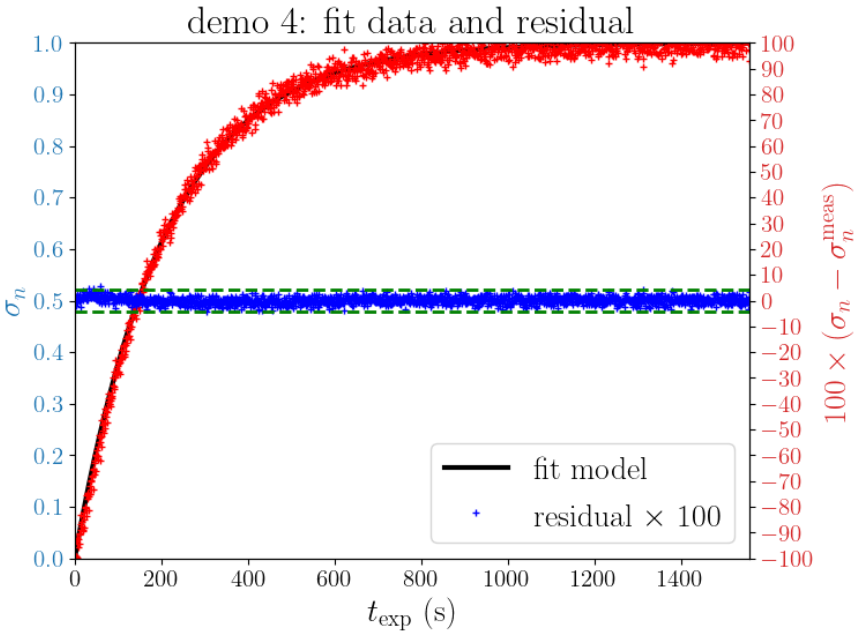

Figure 4 – Fitted data and residual.

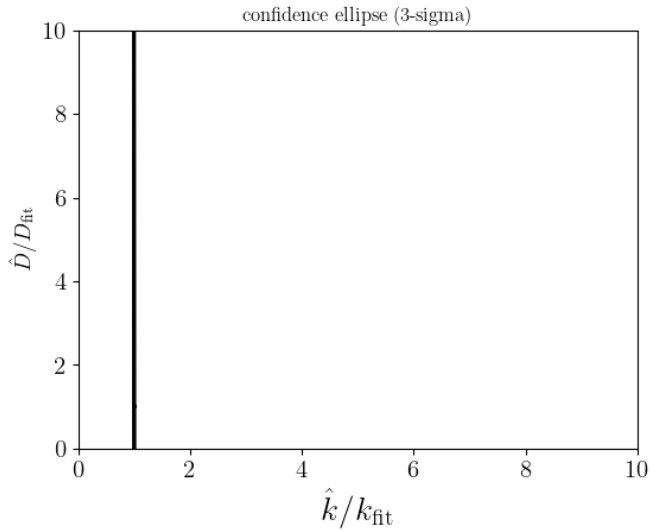

Figure 5 – Asymptotic confidence ellipse.

3.5 Demo 5: Fitting ECR Data Using Various Methods

Demo 5 demonstrates the fitting of ECR data using a range of methods to estimate k and D, evaluate residuals, and compute confidence intervals.

Usage:

Run the script:

```
python -m demos.demo_5
```

Outputs Plot comparing experimental data, fitted results, and residuals obtained using various method

A visualization of the asymptotic confidence region for the parameters.

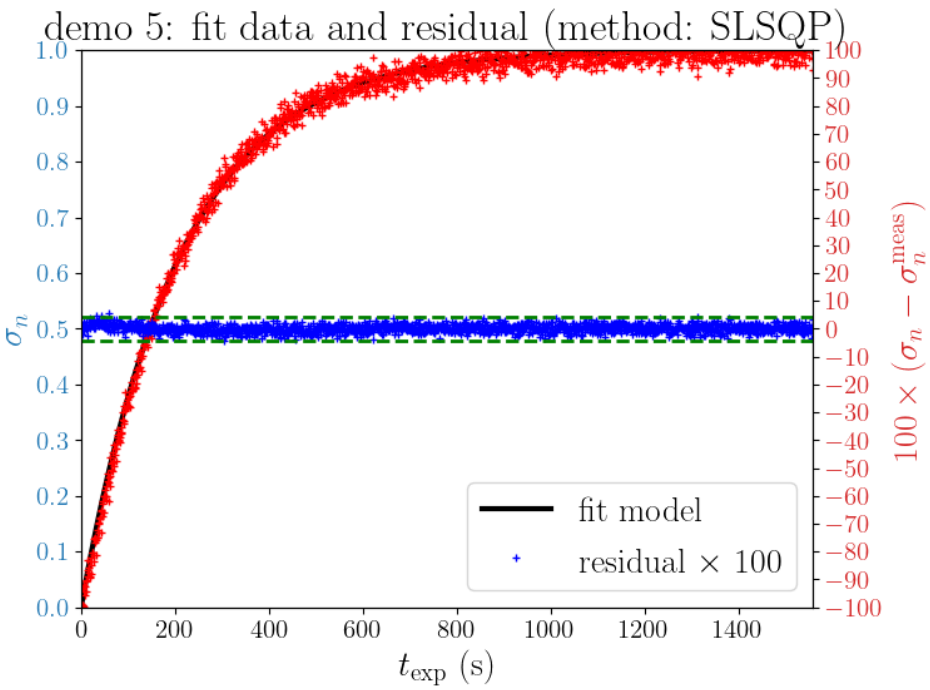

Figure 6 – Fitted data and residual using the SLSQP method.

3.6 Demo 6: Running Synthetic Experiments

Demo 6 simulates synthetic experiments and fits them to evaluate model accuracy and confidence.

Usage:

Run the script:

```
python -m demos.demo_6
```

Output: Synthetic experiment results and asymptotic confidence region.

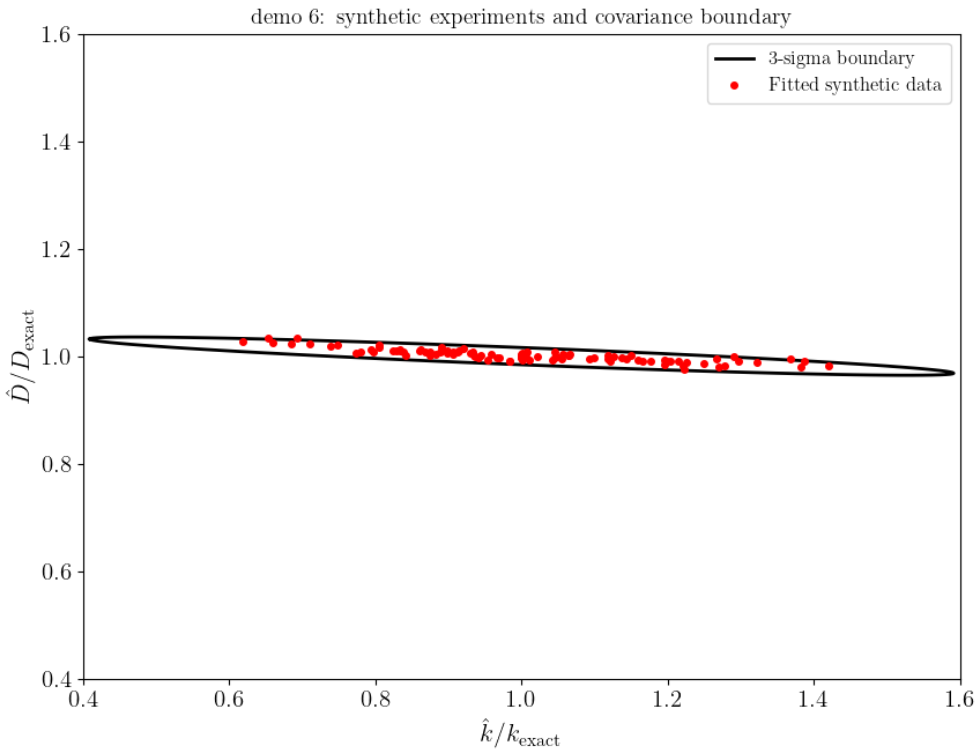

Figure 7 – Synthetic experiment results and asymptotic confidence ellipse.