
impedance.py Documentation

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`impedance.py` is a Python package for making electrochemical impedance spectroscopy (EIS) analysis reproducible and easy-to-use.

Aiming to create a consistent, [scikit-learn-like API](#) for impedance analysis, `impedance.py` contains modules for data preprocessing, validation, model fitting, and visualization.

If you have a feature request or find a bug, please [file an issue](#) or, better yet, make the code improvements and [submit a pull request](#)! The goal is to build an open-source tool that the entire impedance community can improve and use!

CHAPTER 1

Installation

The easiest way to install `impedance.py` is from [PyPI](#) using `pip`:

```
pip install impedance
```

See [Getting started with *impedance.py*](#) for instructions on getting started from scratch.

1.1 Dependencies

`impedance.py` requires:

- Python (≥ 3.7)
- SciPy (≥ 1.0)
- NumPy (≥ 1.14)
- Matplotlib (≥ 3.0)
- Altair (≥ 3.0)

Several example notebooks are provided in the `examples/` directory. Opening these will require Jupyter notebook or Jupyter lab.

Examples and Documentation

Getting started with impedance.py contains a detailed walk through of how to get started from scratch. If you're already familiar with Jupyter/Python, several examples can be found in the `examples/` directory (*Fitting impedance spectra* is a great place to start). The documentation can be found at impedancepy.readthedocs.io.

2.1 Getting started with `impedance.py`

`impedance.py` is a Python package for analyzing electrochemical impedance spectroscopy (EIS) data. The following steps will show you how to get started analyzing your own data using `impedance.py` in a Jupyter notebook.

Hint: If you get stuck or believe you have found a bug, please feel free to open an [issue on GitHub](#).

2.1.1 Step 1: Installation

If you already are familiar with managing Python packages, feel free to skip straight to *Installing packages*. Otherwise, what follows is a quick introduction to the Python package ecosystem:

Installing Miniconda

One of the easiest ways to get started with Python is using Miniconda. Installation instructions for your OS can be found at <https://conda.io/miniconda.html>.

After you have installed conda, you can run the following commands in your Terminal/command prompt/Git BASH to update and test your installation:

1. Update conda's listing of packages for your system: `conda update conda`
2. Test your installation: `conda list`

For a successful installation, a list of installed packages appears.

3. Test that Python 3 is your default Python: `python -V`

You should see something like Python 3.x.x :: Anaconda, Inc.

You can interact with Python at this point, by simply typing `python`.

Setting up a conda environment

(*Optional*) It is recommended that you use virtual environments to keep track of the packages you've installed for a particular project. Much more info on how conda makes this straightforward is given [here](#).

We will start by creating an environment called `impedance-analysis` which contains all the Python base distribution:

```
conda create -n impedance-analysis python=3
```

After conda creates this environment, we need to activate it before we can install anything into it by using:

```
conda activate impedance-analysis
```

We've now activated our conda environment and are ready to install `impedance.py`!

Installing packages

The easiest way to install `impedance.py` and its dependencies (`scipy`, `numpy`, and `matplotlib`) is from [PyPI](#) using `pip`:

```
pip install impedance
```

For this example we will also need Jupyter Lab which we can install with:

```
conda install jupyter jupyterlab
```

We've now got everything in place to start analyzing our EIS data!

Note: The next time you want to use this same environment, all you have to do is open your terminal and type `conda activate impedance-analysis`.

Open Jupyter Lab

(*Optional*) Create a directory in your documents folder for this example:

```
mkdir ~/Documents/impedance-example  
cd ~/Documents/impedance-example
```

Next, we will launch an instance of Jupyter Lab:

```
jupyter lab
```

which should open a new tab in your browser. A tutorial on Jupyter Lab from the Electrochemical Society HackWeek can be found [here](#).

Tip: The code below can be found in the `getting-started.ipynb` notebook

2.1.2 Step 2: Import your data

This example will assume the following dataset is located in your current working directory (feel free to replace it with your data): `exampleData.csv`

For this dataset, importing the data looks something like:

```
from impedance import preprocessing

# Load data from the example EIS result
frequencies, Z = preprocessing.readCSV('./exampleData.csv')

# keep only the impedance data in the first quadrant
frequencies, Z = preprocessing.ignoreBelowX(frequencies, Z)
```

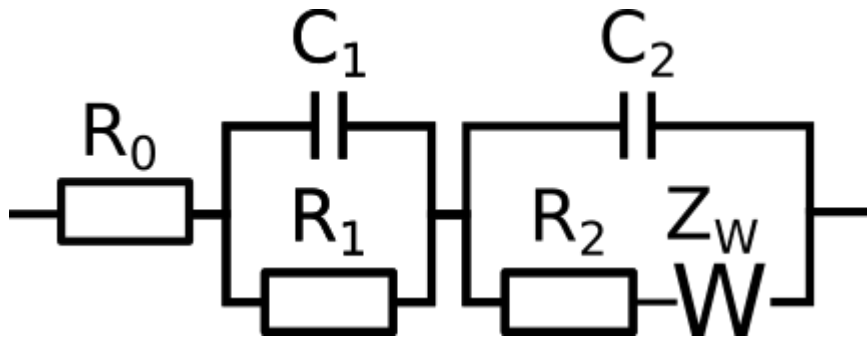
Tip: Functions for reading in files from a variety of vendors (ZPlot, Gamry, Parstat, Autolab, ...) can be found in the `preprocessing` module!

2.1.3 Step 3: Define your impedance model

Next we want to define our impedance model. In order to enable a wide variety of researchers to use the tool, `impedance.py` allows you to define a custom circuit with any combination of [circuit elements](#).

The circuit is defined as a string (i.e. using `'` in Python), where elements in series are separated by a dash (`-`), and elements in parallel are wrapped in a `p(,)`. Each element is defined by the function (in [circuit-elements.py](#)) followed by a single digit identifier.

For example, the circuit below:



would be defined as `R0-p(R1,C1)-p(R2-Wo1,C2)`.

Each circuit, we want to fit also needs to have an initial guess for each of the parameters. These initial guesses are passed in as a list in order the parameters are defined in the circuit string. For example, a good guess for this battery data is `initial_guess = [.01, .01, 100, .01, .05, 100, 1]`.

We create the circuit by importing the `CustomCircuit` object and passing it our circuit string and initial guesses.

```
from impedance.models.circuits import CustomCircuit

circuit = 'R0-p(R1,C1)-p(R2-Wo1,C2)'
initial_guess = [.01, .01, 100, .01, .05, 100, 1]

circuit = CustomCircuit(circuit, initial_guess=initial_guess)
```

2.1.4 Step 4: Fit the impedance model to data

Once we've defined our circuit, fitting it to impedance data is as easy as calling the `.fit()` method and passing it our experimental data!

```
circuit.fit(frequencies, Z)
```

We can access the fit parameters with `circuit.parameters_` or by printing the circuit object itself, `print(circuit)`.

2.1.5 Step 5: Analyze/Visualize the results

For this dataset, the resulting fit parameters are

Parameter	Value
R_0	1.65e-02
R_1	8.68e-03
C_1	3.32e+00
R_2	5.39e-03
$Wo_{1,0}$	6.31e-02
$Wo_{1,1}$	2.33e+02
C_2	2.20e-01

We can get the resulting fit impedance by passing a list of frequencies to the `.predict()` method.

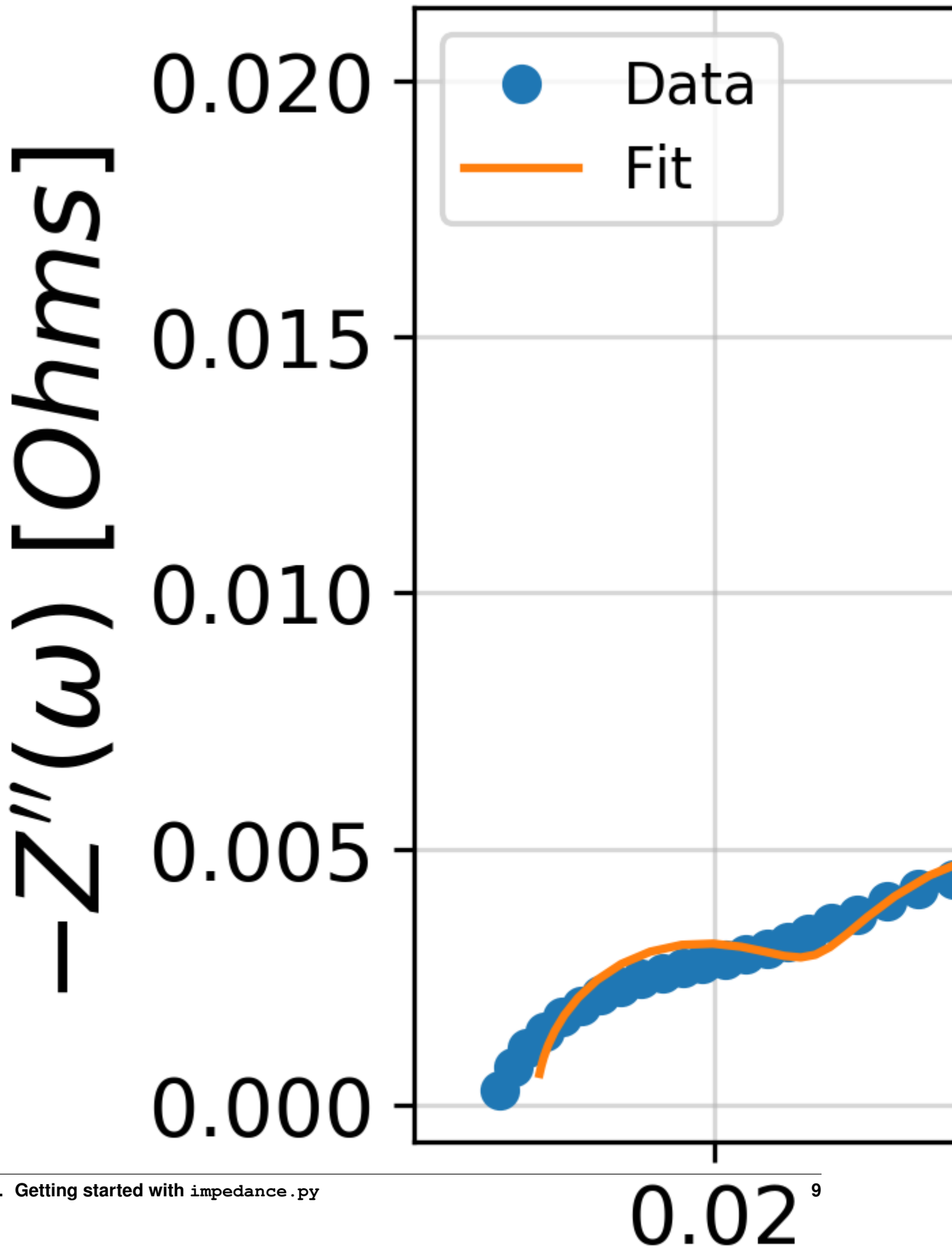
```
Z_fit = circuit.predict(frequencies)
```

To easily visualize the fit, the `plot_nyquist()` function can be handy.

```
import matplotlib.pyplot as plt
from impedance.visualization import plot_nyquist

fig, ax = plt.subplots()
plot_nyquist(ax, Z, fmt='o')
plot_nyquist(ax, Z_fit, fmt='-')

plt.legend(['Data', 'Fit'])
plt.show()
```



Important: Congratulations! You're now up and running with impedance.py

2.2 Examples

2.2.1 Fitting impedance spectra

1. Import and initialize equivalent circuit(s)

To begin we will import the Randles' circuit and a custom circuit from the impedance package. A full list of currently available circuits are available in the [documentation](#).

```
[1]: import sys
     sys.path.append('../..')

     from impedance.models.circuits import Randles, CustomCircuit
```

The classes we just imported represent different equivalent circuit models. To actually use them we want to initialize a specific instance and provide an initial guess for the parameters and any other options.

E.g. for the randles circuit, one of the options is for a constant phase element (CPE) instead of an ideal capacitor.

```
[2]: randles = Randles(initial_guess=[.01, .005, .1, .001, 200])
     randlesCPE = Randles(initial_guess=[.01, .005, .1, .9, .001, 200], CPE=True)
```

Defining the custom circuit works a little differently. Here we pass a string comprised of the circuit elements grouped either in series (separated with a `-`) or in parallel (using the form `p(X, Y)`). Each element can be appended with an integer (e.g. `R0`) or an underscore and an integer (e.g. `CPE_1`) to make keeping track of multiple elements of the same type easier.

```
[3]: customCircuit = CustomCircuit(initial_guess=[.01, .005, .1, .005, .1, .001, 200],
     circuit='R_0-p(R_1,C_1)-p(R_2,C_2)-Wo_1')
```

As of version 0.4, you can now specify values you want to hold constant. For example,

```
[4]: customConstantCircuit = CustomCircuit(initial_guess=[None, .005, .1, .005, .1, .001, 200],
     constants={'R_0': 0.02, 'Wo_1_1': 200},
     circuit='R_0-p(R_1,C_1)-p(R_2,C_2)-Wo_1')
```

Each of the circuit objects we create can be printed in order to see the properties that have been defined for that circuit.

```
[5]: print(customConstantCircuit)

Circuit string: R_0-p(R_1,C_1)-p(R_2,C_2)-Wo_1
Fit: False

Constants:
  R_0 = 2.00e-02 [Ohm]
  Wo_1_1 = 2.00e+02 [sec]

Initial guesses:
  R_1 = 5.00e-03 [Ohm]
```

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```

C_1 = 1.00e-01 [F]
R_2 = 5.00e-03 [Ohm]
C_2 = 1.00e-01 [F]
Wo_1_0 = 1.00e-03 [Ohm]

```

2. Formulate data

Several convenience functions for importing data exist in the `impedance.preprocessing` module, including one for reading simple `.csv` files where frequencies are stored in the first column, real parts of the impedance are in the second column, and imaginary parts of the impedance are in the third column.

```

[6]: from impedance import preprocessing

frequencies, Z = preprocessing.readCSV('../.../data/exampleData.csv')

# keep only the impedance data in the first quadrant
frequencies, Z = preprocessing.ignoreBelowX(frequencies, Z)

```

3. Fit the equivalent circuits to a spectrum

Each of the circuit classes has a `.fit()` method which finds the best fitting parameters.

After fitting a circuit, the fit parameters rather than the initial guesses are shown when printing.

```

[7]: randles.fit(frequencies, Z)
randlesCPE.fit(frequencies, Z)
customCircuit.fit(frequencies, Z)
customConstantCircuit.fit(frequencies, Z)

print(customConstantCircuit)

Circuit string: R_0-p(R_1,C_1)-p(R_2,C_2)-Wo_1
Fit: True

Constants:
  R_0 = 2.00e-02 [Ohm]
  Wo_1_1 = 2.00e+02 [sec]

Initial guesses:
  R_1 = 5.00e-03 [Ohm]
  C_1 = 1.00e-01 [F]
  R_2 = 5.00e-03 [Ohm]
  C_2 = 1.00e-01 [F]
  Wo_1_0 = 1.00e-03 [Ohm]

Fit parameters:
  R_1 = 6.79e-03 (+/- 1.08e-03) [Ohm]
  C_1 = 5.62e+00 (+/- 1.96e+00) [F]
  R_2 = 3.91e-03 (+/- 1.09e-03) [Ohm]
  C_2 = 1.36e+00 (+/- 2.61e-01) [F]
  Wo_1_0 = 5.88e-02 (+/- 1.25e-03) [Ohm]

```

4a. Predict circuit model and visualize with matplotlib

```
[8]: import matplotlib.pyplot as plt
from impedance.visualization import plot_nyquist

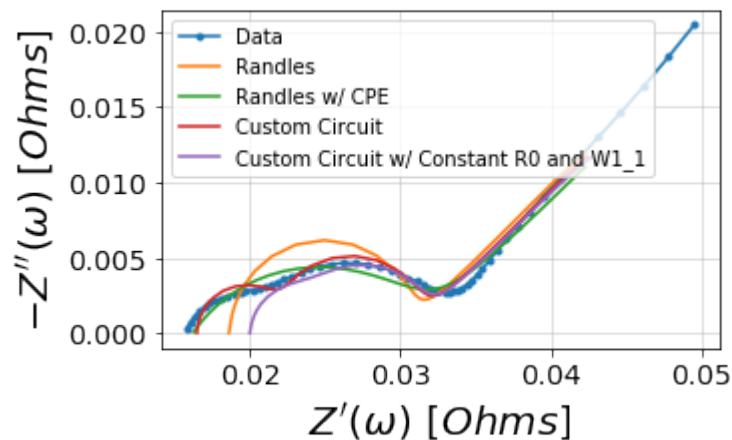
f_pred = np.logspace(5,-2)

randles_fit = randles.predict(f_pred)
randlesCPE_fit = randlesCPE.predict(f_pred)
customCircuit_fit = customCircuit.predict(f_pred)
customConstantCircuit_fit = customConstantCircuit.predict(f_pred)

fig, ax = plt.subplots(figsize=(5,5))

plot_nyquist(ax, Z)
plot_nyquist(ax, randles_fit, fmt='-')
plot_nyquist(ax, randlesCPE_fit, fmt='-')
plot_nyquist(ax, customCircuit_fit, fmt='-')
plot_nyquist(ax, customConstantCircuit_fit, fmt='-')

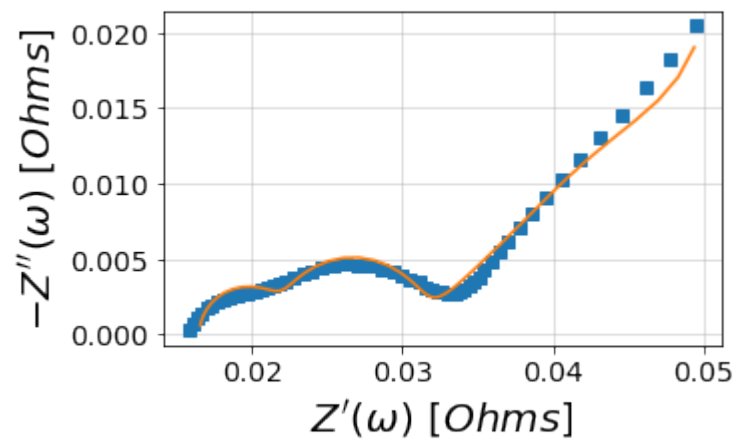
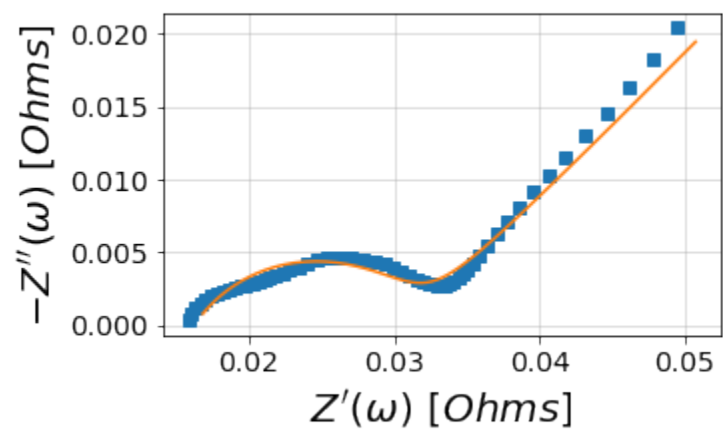
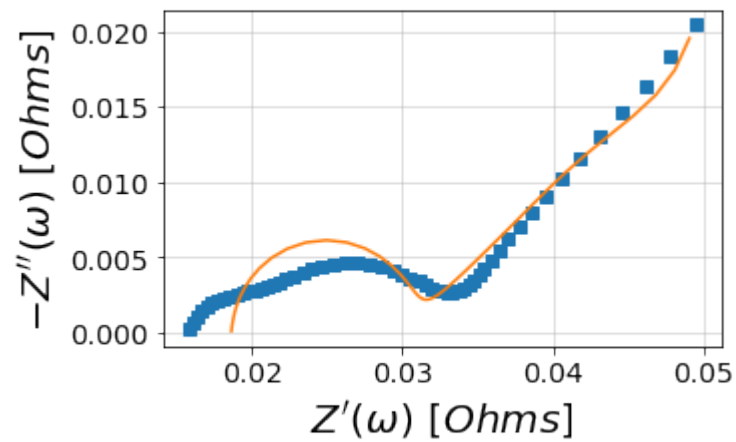
ax.legend(['Data', 'Randles', 'Randles w/ CPE', 'Custom Circuit', 'Custom Circuit w/
↳ Constant R0 and W1_1'])
plt.show()
```

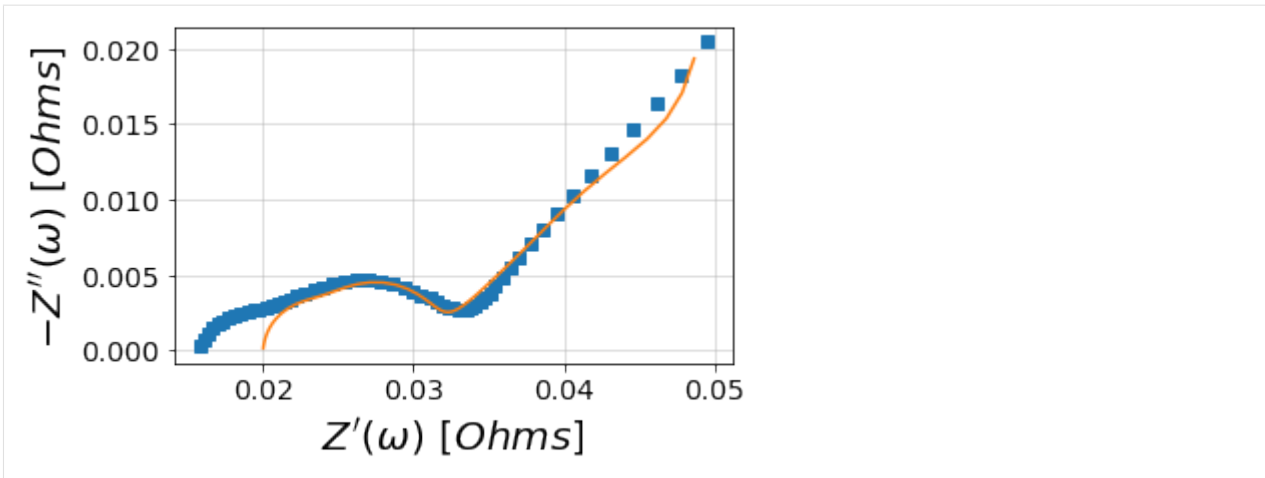


4b. Or use the convenient plotting method included in the package

```
[9]: randles.plot(f_data=frequencies, Z_data=Z, kind='nyquist')
randlesCPE.plot(f_data=frequencies, Z_data=Z, kind='nyquist')
customCircuit.plot(f_data=frequencies, Z_data=Z, kind='nyquist')
customConstantCircuit.plot(f_data=frequencies, Z_data=Z, kind='nyquist')

plt.show()
```



2.2.2 Visualizing impedance spectra

Plotting a basically formatted impedance plot is as easy as 1, 2, 3...

```
[1]: import matplotlib.pyplot as plt
import numpy as np

import sys
sys.path.append('../..')

from impedance.models.circuits import CustomCircuit
from impedance import preprocessing
```

1. Read in data

```
[2]: frequencies, Z = preprocessing.readCSV('../..//data/exampleData.csv')

# keep only the impedance data in the first quadrant
frequencies, Z = preprocessing.ignoreBelowX(frequencies, Z)
```

2. Fit a custom circuit

(If you want to just plot experimental data without fitting a model you should check out the `visualization.plot_*` functions)

```
[3]: circuit = CustomCircuit(initial_guess=[.01, .005, .1, .005, .1, .001, 200], circuit=
    ↪ 'R_0-p(R_1,C_1)-p(R_1,C_1)-Wo_1')

circuit.fit(frequencies, Z)

print(circuit)

Circuit string: R_0-p(R_1,C_1)-p(R_1,C_1)-Wo_1
Fit: True
```

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```

Initial guesses:
  R_0 = 1.00e-02 [Ohm]
  R_1 = 5.00e-03 [Ohm]
  C_1 = 1.00e-01 [F]
  R_1 = 5.00e-03 [Ohm]
  C_1 = 1.00e-01 [F]
  Wo_1_0 = 1.00e-03 [Ohm]
  Wo_1_1 = 2.00e+02 [sec]

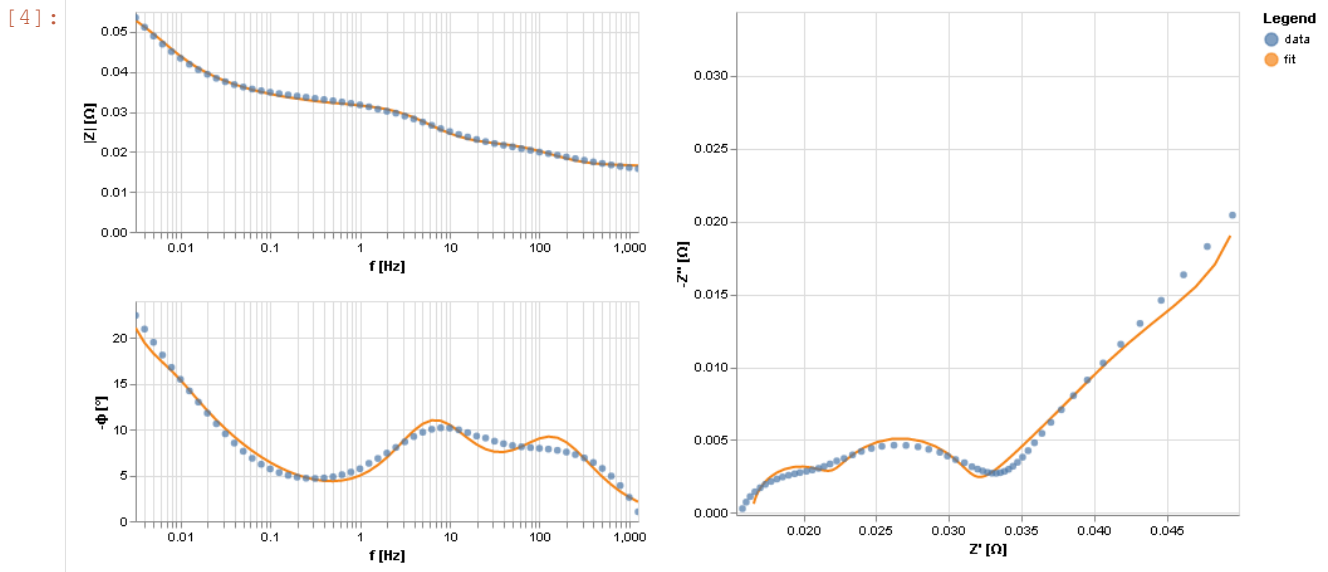
Fit parameters:
  R_0 = 1.65e-02 (+/- 1.54e-04) [Ohm]
  R_1 = 8.77e-03 (+/- 1.89e-04) [Ohm]
  C_1 = 3.28e+00 (+/- 1.85e-01) [F]
  R_1 = 5.31e-03 (+/- 2.06e-04) [Ohm]
  C_1 = 2.32e-01 (+/- 1.90e-02) [F]
  Wo_1_0 = 6.37e-02 (+/- 2.03e-03) [Ohm]
  Wo_1_1 = 2.37e+02 (+/- 1.72e+01) [sec]

```

3. Plot the data and fit

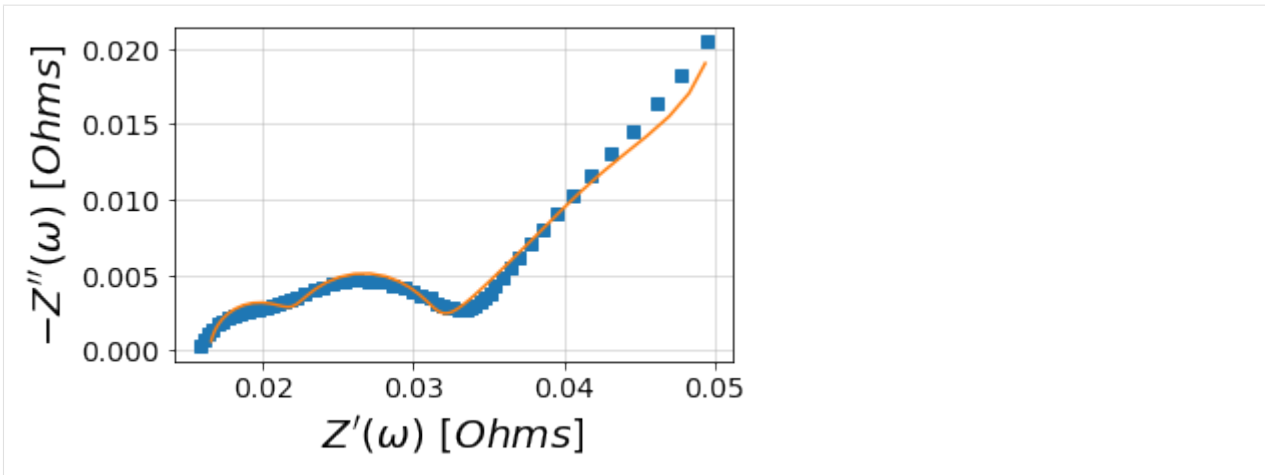
a. Interactive altair plot

```
[4]: circuit.plot(f_data=frequencies, Z_data=Z)
```



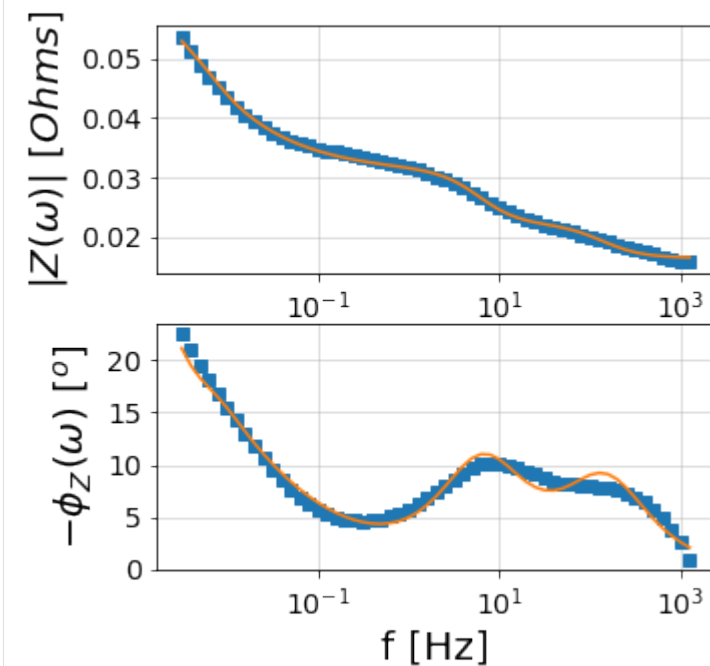
b. Nyquist plot via matplotlib

```
[5]: circuit.plot(f_data=frequencies, Z_data=Z, kind='nyquist')
plt.show()
```



c. Bode plot via matplotlib

```
[6]: circuit.plot(f_data=frequencies, Z_data=Z, kind='bode')
plt.show()
```



Bonus: Easy access to all the customization of matplotlib

Here we plot the data, changing the size of the figure, axes label fontsize, and turning off the grid by accessing the `plt.Axes()` object, `ax`

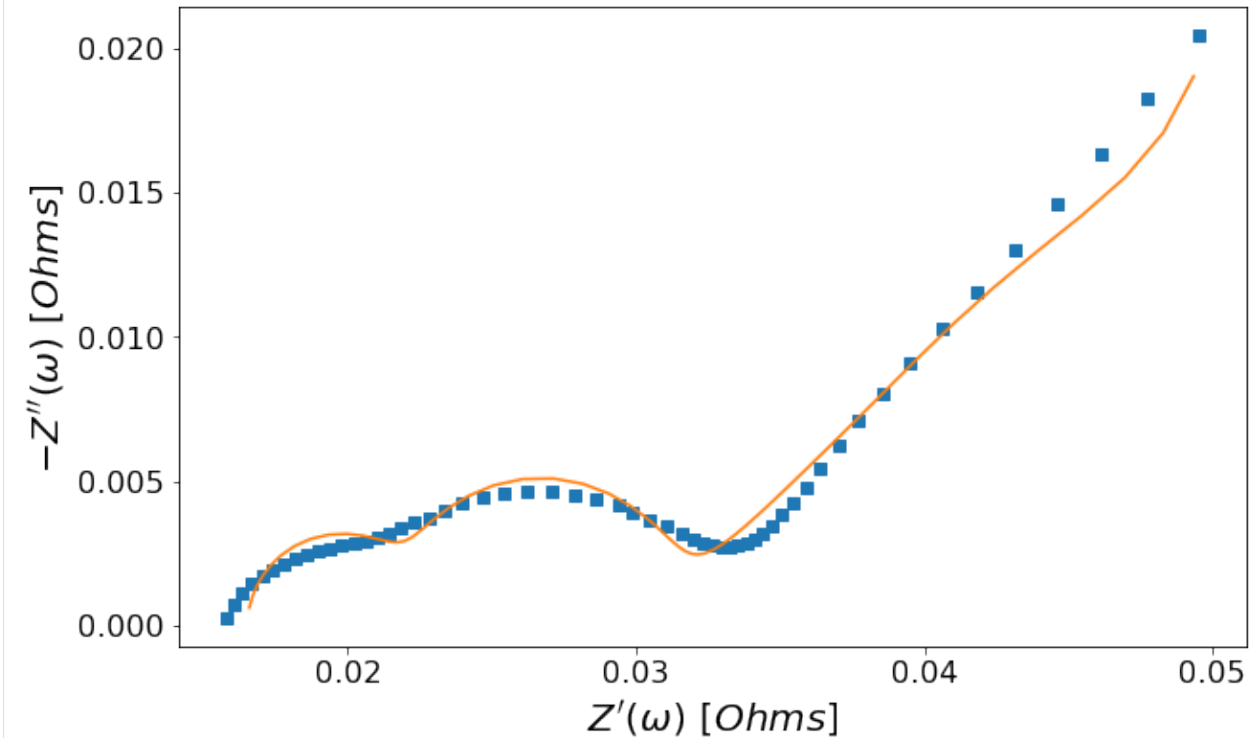
```
[7]: fig, ax = plt.subplots(figsize=(10,10))
ax = circuit.plot(ax, frequencies, Z, kind='nyquist')
```

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```
ax.tick_params(axis='both', which='major', labelsize=16)
ax.grid(False)

plt.show()
```



2.2.3 Model Saving/Loading Example

This set of examples shows how to load and import template models in order to make setting up and reproducing circuit fits easier.

```
[1]: # Load libraries

import impedance.preprocessing as preprocessing
import impedance.models.circuits as circuits
from impedance.visualization import plot_nyquist
import numpy as np
import matplotlib.pyplot as plt

[2]: # Load data from the example EIS result
frequencies, Z = preprocessing.readCSV('../data/exampleData.csv')

# keep only the impedance data in the first quadrant
frequencies, Z = preprocessing.ignoreBelowX(frequencies, Z)
```

Example 1. Importing and Exporting Models

Call the `circuit.save()` function to export the model to a human readable JSON file. The following code generates a test circuit and export it as a template. Here we are using an unfitted model as a template.

```
[3]: test_circuit = circuits.CustomCircuit(initial_guess=[.01, .005, .1, .005, .1, .001,
↪200],
                                         circuit='R0-p(R1,C1)-p(R2,C2)-Wo1')

print(test_circuit)

test_circuit.save('template_model.json')
```

```
Circuit string: R0-p(R1,C1)-p(R2,C2)-Wo1
Fit: False
```

Initial guesses:

```
    R0 = 1.00e-02 [Ohm]
    R1 = 5.00e-03 [Ohm]
    C1 = 1.00e-01 [F]
    R2 = 5.00e-03 [Ohm]
    C2 = 1.00e-01 [F]
    Wo1_0 = 1.00e-03 [Ohm]
    Wo1_1 = 2.00e+02 [sec]
```

Call the `model_io.model_import` function to import the model back as a template.

```
[4]: loaded_template = circuits.CustomCircuit()
loaded_template.load('template_model.json')

print("Loaded Template")
print(loaded_template)
```

```
R0-p(R1,C1)-p(R2,C2)-Wo1
Loaded Template
```

```
Circuit string: R0-p(R1,C1)-p(R2,C2)-Wo1
Fit: False
```

Initial guesses:

```
    R0 = 1.00e-02 [Ohm]
    R1 = 5.00e-03 [Ohm]
    C1 = 1.00e-01 [F]
    R2 = 5.00e-03 [Ohm]
    C2 = 1.00e-01 [F]
    Wo1_0 = 1.00e-03 [Ohm]
    Wo1_1 = 2.00e+02 [sec]
```

Example 2. Using imported template model to fit data

After the model has been imported as a template, it can be used as a starting point to fit data. This saves on needing to configure the initial parameters each time a fit is performed and to persist starting conditions across several fitting sessions.

```
[5]: fig, ax = plt.subplots(figsize=(5,5))
f_pred = np.logspace(5,-2)
loaded_template.fit(frequencies, Z)

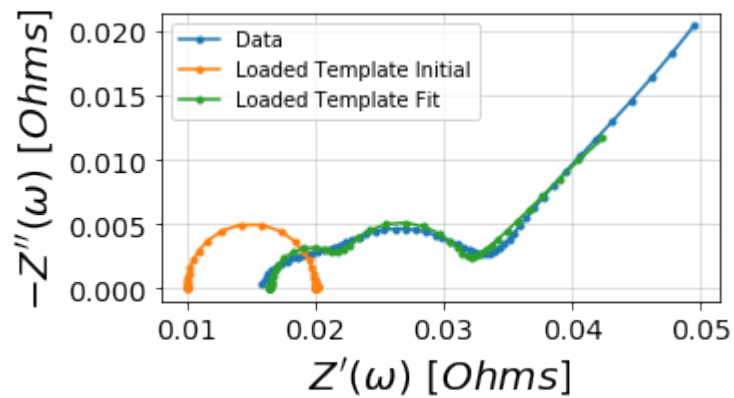
imported_circuit_init = loaded_template.predict(f_pred, use_initial = True)
imported_circuit_fit = loaded_template.predict(f_pred)

plot_nyquist(ax, Z)
plot_nyquist(ax, imported_circuit_init)
plot_nyquist(ax, imported_circuit_fit)

ax.legend(['Data', 'Loaded Template Initial', 'Loaded Template Fit'])

plt.show()
print(loaded_template)
```

Simulating circuit based on initial parameters



Circuit string: R0-p(R1,C1)-p(R2,C2)-Wol
Fit: True

Initial guesses:

```
R0 = 1.00e-02 [Ohm]
R1 = 5.00e-03 [Ohm]
C1 = 1.00e-01 [F]
R2 = 5.00e-03 [Ohm]
C2 = 1.00e-01 [F]
Wol_0 = 1.00e-03 [Ohm]
Wol_1 = 2.00e+02 [sec]
```

Fit parameters:

```
R0 = 1.65e-02 (+/- 1.54e-04) [Ohm]
R1 = 8.77e-03 (+/- 1.89e-04) [Ohm]
C1 = 3.28e+00 (+/- 1.85e-01) [F]
R2 = 5.31e-03 (+/- 2.06e-04) [Ohm]
C2 = 2.32e-01 (+/- 1.90e-02) [F]
Wol_0 = 6.37e-02 (+/- 2.03e-03) [Ohm]
Wol_1 = 2.37e+02 (+/- 1.72e+01) [sec]
```

Example 3. Using fitted data as a starting point for new fits

Consider the case where a successful fit has been performed and a new set of EIS data is obtained which is similar to the first spectrum. It is useful to use the successfully fitted parameters as a starting point for subsequent fits.

```
[6]: # Export the fitted model as a template

loaded_template.save('fitted_template.json')
```

Using the exported model's fitted parameters, generate a new circuit using the fitted parameters as initial guesses by supplying the `fitted_as_initial` parameter as `True`.

```
[7]: fitted_template = circuits.CustomCircuit()
fitted_template.load('fitted_template.json', fitted_as_initial=True)
print(fitted_template)
```

```
R0-p(R1,C1)-p(R2,C2)-Wo1
```

```
Circuit string: R0-p(R1,C1)-p(R2,C2)-Wo1
Fit: False
```

```
Initial guesses:
```

```
    R0 = 1.65e-02 [Ohm]
```

```
    R1 = 8.77e-03 [Ohm]
```

```
    C1 = 3.28e+00 [F]
```

```
    R2 = 5.31e-03 [Ohm]
```

```
    C2 = 2.32e-01 [F]
```

```
    Wo1_0 = 6.37e-02 [Ohm]
```

```
    Wo1_1 = 2.37e+02 [sec]
```

Z2 is a similar impedance spectra that we can fit using the previous fitted parameters as starting points. It has been shifted by 5 mOhm in the real axis and the data has been scaled by 1.5x.

```
[8]: Z2 = (0.005 + Z.real)*1.5 + 1.5j*Z.imag
```

```
[9]: fig, ax = plt.subplots(figsize=(10,10))
f_pred = np.logspace(5,-2)
fitted_template.fit(frequencies, Z2)

imported_circuit_init = fitted_template.predict(f_pred, use_initial = True)
imported_circuit_fit = fitted_template.predict(f_pred)

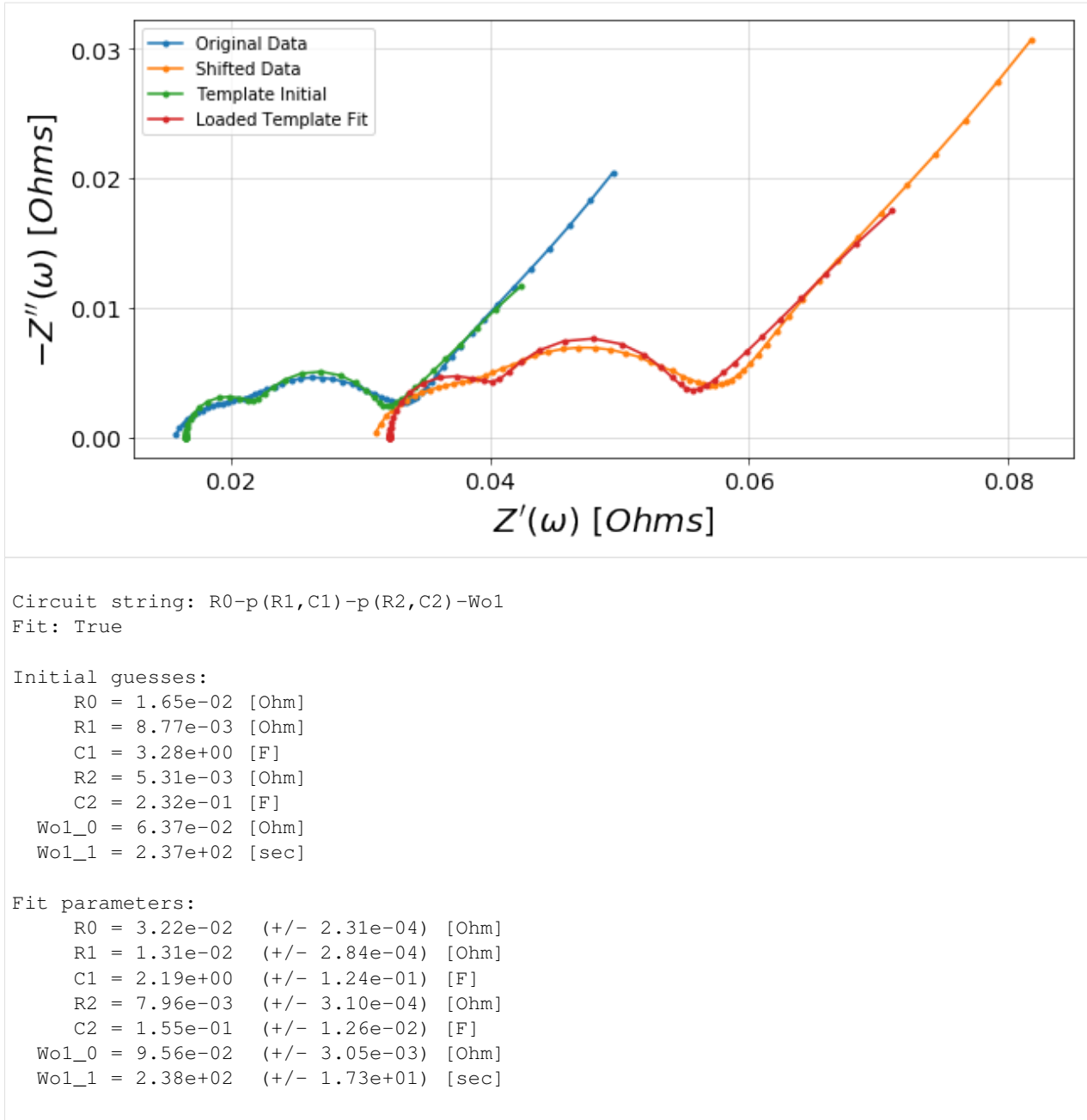
plot_nyquist(ax, Z)
plot_nyquist(ax, Z2)
plot_nyquist(ax, imported_circuit_init)
plot_nyquist(ax, imported_circuit_fit)

ax.legend(['Original Data', 'Shifted Data', 'Template Initial', 'Loaded Template Fit
→'])

plt.show()

print(fitted_template)
```

```
Simulating circuit based on initial parameters
```

2.2.4 Validation of EIS data

The Kramers-Kronig Relations

Electrochemical impedance spectroscopy (EIS) is built on linear systems theory which requires that the system satisfy conditions of causality, linearity, and stability. The Kramers-Kronig relations consist of a set of transformations that can be used to predict one component of the impedance from the other over the frequency limits from zero to infinity. For example, one might calculate the imaginary component of the impedance from the measured real component,

$$Z''(\omega) = -\frac{2\omega}{\pi} \int_0^\infty \frac{Z'(x) - Z'(\omega)}{x^2 - \omega^2} dx$$

where $Z'(\omega)$ and $Z''(\omega)$ are the real and imaginary components of the impedance as a function of frequency, ω . Similarly, the real part of the impedance spectrum can be calculated from the imaginary part by

$$Z'(\omega) = Z'(\infty) + \frac{2}{\pi} \int_0^\infty \frac{xZ''(x) - \omega Z''(\omega)}{x^2 - \omega^2} dx$$

The residual error between the predicted and measured impedance can then be used to determine consistency with the Kramers-Kronig relations.

Practically, however, the 0 to ∞ frequency range required for integration can be difficult to measure experimentally, so several other methods have been developed to ensure Kramers-Kronig relations are met:

- *Measurement models*
- *The Lin-KK method*

Measurement models

```
[1]: import matplotlib.pyplot as plt
import numpy as np

import sys
sys.path.append('../..')

from impedance.models.circuits import CustomCircuit
from impedance import preprocessing

[2]: # Load data from the example EIS result
f, Z = preprocessing.readCSV('../..data/exampleData.csv')

# keep only the impedance data in the first quadrant
f, Z = preprocessing.ignoreBelowX(f, Z)

mask = f < 1000
f = f[mask]
Z = Z[mask]

[3]: N = 10

circuit = 'R_0'
initial_guess = [.015]
for i in range(N):
    circuit += f'-p(R_{i % 9 + 1},C_{i % 9 + 1})'
    initial_guess.append(.03/N)
    initial_guess.append(10**(3 - 6*i/N))

meas_model = CustomCircuit(initial_guess=initial_guess, circuit=circuit)

[4]: meas_model.fit(f, Z)

print(meas_model)

Circuit string: R_0-p(R_1,C_1)-p(R_2,C_2)-p(R_3,C_3)-p(R_4,C_4)-p(R_5,C_5)-p(R_6,C_6)-
→p(R_7,C_7)-p(R_8,C_8)-p(R_9,C_9)-p(R_1,C_1)
Fit: True
```

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Initial guesses:

```

R_0 = 1.50e-02 [Ohm]
R_1 = 3.00e-03 [Ohm]
C_1 = 1.00e+03 [F]
R_2 = 3.00e-03 [Ohm]
C_2 = 2.51e+02 [F]
R_3 = 3.00e-03 [Ohm]
C_3 = 6.31e+01 [F]
R_4 = 3.00e-03 [Ohm]
C_4 = 1.58e+01 [F]
R_5 = 3.00e-03 [Ohm]
C_5 = 3.98e+00 [F]
R_6 = 3.00e-03 [Ohm]
C_6 = 1.00e+00 [F]
R_7 = 3.00e-03 [Ohm]
C_7 = 2.51e-01 [F]
R_8 = 3.00e-03 [Ohm]
C_8 = 6.31e-02 [F]
R_9 = 3.00e-03 [Ohm]
C_9 = 1.58e-02 [F]
R_1 = 3.00e-03 [Ohm]
C_1 = 3.98e-03 [F]

```

Fit parameters:

```

R_0 = 1.63e-02 (+/- 3.51e-05) [Ohm]
R_1 = 6.04e+04 (+/- 1.71e-06) [Ohm]
C_1 = 3.81e+03 (+/- 4.27e+01) [F]
R_2 = 1.33e-02 (+/- 2.06e-04) [Ohm]
C_2 = 2.78e+03 (+/- 1.14e+02) [F]
R_3 = 2.49e-03 (+/- 2.54e-04) [Ohm]
C_3 = 7.19e+01 (+/- 1.58e+01) [F]
R_4 = 2.12e-03 (+/- 1.05e-04) [Ohm]
C_4 = 5.74e+02 (+/- 6.43e+01) [F]
R_5 = 5.61e-03 (+/- 2.36e-04) [Ohm]
C_5 = 1.48e+03 (+/- 5.49e+01) [F]
R_6 = 5.12e-03 (+/- 6.90e-04) [Ohm]
C_6 = 7.77e+00 (+/- 2.09e+00) [F]
R_7 = 3.72e-03 (+/- 7.13e-04) [Ohm]
C_7 = 3.63e+00 (+/- 3.64e-01) [F]
R_8 = 2.43e-03 (+/- 2.01e-04) [Ohm]
C_8 = 1.11e+00 (+/- 1.78e-01) [F]
R_9 = 3.18e-03 (+/- 1.96e-04) [Ohm]
C_9 = 1.85e-01 (+/- 8.37e-03) [F]
R_1 = 6.01e-06 (+/- 3.51e-05) [Ohm]
C_1 = 2.30e-30 (+/- 3.71e+02) [F]

```

```
[5]: from impedance.visualization import plot_nyquist, plot_residuals
```

```

res_meas_real = (Z - meas_model.predict(f)).real/np.abs(Z)
res_meas_imag = (Z - meas_model.predict(f)).imag/np.abs(Z)

```

```

fig = plt.figure(figsize=(5,8))
gs = fig.add_gridspec(3, 1)
ax1 = fig.add_subplot(gs[2,:])
ax2 = fig.add_subplot(gs[2,:])

```

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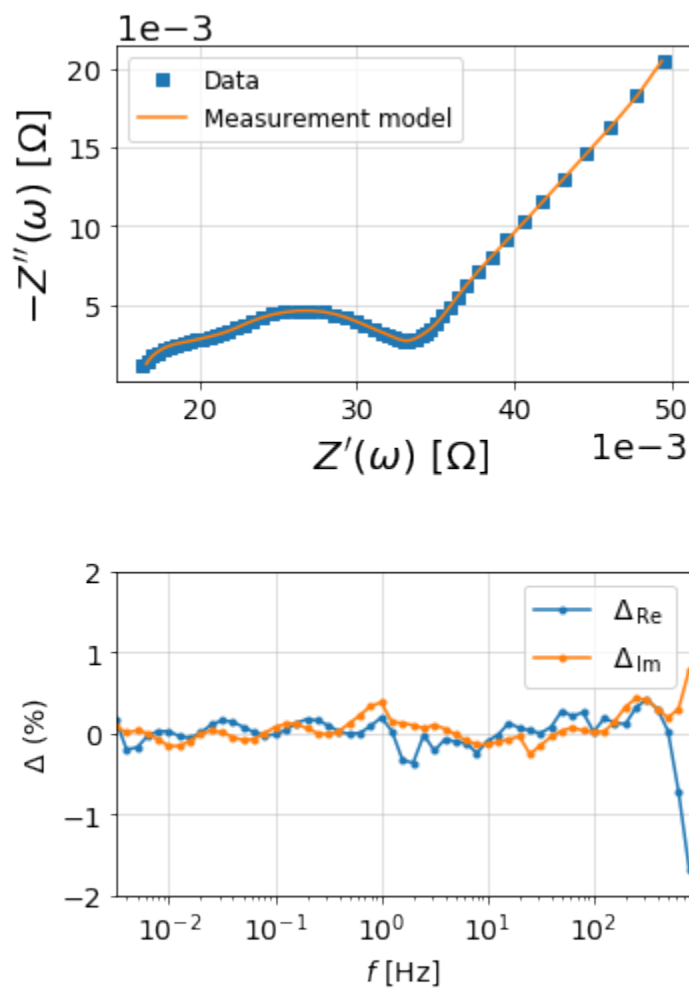
```
# plot original data
plot_nyquist(ax1, Z, fmt='s')

# plot measurement model
plot_nyquist(ax1, meas_model.predict(f), fmt='-', scale=1e3, units='\Omega')

ax1.legend(['Data', 'Measurement model'], loc=2, fontsize=12)

# Plot residuals
plot_residuals(ax2, f, res_meas_real, res_meas_imag, y_limits=(-2,2))

plt.tight_layout()
plt.show()
```



The Lin-KK method

The lin-KK method from Schönleber et al. [1] is a quick test for checking the validity of EIS data. The validity of an impedance spectrum is analyzed by its reproducibility by a Kramers-Kronig (KK) compliant equivalent circuit. In

particular, the model used in the lin-KK test is an ohmic resistor, R_{Ohm} , and M RC elements.

$$\hat{Z} = R_{Ohm} + \sum_{k=1}^M \frac{R_k}{1 + j\omega\tau_k}$$

The M time constants, τ_k , are distributed logarithmically,

$$\tau_1 = \frac{1}{\omega_{max}}; \tau_M = \frac{1}{\omega_{min}}; \tau_k = 10^{\log(\tau_{min}) + \frac{k-1}{M-1} \log(\frac{\tau_{max}}{\tau_{min}})}$$

and are not fit during the test (only R_{Ohm} and R_k are free parameters).

In order to prevent under- or over-fitting, Schönleber et al. propose using the ratio of positive resistor mass to negative resistor mass as a metric for finding the optimal number of RC elements.

$$\mu = 1 - \frac{\sum_{R_k \geq 0} |R_k|}{\sum_{R_k < 0} |R_k|}$$

The argument `c` defines the cutoff value for μ . The algorithm starts at $M = 3$ and iterates up to `max_M` until a $\mu < c$ is reached. The default of 0.85 is simply a heuristic value based off of the experience of Schönleber et al.

If the argument `c` is `None`, then the automatic determination of RC elements is turned off and the solution is calculated for `max_M` RC elements. This manual mode should be used with caution as under- and over-fitting should be avoided.

[1] Schönleber, M. et al. A Method for Improving the Robustness of linear Kramers-Kronig Validity Tests. *Electrochimica Acta* 131, 20–27 (2014) doi: [10.1016/j.electacta.2014.01.034](https://doi.org/10.1016/j.electacta.2014.01.034).

```
[6]: import matplotlib.pyplot as plt
import numpy as np

import sys
sys.path.append('../..')

from impedance.validation import linKK

[7]: # Load data from the example EIS result
f, Z = preprocessing.readCSV('../..../data/exampleData.csv')

# keep only the impedance data in the first quadrant
f, Z = preprocessing.ignoreBelowX(f, Z)

mask = f < 1000
f = f[mask]
Z = Z[mask]

[8]: M, mu, Z_linKK, res_real, res_imag = linKK(f, Z, c=.5, max_M=100, fit_type='complex',
↪add_cap=True)

print('\nCompleted Lin-KK Fit\nM = {:d}\nmu = {:.2f}'.format(M, mu))

10 1.0 8.144660459067897e-05
20 0.8929547688006024 5.100216832596417e-05

Completed Lin-KK Fit
M = 26
mu = 0.31
```

```
[9]: from impedance.visualization import plot_nyquist, plot_residuals

fig = plt.figure(figsize=(5,8))
gs = fig.add_gridspec(3, 1)
ax1 = fig.add_subplot(gs[2,:])
ax2 = fig.add_subplot(gs[2,:])

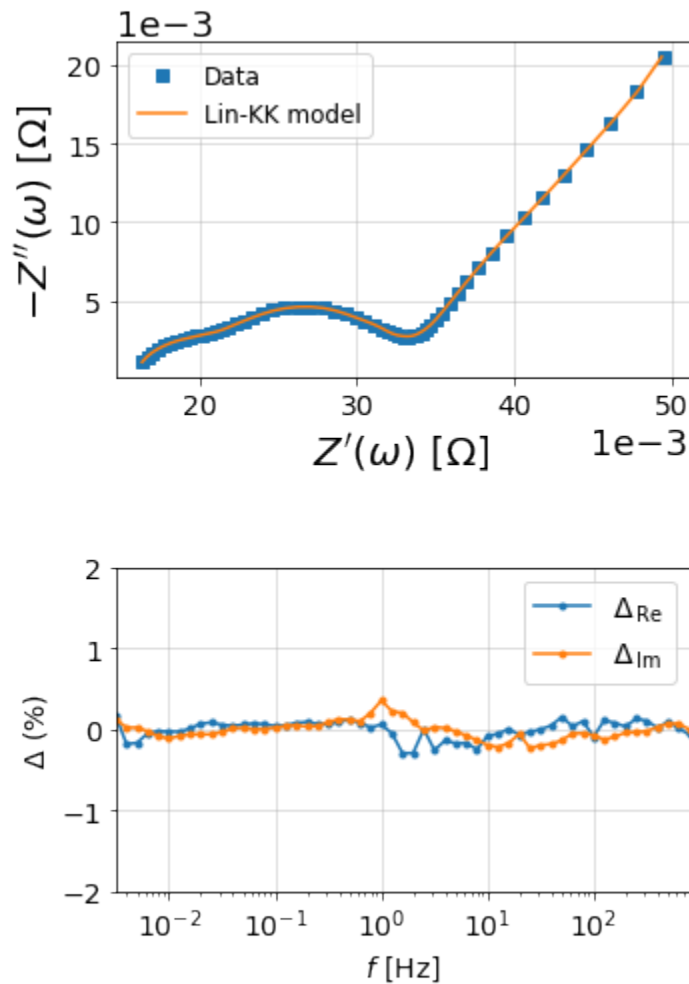
# plot original data
plot_nyquist(ax1, Z, fmt='s')

# plot measurement model
plot_nyquist(ax1, Z_linKK, fmt='-', scale=1e3, units='\Omega')

ax1.legend(['Data', 'Lin-KK model'], loc=2, fontsize=12)

# Plot residuals
plot_residuals(ax2, f, res_real, res_imag, y_limits=(-2,2))

plt.tight_layout()
plt.show()
```



2.2.5 Looping through and fitting multiple impedance data sets

```
[1]: import os
import sys
sys.path.append('../..../')

import glob
import numpy as np
```

1. Find all files that match a specified pattern

Using a search string to find .z files that contain “Circuit” at the beginning and EIS towards the end

```
[2]: directory = r'../..../data/'
all_files = glob.glob(os.path.join(directory, 'Circuit*EIS*.z'))
all_files

[2]: ['../..../data\\Circuit1_EIS_1.z',
'../..../data\\Circuit1_EIS_2.z',
'../..../data\\Circuit2_EIS_1.z',
'../..../data\\Circuit2_EIS_2.z',
'../..../data\\Circuit3_EIS_1.z',
'../..../data\\Circuit3_EIS_2.z']
```

2. Use preprocessing module to read in ZPlot data

```
[3]: from impedance import preprocessing
# Initialize some empty lists for the frequencies and Z data
freqs = []
Zs = []

# Now loop through file names in our list and extract data one by one
for filename in all_files:
    f, Z = preprocessing.readZPlot(filename)
    freqs.append(f)
    Zs.append(Z)

# Check to see if we extracted data for all the files
print(np.shape(Zs), np.shape(all_files))

(6,) (6,)
```

3. Create a list of circuit models

```
[4]: from impedance.models.circuits import CustomCircuit
# This data comes from dummy circuits I made to check measurement bias in
# our potentiostat, so I know a priori its an R-RC circuit

circuits = []

circ_string = 'R0-p(R1,C1)'
initial_guess = [100, 400, 1e-5]
```

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```
# Now loop through data list to create circuits and fit them
for f, Z, filename in zip(freqs, Zs, all_files):
    name = filename.split('/')[-1]
    circuit = CustomCircuit(circ_string, initial_guess=initial_guess, name=name)
    circuit.fit(f, Z)
    circuits.append(circuit)
```

We now have a list of our circuit class objects, all fit to different sets of data. As you may notice from the file names, there are three unique circuits each with a replicate set of data. We expect each of the replicates to fit similarly.

```
[5]: for circuit in circuits:
      print(circuit)
```

```
Name: data\Circuit1_EIS_1.z
Circuit string: R0-p(R1,C1)
Fit: True
```

```
Initial guesses:
```

```
    R0 = 1.00e+02 [Ohm]
    R1 = 4.00e+02 [Ohm]
    C1 = 1.00e-05 [F]
```

```
Fit parameters:
```

```
    R0 = 2.91e+01 (+/- 3.63e-02) [Ohm]
    R1 = 4.67e+01 (+/- 4.69e-02) [Ohm]
    C1 = 1.04e-05 (+/- 2.95e-08) [F]
```

```
Name: data\Circuit1_EIS_2.z
Circuit string: R0-p(R1,C1)
Fit: True
```

```
Initial guesses:
```

```
    R0 = 1.00e+02 [Ohm]
    R1 = 4.00e+02 [Ohm]
    C1 = 1.00e-05 [F]
```

```
Fit parameters:
```

```
    R0 = 2.91e+01 (+/- 3.58e-02) [Ohm]
    R1 = 4.67e+01 (+/- 4.64e-02) [Ohm]
    C1 = 1.04e-05 (+/- 2.91e-08) [F]
```

```
Name: data\Circuit2_EIS_1.z
Circuit string: R0-p(R1,C1)
Fit: True
```

```
Initial guesses:
```

```
    R0 = 1.00e+02 [Ohm]
    R1 = 4.00e+02 [Ohm]
    C1 = 1.00e-05 [F]
```

```
Fit parameters:
```

```
    R0 = 1.50e+02 (+/- 3.23e-01) [Ohm]
    R1 = 5.02e+02 (+/- 3.57e-01) [Ohm]
```

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```

C1 = 3.12e-08  (+/- 7.79e-11) [F]

Name: data\Circuit2_EIS_2.z
Circuit string: R0-p(R1,C1)
Fit: True

Initial guesses:
  R0 = 1.00e+02 [Ohm]
  R1 = 4.00e+02 [Ohm]
  C1 = 1.00e-05 [F]

Fit parameters:
  R0 = 1.50e+02  (+/- 3.19e-01) [Ohm]
  R1 = 5.02e+02  (+/- 3.53e-01) [Ohm]
  C1 = 3.12e-08  (+/- 7.70e-11) [F]

Name: data\Circuit3_EIS_1.z
Circuit string: R0-p(R1,C1)
Fit: True

Initial guesses:
  R0 = 1.00e+02 [Ohm]
  R1 = 4.00e+02 [Ohm]
  C1 = 1.00e-05 [F]

Fit parameters:
  R0 = 1.51e+03  (+/- 2.62e+00) [Ohm]
  R1 = 4.63e+03  (+/- 3.14e+00) [Ohm]
  C1 = 2.02e-08  (+/- 5.39e-11) [F]

Name: data\Circuit3_EIS_2.z
Circuit string: R0-p(R1,C1)
Fit: True

Initial guesses:
  R0 = 1.00e+02 [Ohm]
  R1 = 4.00e+02 [Ohm]
  C1 = 1.00e-05 [F]

Fit parameters:
  R0 = 1.51e+03  (+/- 2.68e+00) [Ohm]
  R1 = 4.63e+03  (+/- 3.21e+00) [Ohm]
  C1 = 2.02e-08  (+/- 5.52e-11) [F]

```

Now we'll get the impedance predicted by the fit parameters

```

[6]: fits = []
    for f, circuit in zip(freqs, circuits):
        fits.append(circuit.predict(f))

```

4. Plot the data and fits

Now we can visualize the data and fits. For now we'll place them all on the same axis

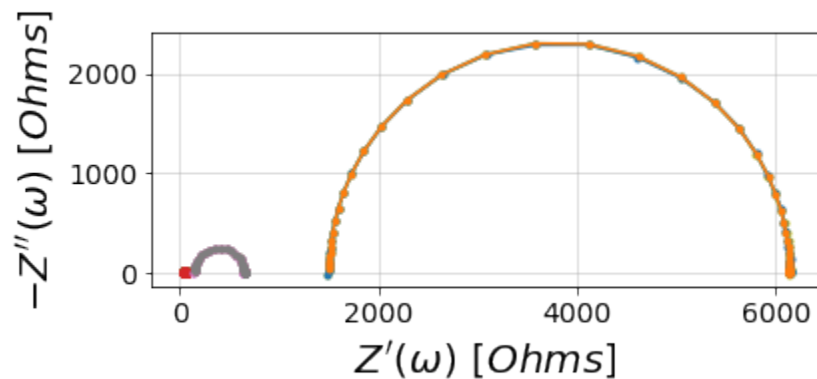
```
[7]: import matplotlib.pyplot as plt
      from impedance.visualization import plot_nyquist, plot_bode
```

```
[8]: fig, ax = plt.subplots()

      for fit, Z in zip(fits, Zs):
          # Plotting data
          plot_nyquist(ax, Z)

          # Plotting fit
          plot_nyquist(ax, fit)

      plt.show()
```

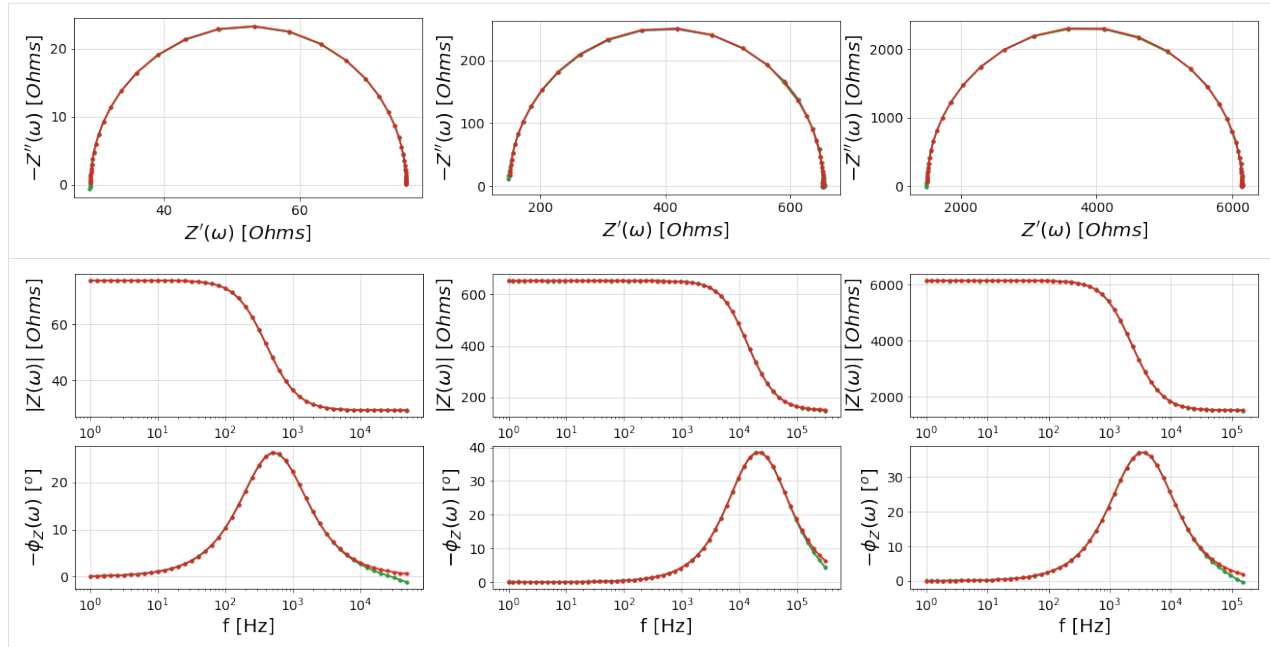


Since the circuits have different orders of magnitude impedance, this looks bad so let's put each pair of data on separate axes.

```
[9]: # Nyquist plots
      fig, axes = plt.subplots(ncols=3, figsize=(22,6))
      for circuit, Z, fit in zip(circuits, Zs, fits):
          n = int(circuit.name.split('Circuit')[-1].split('_')[0])
          plot_nyquist(axes[n - 1], Z)
          plot_nyquist(axes[n - 1], fit)

      # Bode plots
      fig, axes = plt.subplots(nrows=2, ncols=3, figsize=(22,6))
      for circuit, f, Z, fit in zip(circuits, freqs, Zs, fits):
          n = int(circuit.name.split('Circuit')[-1].split('_')[0])
          plot_bode([axes[0][n - 1], axes[1][n - 1]], f, Z)
          plot_bode([axes[0][n - 1], axes[1][n - 1]], f, fit)

      plt.show()
```



2.3 Preprocessing

Methods for preprocessing impedance data from instrument files

`impedance.preprocessing.cropFrequencies(frequencies, Z, freqmin=0, freqmax=None)`

Trim out all data points below the X-axis

Parameters

frequencies [np.ndarray] Array of frequencies

Z [np.ndarray of complex numbers] Array of complex impedances

freqmin [float] Minimum frequency, omit for no lower frequency limit

freqmax [float] Max frequency, omit for no upper frequency limit

Returns

frequencies_final [np.ndarray] Array of frequencies after filtering

Z_final [np.ndarray of complex numbers] Array of complex impedances after filtering

`impedance.preprocessing.ignoreBelowX(frequencies, Z)`

Trim out all data points below the X-axis

Parameters

frequencies [np.ndarray] Array of frequencies

Z [np.ndarray of complex numbers] Array of complex impedances

Returns

frequencies [np.ndarray] Array of frequencies after filtering

Z [np.ndarray of complex numbers] Array of complex impedances after filtering

`impedance.preprocessing.readAutolab(filename)`
function for reading comma-delimited files from Autolab

Parameters

filename: `string` Filename of file to extract impedance data from

Returns

frequencies `[np.ndarray]` Array of frequencies

impedance `[np.ndarray of complex numbers]` Array of complex impedances

`impedance.preprocessing.readBioLogic(filename)`
function for reading the .mpt file from Biologic EC-lab software

Parameters

filename: `string` Filename of .csv file to extract impedance data from

Returns

frequencies `[np.ndarray]` Array of frequencies

impedance `[np.ndarray of complex numbers]` Array of complex impedances

`impedance.preprocessing.readCHInstruments(filename)`
function for reading the .txt file from CHInstruments

Parameters

filename: `string` Filename of .txt file to extract impedance data from

Returns

frequencies `[np.ndarray]` Array of frequencies

impedance `[np.ndarray of complex numbers]` Array of complex impedances

`impedance.preprocessing.readFile(filename, instrument=None)`
A wrapper for reading in many common types of impedance files

Parameters

filename: `string` Filename to extract impedance data from

instrument: `string` Type of instrument file

Returns

frequencies `[np.ndarray]` Array of frequencies

impedance `[np.ndarray of complex numbers]` Array of complex impedances

`impedance.preprocessing.readGamry(filename)`
function for reading the .DTA file from Gamry

Parameters

filename: `string` Filename of .DTA file to extract impedance data from

Returns

frequencies `[np.ndarray]` Array of frequencies

impedance `[np.ndarray of complex numbers]` Array of complex impedances

`impedance.preprocessing.readParstat(filename)`
function for reading the .txt file from Parstat

Parameters

filename: `string` Filename of .txt file to extract impedance data from

Returns

frequencies `[np.ndarray]` Array of frequencies

impedance `[np.ndarray of complex numbers]` Array of complex impedances

`impedance.preprocessing.readPowerSuite(filename)`
function for reading the .txt file from Parstat

Parameters

filename: `string` Filename of .txt file to extract impedance data from

Returns

frequencies `[np.ndarray]` Array of frequencies

impedance `[np.ndarray of complex numbers]` Array of complex impedances

`impedance.preprocessing.readVersaStudio(filename)`
function for reading the .PAR file from VersaStudio

Parameters

filename: `string` Filename of .PAR file to extract impedance data from

Returns

frequencies `[np.ndarray]` Array of frequencies

impedance `[np.ndarray of complex numbers]` Array of complex impedances

`impedance.preprocessing.readZPlot(filename)`
function for reading the .z file from Scribner's ZPlot

Parameters

filename: `string` Filename of .z file to extract impedance data from

Returns

frequencies `[np.ndarray]` Array of frequencies

impedance `[np.ndarray of complex numbers]` Array of complex impedances

2.4 Validation

Interpreting EIS data fundamentally relies on the the system conforming to conditions of causality, linearity, and stability. For an example of how the adherence to the Kramers-Kronig relations, see the [Validation Example Jupyter Notebook](#)

2.4.1 Lin-KK method

Validating your data with the lin-KK model requires fitting an optimal number of RC-elements and analysis of the residual errors.

`impedance.validation.calc_mu(Rs)`
Calculates mu for use in LinKK

```
impedance.validation.eval_linKK(elements, ts, f)
```

Builds a circuit of RC elements to be used in LinKK

```
impedance.validation.fit_linKK(f, ts, M, Z, fit_type='real', add_cap=False)
```

Fits the linKK model using linear regression

Parameters

f: `np.ndarray` measured frequencies

ts: `np.ndarray` logarithmically spaced time constants of RC elements

M: `int` the number of RC elements

Z: `np.ndarray of complex numbers` measured impedances

fit_type: `str` selects which components of data are fit ('real', 'imag', or 'complex')

add_cap: `bool` option to add a serial capacitance that helps validate data with no low-frequency intercept

Returns

elements: `np.ndarray` values of fit R_k in RC elements and series R_0 , L, and optionally C.

mu: `np.float` under- or over-fitting measure

Notes

Since we have a system of equations, $Ax = b$, that's linear wrt R_k , we can fit the model by calculating the pseudo-inverse of A. Ax is our model fit, \hat{Z} , and b is the normalized real or imaginary component of the impedance data, $Re(Z)/|Z|$ or $Im(Z)/|Z|$, respectively.

$\hat{Z} = R_0 + \sum_{k=1}^M (R_k/|Z|(1 + j * w * \tau_k))$. x is an $(M+1) \times 1$ matrix where the first row contains R_0 and subsequent rows contain R_k values. A is an $N \times (M+1)$ matrix, where N is the number of data points, and M is the number of RC elements.

Examples

Fitting the real part of data, the first column of A contains values of $\frac{1}{|Z|}$, the second column contains $Re(1/|Z|(1 + j * w * \tau_1))$, the third contains $Re(1/|Z|(1 + j * w * \tau_2))$ and so on. The R_k values within the x matrix are found using `numpy.linalg.pinv` when `fit_type = 'real'` or `'imag'`. When `fit_type = 'complex'` the coefficients are found “manually” using $r = \|A'x - b'\|^2 + \|A''x - b''\|^2$ according to Eq 14 of Schonleber [1].

[1] Schönleber, M. et al. A Method for Improving the Robustness of linear Kramers-Kronig Validity Tests. *Electrochimica Acta* 131, 20–27 (2014) doi: [10.1016/j.electacta.2014.01.034](https://doi.org/10.1016/j.electacta.2014.01.034).

```
impedance.validation.get_tc_distribution(f, M)
```

Returns the distribution of time constants for the linKK method

```
impedance.validation.linKK(f, Z, c=0.85, max_M=50, fit_type='real', add_cap=False)
```

A method for implementing the Lin-KK test for validating linearity [1]

Parameters

f: `np.ndarray` measured frequencies

Z: `np.ndarray of complex numbers` measured impedances

c: `np.float` cutoff for mu

max_M: int the maximum number of RC elements

fit_type: str selects which components of data are fit ('real', 'imag', or 'complex')

add_cap: bool option to add a serial capacitance that helps validate data with no low-frequency intercept

Returns

M: int number of RC elements used

mu: np.float under- or over-fitting measure

Z_fit: np.ndarray of complex numbers impedance of fit at input frequencies

resids_real: np.ndarray real component of the residuals of the fit at input frequencies

resids_imag: np.ndarray imaginary component of the residuals of the fit at input frequencies

Notes

The lin-KK method from Schönleber et al. [1] is a quick test for checking the validity of EIS data. The validity of an impedance spectrum is analyzed by its reproducibility by a Kramers-Kronig (KK) compliant equivalent circuit. In particular, the model used in the lin-KK test is an ohmic resistor, R_{Ohm} , and M RC elements.

$$\hat{Z} = R_{Ohm} + \sum_{k=1}^M \frac{R_k}{1 + j\omega\tau_k}$$

The M time constants, τ_k , are distributed logarithmically,

$$\tau_1 = \frac{1}{\omega_{max}}; \tau_M = \frac{1}{\omega_{min}}; \tau_k = 10^{\log(\tau_{min}) + \frac{k-1}{M-1} \log(\frac{\tau_{max}}{\tau_{min}})}$$

and are not fit during the test (only R_{Ohm} and R_k are free parameters).

In order to prevent under- or over-fitting, Schönleber et al. propose using the ratio of positive resistor mass to negative resistor mass as a metric for finding the optimal number of RC elements.

$$\mu = 1 - \frac{\sum_{R_k \geq 0} |R_k|}{\sum_{R_k < 0} |R_k|}$$

The argument `c` defines the cutoff value for μ . The algorithm starts at $M = 3$ and iterates up to `max_M` until a $\mu < c$ is reached. The default of 0.85 is simply a heuristic value based off of the experience of Schönleber et al., but a lower value may give better results.

If the argument `c` is `None`, then the automatic determination of RC elements is turned off and the solution is calculated for `max_M` RC elements. This manual mode should be used with caution as under- and over-fitting should be avoided.

[1] Schönleber, M. et al. A Method for Improving the Robustness of linear Kramers-Kronig Validity Tests. *Electrochimica Acta* 131, 20–27 (2014) doi: [10.1016/j.electacta.2014.01.034](https://doi.org/10.1016/j.electacta.2014.01.034).

`impedance.validation.residuals_linKK(elements, ts, Z, f, residuals='real')`

Calculates the residual between the data and a LinKK fit

2.5 Circuits

class `impedance.models.circuits.circuits.BaseCircuit` (`initial_guess=[]`, `constants=None`, `name=None`)

Base class for equivalent circuit models

Methods

<code>fit(frequencies, impedance[, method, bounds])</code>	Fit the circuit model
<code>get_param_names()</code>	Converts circuit string to names and units
<code>load(filepath[, fitted_as_initial])</code>	Imports a model from JSON
<code>plot([ax, f_data, Z_data, kind])</code>	visualizes the model and optional data as a nyquist,
<code>predict(frequencies[, use_initial])</code>	Predict impedance using an equivalent circuit model
<code>save(filepath)</code>	Exports a model to JSON

fit (*frequencies, impedance, method=None, bounds=None*)

Fit the circuit model

Parameters

frequencies: **numpy array** Frequencies

impedance: **numpy array of dtype ‘complex128’** Impedance values to fit

method: {‘lm’, ‘trf’, ‘dogbox’}, **optional** Name of method to pass to `scipy.optimize.curve_fit`

bounds: **2-tuple of array_like, optional** Lower and upper bounds on parameters. Defaults to bounds on all parameters of 0 and `np.inf`, except the CPE alpha which has an upper bound of 1

Returns

self: returns an instance of self

get_param_names ()

Converts circuit string to names and units

load (*filepath, fitted_as_initial=False*)

Imports a model from JSON

Parameters

filepath: **str** filepath to JSON file to load model from

fitted_as_initial: **bool** If true, loads the model’s fitted parameters as initial guesses

Otherwise, loads the model’s initial and fitted parameters as a completed model

plot (*ax=None, f_data=None, Z_data=None, kind=‘altair’, **kwargs*)

visualizes the model and optional data as a nyquist, bode, or altair (interactive) plots

Parameters

ax: **matplotlib.axes** axes to plot on

f_data: **np.array of type float** Frequencies of input data (for Bode plots)

Z_data: **np.array of type complex** Impedance data to plot

kind: {‘altair’, ‘nyquist’, ‘bode’} type of plot to visualize

Returns

ax: **matplotlib.axes** axes of the created nyquist plot

Other Parameters

****kwargs** [optional]

If kind is ‘nyquist’ or ‘bode’, used to specify additional *matplotlib.pyplot.Line2D* properties like linewidth, line color, marker color, and labels.

If kind is ‘altair’, used to specify nyquist height as *size*

predict (*frequencies*, *use_initial=False*)

Predict impedance using an equivalent circuit model

Parameters

frequencies: ndarray of numeric dtype

use_initial: boolean If true and the model was previously fit use the initial parameters instead

Returns

impedance: ndarray of dtype ‘complex128’ Predicted impedance

save (*filepath*)

Exports a model to JSON

Parameters

filepath: str Destination for exporting model object

class impedance.models.circuits.circuits.**CustomCircuit** (*circuit=*”, ***kwargs*)

Methods

<code>fit(frequencies, impedance[, method, bounds])</code>	Fit the circuit model
<code>get_param_names()</code>	Converts circuit string to names and units
<code>load(filepath[, fitted_as_initial])</code>	Imports a model from JSON
<code>plot([ax, f_data, Z_data, kind])</code>	visualizes the model and optional data as a nyquist,
<code>predict(frequencies[, use_initial])</code>	Predict impedance using an equivalent circuit model
<code>save(filepath)</code>	Exports a model to JSON

class impedance.models.circuits.circuits.**Randles** (*CPE=False*, ***kwargs*)

A Randles circuit model class

Methods

<code>fit(frequencies, impedance[, method, bounds])</code>	Fit the circuit model
<code>get_param_names()</code>	Converts circuit string to names and units
<code>load(filepath[, fitted_as_initial])</code>	Imports a model from JSON
<code>plot([ax, f_data, Z_data, kind])</code>	visualizes the model and optional data as a nyquist,
<code>predict(frequencies[, use_initial])</code>	Predict impedance using an equivalent circuit model
<code>save(filepath)</code>	Exports a model to JSON

2.6 Circuit Elements

`impedance.models.circuits.elements.C(p,f)`
defines a capacitor

$$Z = \frac{1}{C \times j2\pi f}$$

`impedance.models.circuits.elements.CPE(p,f)`
defines a constant phase element

Notes

$$Z = \frac{1}{Q \times (j2\pi f)^\alpha}$$

where $Q = p[0]$ and $\alpha = p[1]$.

`impedance.models.circuits.elements.G(p,f)`
defines a Gerischer Element as represented in [1]

Notes

$$Z = \frac{R_G}{\sqrt{1 + j2\pi f t_G}}$$

where $R_G = p[0]$ and $t_G = p[1]$

Gerischer impedance is also commonly represented as [2]:

$$Z = \frac{Z_o}{\sqrt{K + j2\pi f}}$$

where $Z_o = \frac{R_G}{\sqrt{t_G}}$ and $K = \frac{1}{t_G}$ with units $\Omega sec^{1/2}$ and sec^{-1} , respectively.

[1] Y. Lu, C. Kreller, and S.B. Adler, Journal of The Electrochemical Society, 156, B513-B525 (2009)
[doi:10.1149/1.3079337](https://doi.org/10.1149/1.3079337).

[2] M. González-Cuenca, W. Zipprich, B.A. Boukamp, G. Pudmich, and F. Tietz, Fuel Cells, 1, 256-264 (2001)
[doi:10.1016/0013-4686\(93\)85083-B](https://doi.org/10.1016/0013-4686(93)85083-B).

`impedance.models.circuits.elements.Gs(p,f)`
defines a finite-length Gerischer Element as represented in [1]

Notes

$$Z = \frac{R_G}{\sqrt{1 + j2\pi f t_G \tanh(\phi \sqrt{1 + j2\pi f t_G})}}$$

where $R_G = p[0]$, $t_G = p[1]$ and $\phi = p[2]$

[1] R.D. Green, C.C Liu, and S.B. Adler, Solid State Ionics, 179, 647-660 (2008) [doi:10.1016/j.ssi.2008.04.024](https://doi.org/10.1016/j.ssi.2008.04.024).

`impedance.models.circuits.elements.K(p,f)`
An RC element for use in lin-KK model

Notes

$$Z = \frac{R}{1 + j\omega\tau_k}$$

`impedance.models.circuits.elements.L(p, f)`
defines an inductor

$$Z = L \times j2\pi f$$

`impedance.models.circuits.elements.La(p, f)`
defines a modified inductance element as represented in [1]

Notes

$$Z = L \times (j2\pi f)^\alpha$$

where $L = p[0]$ and $\alpha = p[1]$

[1] EC-Lab Application Note 42, BioLogic Instruments (2019).

`impedance.models.circuits.elements.R(p, f)`
defines a resistor

Notes

$$Z = R$$

`impedance.models.circuits.elements.T(p, f)`
A macrohomogeneous porous electrode model from Paasch et al. [1]

Notes

$$Z = A \frac{\coth \beta}{\beta} + B \frac{1}{\beta \sinh \beta}$$

where

$$A = d \frac{\rho_1^2 + \rho_2^2}{\rho_1 + \rho_2} \quad B = d \frac{2\rho_1\rho_2}{\rho_1 + \rho_2}$$

and

$$\beta = (a + j\omega b)^{1/2} \quad a = \frac{kd^2}{K} \quad b = \frac{d^2}{K}$$

[1] G. Paasch, K. Micka, and P. Gersdorf, *Electrochimica Acta*, 38, 2653–2662 (1993) doi: [10.1016/0013-4686\(93\)85083-B](https://doi.org/10.1016/0013-4686(93)85083-B).

`impedance.models.circuits.elements.W(p, f)`
defines a semi-infinite Warburg element

Notes

$$Z = \frac{A_W}{\sqrt{2\pi f}}(1 - j)$$

`impedance.models.circuits.elements.Wo(p, f)`
 defines an open (finite-space) Warburg element

Notes

$$Z = \frac{Z_0}{\sqrt{j\omega\tau}} \coth \sqrt{j\omega\tau}$$

where $Z_0 = p[0]$ (Ohms) and $\tau = p[1]$ (sec) = $\frac{L^2}{D}$

`impedance.models.circuits.elements.Ws(p, f)`
 defines a short (finite-length) Warburg element

Notes

$$Z = \frac{Z_0}{\sqrt{j\omega\tau}} \tanh \sqrt{j\omega\tau}$$

where $Z_0 = p[0]$ (Ohms) and $\tau = p[1]$ (sec) = $\frac{L^2}{D}$

`impedance.models.circuits.elements.element_metadata(num_params, units)`
 decorator to store metadata for a circuit element

Parameters

num_params [int] number of parameters for an element

units [list of str] list of units for the element parameters

`impedance.models.circuits.elements.p(parallel)`
 adds elements in parallel

Notes

$$Z = \frac{1}{\frac{1}{Z_1} + \frac{1}{Z_2} + \dots + \frac{1}{Z_n}}$$

`impedance.models.circuits.elements.s(series)`
 sums elements in series

Notes

$$Z = Z_1 + Z_2 + \dots + Z_n$$

2.7 Fitting

`impedance.models.circuits.fitting.buildCircuit` (*circuit, frequencies, *parameters, constants=None, eval_string="", index=0*)
 recursive function that transforms a circuit, parameters, and frequencies into a string that can be evaluated

Parameters

circuit: str
frequencies: list/tuple/array of floats
parameters: list/tuple/array of floats
constants: dict

Returns

eval_string: str Python expression for calculating the resulting fit
index: int Tracks parameter index through recursive calling of the function

`impedance.models.circuits.fitting.circuit_fit` (*frequencies, impedances, circuit, initial_guess, constants, method=None, bounds=None, bootstrap=False*)

Main function for fitting an equivalent circuit to data

Parameters

frequencies [numpy array] Frequencies
impedances [numpy array of dtype 'complex128'] Impedances
circuit [string] string defining the equivalent circuit to be fit
initial_guess [list of floats] initial guesses for the fit parameters
constants [dictionary] parameters and their values to hold constant during fitting (e.g. {"RO": 0.1})
method [{ 'lm', 'trf', 'dogbox' }, optional] Name of method to pass to `scipy.optimize.curve_fit`
bounds [2-tuple of array_like, optional] Lower and upper bounds on parameters. Defaults to bounds on all parameters of 0 and `np.inf`, except the CPE alpha which has an upper bound of 1

Returns

p_values [list of floats] best fit parameters for specified equivalent circuit
p_errors [list of floats] one standard deviation error estimates for fit parameters

Notes

Need to do a better job of handling errors in fitting. Currently, an error of -1 is returned.

`impedance.models.circuits.fitting.rmse` (*a, b*)

A function which calculates the root mean squared error between two vectors.

Notes

$$RMSE = \sqrt{\frac{1}{n}(a - b)^2}$$

`impedance.models.circuits.fitting.wrapCircuit` (*circuit, constants*)
wraps function so we can pass the circuit string

2.8 Frequently Asked Questions

2.8.1 What method does impedance.py use for fitting equivalent circuit models?

Fitting is performed by non-linear least squares regression of the circuit model to impedance data via `curve_fit` from the `scipy.optimize` package.[1] Real and imaginary components are fit simultaneously with uniform weighting, i.e. the objective function to minimize is,

$$\chi^2 = \sum_{n=0}^N [Z'_{data}(\omega_n) - Z'_{model}(\omega_n)]^2 + [Z''_{data}(\omega_n) - Z''_{model}(\omega_n)]^2$$

where N is the number of frequencies and Z' and Z'' are the real and imaginary components of the impedance, respectively. The default optimization method is the Levenberg-Marquardt algorithm (`method='lm'`) for unconstrained problems and the Trust Region Reflective algorithm (`method='trf'`) if bounds are provided. See the [SciPy documentation](#) for more details and options.

[1] Virtanen, P., Gommers, R., Oliphant, T.E. et al. SciPy 1.0: fundamental algorithms for scientific computing in Python. Nat Methods 17, 261–272 (2020). doi: [10.1038/s41592-019-0686-2](https://doi.org/10.1038/s41592-019-0686-2)

2.8.2 How do I cite impedance.py?

If you use impedance.py in published work, please consider citing <https://joss.theoj.org/papers/10.21105/joss.02349> as

```
@article{Murbach2020,
  doi = {10.21105/joss.02349},
  url = {https://doi.org/10.21105/joss.02349},
  year = {2020},
  publisher = {The Open Journal},
  volume = {5},
  number = {52},
  pages = {2349},
  author = {Matthew D. Murbach and Brian Gerwe and Neal Dawson-Elli and Lok-kun_
↪Tsui},
  title = {impedance.py: A Python package for electrochemical impedance analysis},
  journal = {Journal of Open Source Software}
}
```

2.8.3 How can I contribute to impedance.py?

First off, thank you for your interest in contributing to the open-source electrochemical community! We're excited to welcome all contributions including suggestions for new features, bug reports/fixes, examples/documentation, and additional impedance analysis functionality.

Feature requests and bug reports

If you want to make a suggestion for a new feature, please [make an issue](#) including as much detail as possible. If you're requesting a new circuit element or data file type, there are special issue templates that you can select and use.

Contributing code

The preferred method for contributing code to impedance.py is to fork the repository on GitHub and submit a “pull request” (PR). More detailed information on how to get started developing impedance.py can be found in [CONTRIBUTING.md](#).

Feel free to reach out via GitHub issues with any questions!

CHAPTER 3

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