pyDRTtools Documentation

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1. Introduction

pyDRTtools is a Python-based graphic user interface (GUI) for the analysis of electrochemical impedance spectroscopy (EIS) data using the distribution of relaxation times (DRT) method. The computation of the DRT is based on Bayesian ridge regression (also known as Tikhonov regularization). The DRT is discretized using piecewise linear or radial basis functions (RBFs). A snapshot of the DRTtools GUI is shown below in Figure 1.

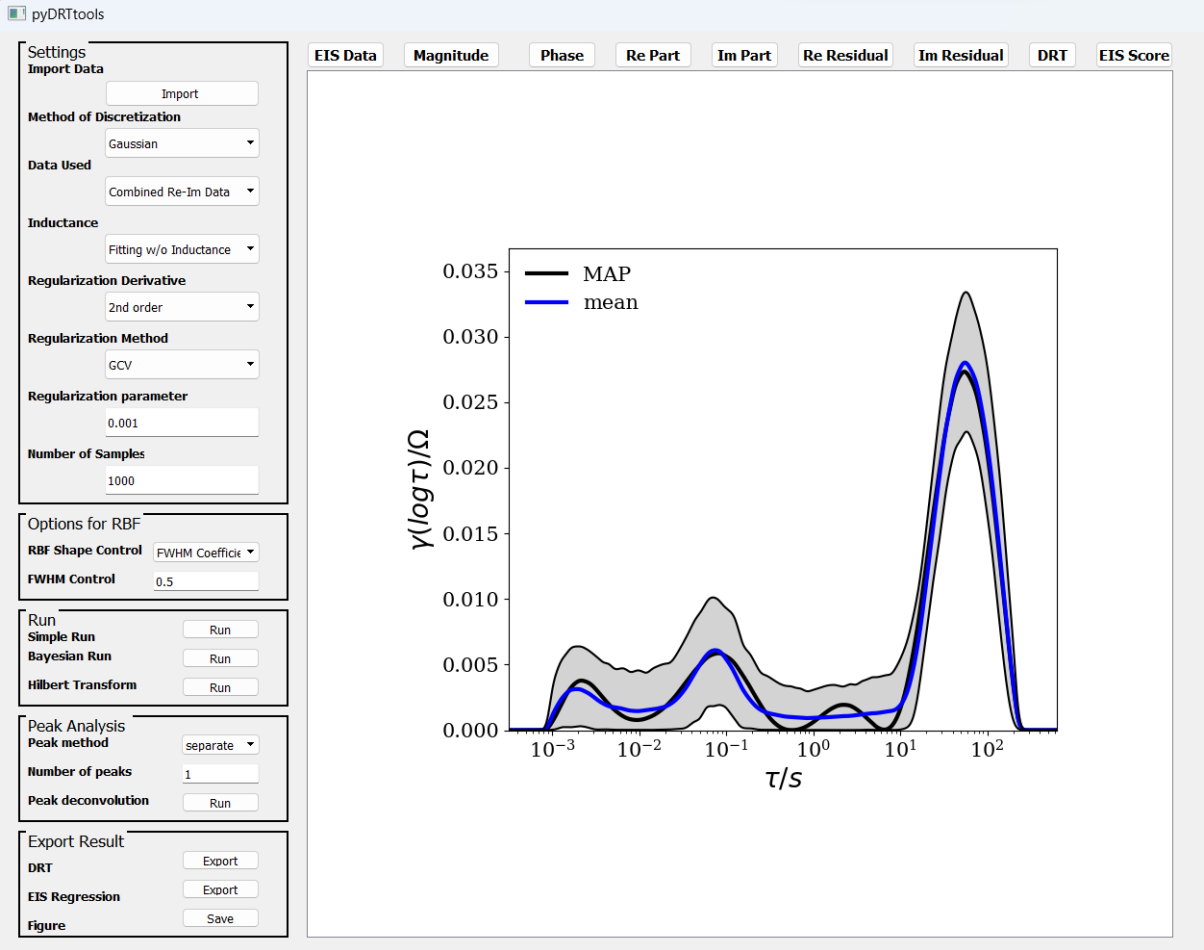


Figure 1– A snapshot of the pyDRTtools GUI.

To launch pyDRTtools, users should **run "launch_gui()"** in the anaconda prompt. When results generated by the pyDRTtools are used in journal/conference articles and other academic works, users should cite the following two references:

[1] T.H. Wan, M. Saccoccio, C. Chen, F. Ciucci, Influence of the Discretization Methods on the Distribution of Relaxation Times Deconvolution: Implementing Radial Basis Functions with DRTtools, Electrochimica Acta, 184 (2015) 483-499.

(**Link:** doi.org/10.1016/j.electacta.2015.09.097)

[2] A. Maradesa, B. Py, T.H. Wan, M.B. Effat, F. Ciucci, Selecting the Regularization Parameter in the Distribution of Relaxation Times, Journal of the Electrochemical Society, 170 (2023) 030502.

(**Link:** https://doi.org/10.1149/1945-7111/acbca4)

[3] Saccoccio, M., Wan. T. H., Chen, C., & Ciucci, F. Optimal regularization in distribution of relaxation times applied to electrochemical impedance spectroscopy: Ridge and lasso regression methods - A theoretical and experimental study. Electrochimica Acta, 147, 470-482.

(**Link:** https://doi.org/10.1016/j.electacta.2014.09.058)

If the credibility interval function is used for academic works, users should also cite the following two papers:

[4] F. Ciucci, C. Chen, Analysis of Electrochemical Impedance Spectroscopy Data Using the Distribution of Relaxation Times: A Bayesian and Hierarchical Bayesian Approach, Electrochimica Acta, 167 (2015) 439-454.

(**Link:** doi.org/10.1016/j.electacta.2015.03.123)

[5] M.B. Effat, F. Ciucci, Bayesian and Hierarchical Bayesian Based Regularization for Deconvolving the Distribution of Relaxation Times from Electrochemical Impedance Spectroscopy Data, Electrochimica Acta, 247 (2017) 1117-1129.

(**Link:** doi.org/10.1016/j.electacta.2017.07.050)

If the Hilbert Transform function is used for academic works, users should also cite the following paper:

[6] J. Liu, T.H. Wan, F. Ciucci, A Bayesian View on the Hilbert transform and the Kramers-Kronig Transform of Electrochemical Impedance Data: Probabilistic Estimates and Quality Scores, Electrochimica Acta, 357 (2020) 136864.

(**Link:** doi.org/10.1016/j.electacta.2020.136864)

Users are encouraged to read other articles from our group. A list of related references is given in Section 7 of this document. Users can also refer to the following Github link:

https://github.com/ciuccislab.

2. Installation Procedure

Since the pyDRTtools were developed in the Python language, Anaconda needs to be first installed. The installation can be done in two ways. Users can choose any of the following ways to installed pyDRTtools:

First

Create a virtual environment, activate the environment, install depenedencies, install pyDRTtools via "pip", and launch GUI from the command line

Create a virtual environment called "DRT"

```
1  conda create --name DRT python=3.9 pip ipython pandas matplotlib scikit-learn, ipython
```

Activate the environment

2 conda activate DRT

Install dependencies

3 pip install cvxopt cvxpy PyQt5

Install pyDRTtools via "pip"

4 pip install -i https://test.pypi.org/simple/ pyDRTtools==0.2.8.76

Activate ipython command line and run the following to launch the GUI

5 from pyDRTtools.GUI import launch_gui

launch_gui()

```
Type 'copyright', 'credits' or 'license' for more information
IPython 7.31.1 -- An enhanced Interactive Python. Type '?' for help.

In [1]: from pyDRTtools.GUI import launch_gui

In [2]: launch_gui()
```

Second

The pyDRTtools package can be obtained by either downloaded directly from Github (https://github.com/ciuccislab) or clone "git clone" to have pyDRTtools local repository on your computer. The following steps show how to do the installation:

1 Open your anaconda prompt and navigate to the pyDRTtools source folder directory (see

Figure 2 (a) for the procedure)

2 Install depencencies: "pip install -r requirements.txt" as shown in

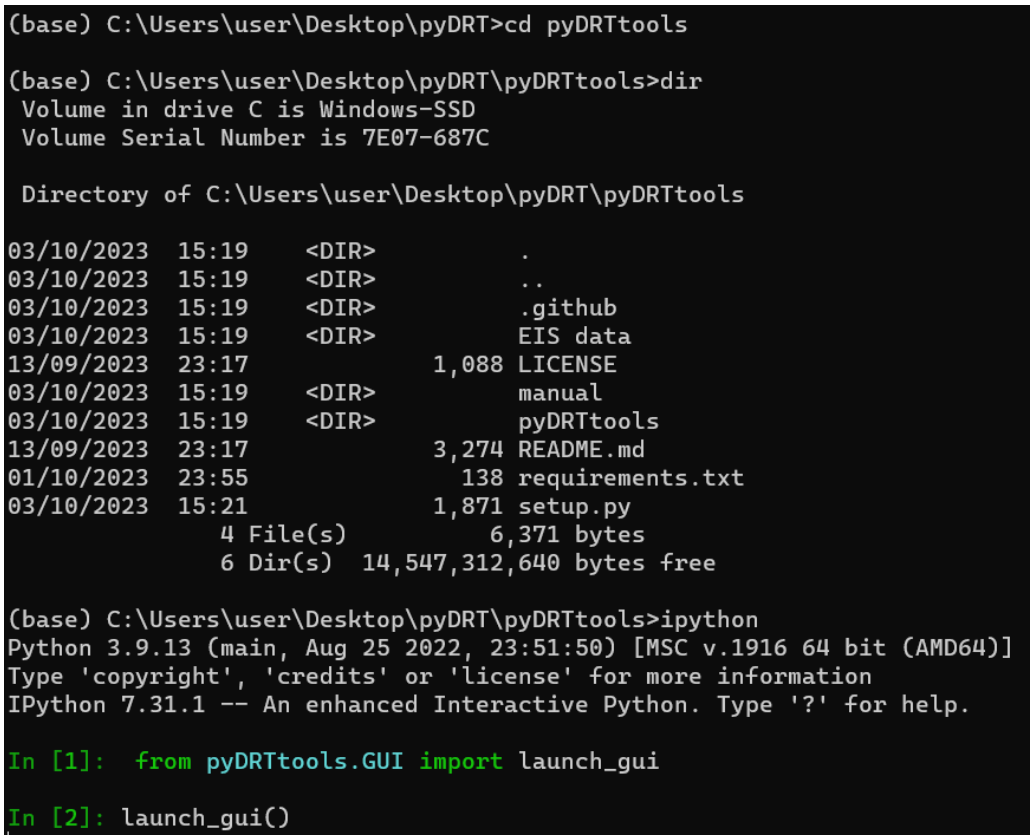
Figure 2 (b).

3 Then, use "ipython" to launch pyDRTtool GUI

from pyDRTtools.GUI import launch_gui

launch_gui()

(a)


(base) C:\Users\user\Desktop\pyDRT>cd pyDRTtools
(base) C:\Users\user\Desktop\pyDRT\pyDRTtools>dir
Volume in drive C is Windows-SSD
Volume Serial Number is 7E07-687C
Directory of C:\Users\user\Desktop\pyDRT\pyDRTtools
03/10/2023 15:19 <DIR> .
03/10/2023 15:19 <DIR> ..
03/10/2023 15:19 <DIR> .github
03/10/2023 15:19 <DIR> EIS data
13/09/2023 23:17 1,088 LICENSE
03/10/2023 15:19 <DIR> manual
03/10/2023 15:19 <DIR> pyDRTtools
13/09/2023 23:17 3,274 README.md
01/10/2023 23:55 138 requirements.txt
03/10/2023 15:21 1,871 setup.py
4 File(s) 6,371 bytes
6 Dir(s) 14,547,312,640 bytes free
(base) C:\Users\user\Desktop\pyDRT\pyDRTtools>ipython
Python 3.9.13 (main, Aug 25 2022, 23:51:50) [MSC v.1916 64 bit (AMD64)]
Type 'copyright', 'credits' or 'license' for more information
IPython 7.31.1 -- An enhanced Interactive Python. Type '?' for help.
In [1]: from pyDRTtools.GUI import launch_gui
In [2]: launch_gui()

(b)

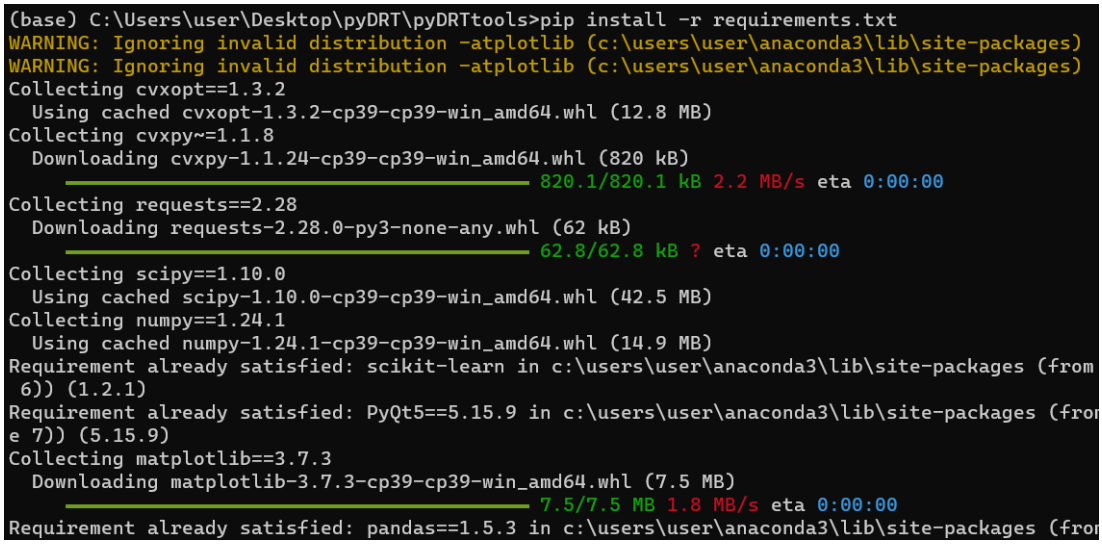


Figure 2 – Download of the required modules for running the pyDRTtools.

The complete procedure can be viewed in the video entitled ‘installation guide for pyDRTtools’.

3. General Settings

The general setting panel allows users to import EIS data and set their DRT deconvolution preferences as shown in Figure 3. The basic options include the discretization method, the selection of a specific part of the spectrum, the inclusion of an inductor, the selection of the derivative order, the selection of the regularization method, and the number of samples drawn during the Bayesian run.

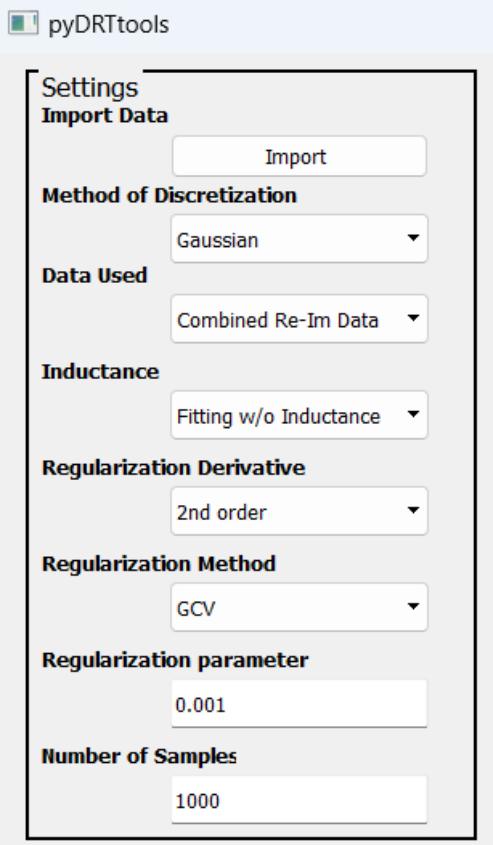


Figure 3 – The general settings sub-panel.

3.1 Importing Data

Data can be imported to pyDRTtools from .mat, .csv, or .txt files. One should click the import data button to import the data file. Upon clicking the import button, the file management panel will open, allowing users to navigate their files/folders. The .csv and .txt file to be imported should have 3 columns. From left to right, the first column corresponds to frequencies. The second column is the real part of the EIS data. The third column is the imaginary part of the EIS data. No column labels should be included. In Figure 2, users can find examples of .csv and .txt files.

(a)

	A	B	C	D
1	999.0404	0.112363	0.003183	
2	891.4258	0.112503	0.002607	
3	794.2377	0.112551	0.001995	
4	707.5095	0.112699	0.001453	
5	631.0095	0.112815	0.001029	
6	562.3392	0.11302	0.000613	
7	500.8012	0.113232	0.000216	
8	446.8588	0.113367	-0.00016	
9	397.5826	0.11362	-0.00045	
10	354.6595	0.113759	-0.00071	
11	316.3158	0.113991	-0.00099	
12	281.8943	0.114189	-0.00122	

(b)

LIB_data - Notepad

File Edit Format View Help

```
999.040405      0.112362966     0.00318273902
891.425842      0.112503432     0.00260713021
794.237671      0.112550855     0.00199478003
707.50946       0.112699494     0.00145304354
631.009521      0.112815008     0.00102882599
562.339172      0.113019735     0.000612545933
500.801239      0.113232359     0.000216439541
446.858795      0.113367356     -0.000163132951
397.582581      0.113620296     -0.00045187716
354.659485      0.11375922      -0.000712261535
316.315765      0.113991261     -0.000993279391
281.894287      0.114189491     -0.00121764559
```

Figure 4 – Examples of importable (a) .csv and (b) .txt files.

The decimal mark for the imported .txt file can either be a dot or a comma. If users wish to import a .mat file, the data should be saved as three separate vectors, “freq” (frequency data), “Z_prime” (real part of the EIS data), and “Z_double_prime” (imaginary part of the EIS data).

Moreover, it is highly recommended that the frequency data be equally spaced in the logarithm scale to reduce the computational effort. The data should be arranged so that the frequencies are in descending order. After importing, the EIS data will be plotted in a complex plot, as shown in Figure 5.

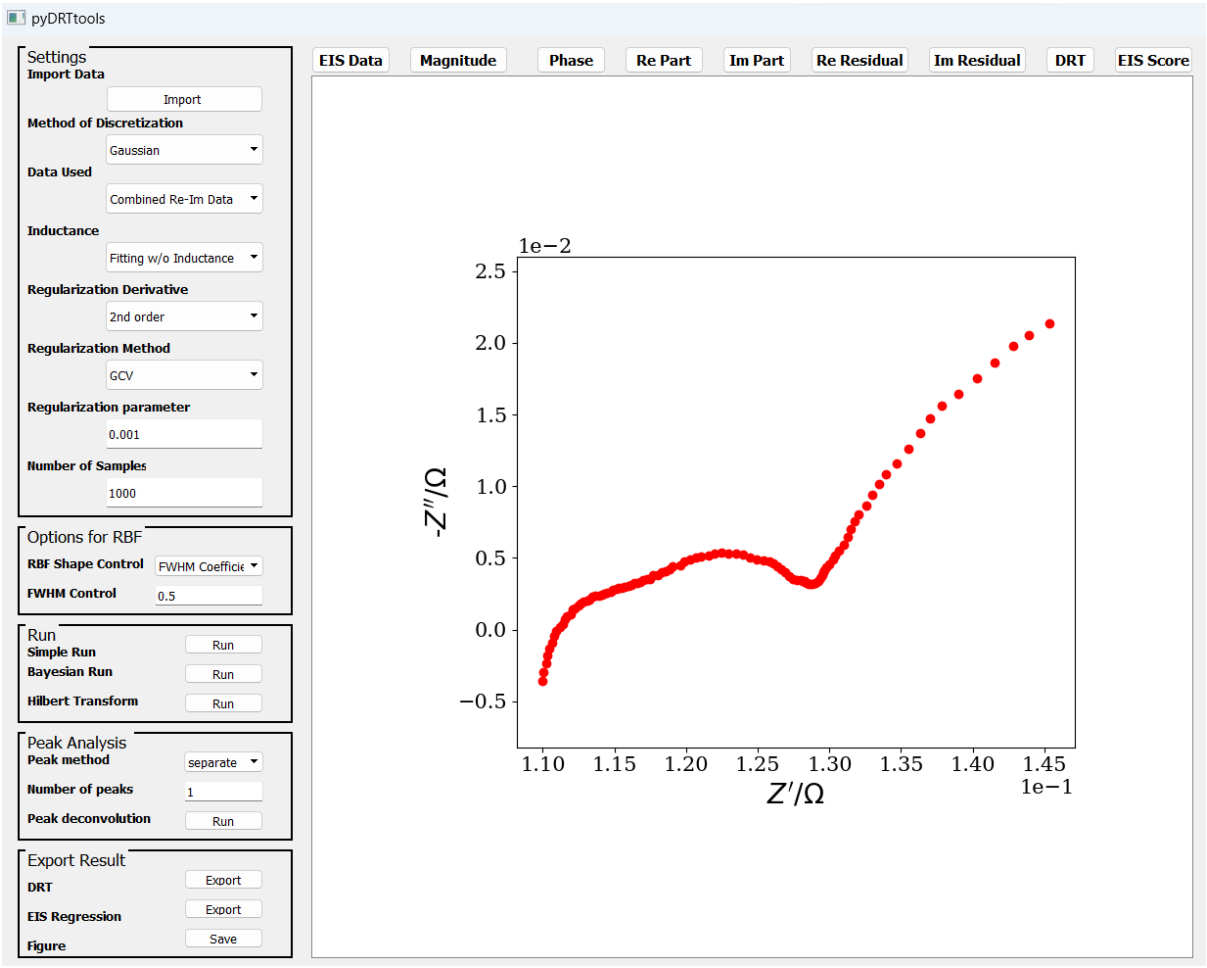


Figure 5 – The Nyquist plot of the imported experimental EIS data.

3.2 Discretization

Users can choose a suitable discretization method using the scroll-down menu. The available methods include piecewise linear and RBF discretizations.

For the piecewise linear discretization,

$$\phi_m(\ln\tau)=\begin{cases} 1-\dfrac{\ln\tau-\ln\tau_m}{\ln\tau_{m-1}-\ln\tau_m}, & \tau_{m-1}\le\tau\le\tau_m \\ 1-\dfrac{\ln\tau-\ln\tau_m}{\ln\tau_{m+1}-\ln\tau_m}, & \tau_m<\tau\le\tau_{m+1} \\ 0, & \tau<\tau_{m-1}\text{ or }\tau_{m+1}<\tau \end{cases} \quad (1)$$

where τ_m is the relaxation time of the m^{th} collocation point.

For RBF discretization, users can choose among Gaussian, C^2 Matérn, C^4 Matérn, C^6 Matérn, Cauchy, inverse quadric, and inverse quadratic functions. The available RBFs are listed in Figure 5 and Table 1.

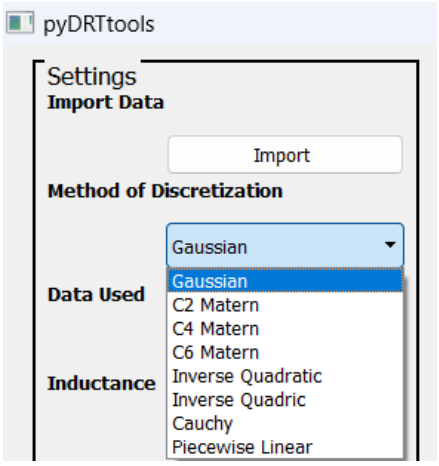


Figure 6 – The "Method of Discretization" drop-down option.

Table 1 –RBFs used by pyDRTtools where $x = |\ln\tau - \ln\tau_m|$ and μ is the shape factor of the RBFs. The Gaussian function is set as the default discretization function.

Function	$\phi_\mu(x)$
Gaussian	$\exp(-(\mu x)^2)$
C^2 Matérn	$\exp(-\lvert\mu x\rvert)\,(1+\lvert\mu x\rvert)$
C^4 Matérn	$\exp(-\lvert\mu x\rvert)\left(1+\lvert\mu x\rvert+\frac{1}{3}\lvert\mu x\rvert^2\right)$
C^6 Matérn	$\exp(-\lvert\mu x\rvert)\left(1+\lvert\mu x\rvert+\frac{2}{5}\lvert\mu x\rvert^2+\frac{1}{15}\lvert\mu x\rvert^3\right)$
Inverse Quadratic	$1/(1+(\mu x)^2)$
Inverse Quadric	$1/\sqrt{1+(\mu x)^2}$
Cauchy	$1/(1+\lvert\mu x\rvert)$

3.3 Data Used

Users can then select which part of the EIS data, either real ("Re Data"), imaginary ("Im Data"), or both real and imaginary parts ("Combined Re-Im Data"), can be used for the computation of the DRT. The "Combined Re-Im Data" is set as the default option.

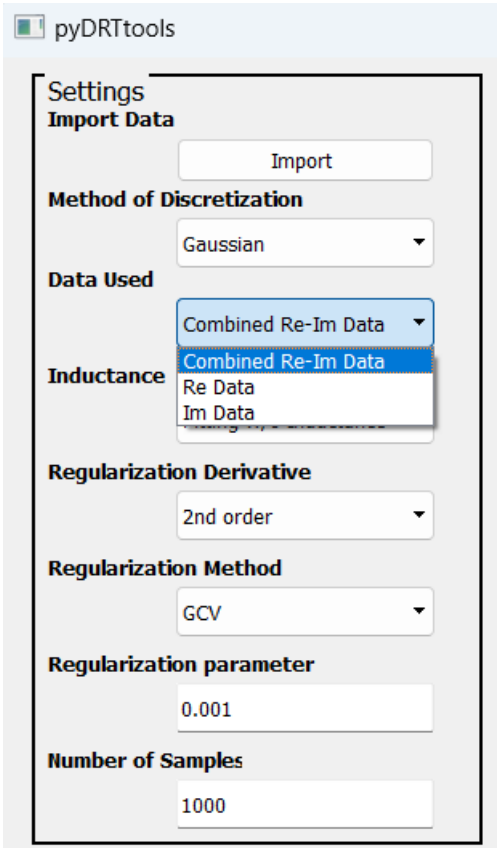


Figure 7 – The "Data Used" drop-down option.

3.4 Inductance

pyDRTtools gives three options for treating the inductive features: 1) fitting without inductance; 2) fitting with inductance; and 2) discarding the inductance.

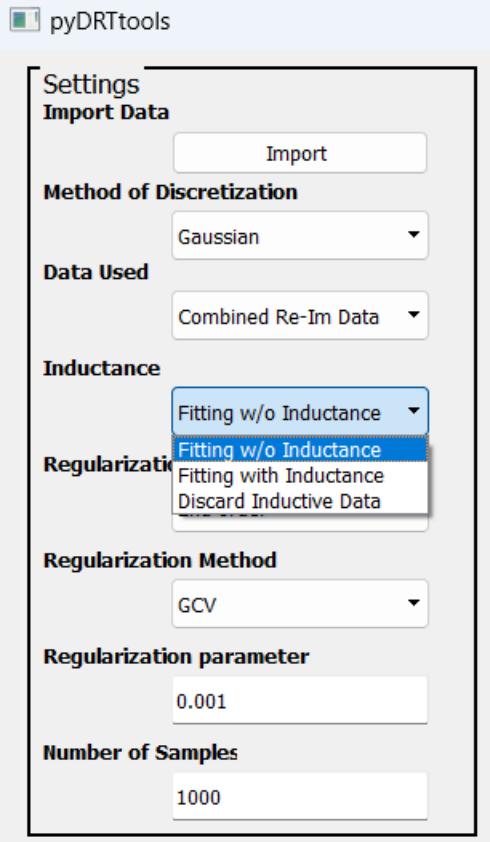


Figure 8 – The "Inductance Included" drop-down option.

The 1st option, "Fitting w/o Inductance," corresponds to using the following DRT model:

$$Z_{\mathrm{DRT}}=R_{\infty}+\int_{-\infty}^{+\infty}\frac{\gamma(\ln\tau)}{1+i2\pi f\tau}\mathrm{d}\ln\tau \tag{2}$$

where R_{∞} is the Ohmic resistance, and $\gamma(\ln\tau)$, the DRT, is a suitable function that describes the time relaxation characteristics of the electrochemical system studied.

The 2nd option, "Fitting with Inductance", corresponds to fitting the EIS data with an inductive element as well. In other words, we fit the EIS data with the following model:

$$Z_{\mathrm{DRT}}=R_{\infty}+i\,2\pi f L_0+\int_{-\infty}^{+\infty}\frac{\gamma(\ln\tau)}{1+i2\pi f\tau}\mathrm{d}\ln\tau \tag{3}$$

where the additional term compared to (2), *i.e.*, $i\,2\pi f L_0$, denotes the contribution of an inductor.

Moreover, users can also discard all the inductance data, i.e., EIS data with positive imaginary part, using the 3rd option 'Discard Inductive Data'.

3.5 Regularization Derivative

Users can choose the order of the derivative used in the penalty. If the "1st-order" option is chosen, the norm of the first-order derivative of $\gamma(\ln\tau)$, *i.e.*, $\left\|\frac{\mathrm{d}\gamma(\ln\tau)}{\mathrm{d}\ln\tau}\right\|^2$, is used as the penalty.

If the "2nd-order" option is chosen, the norm of the second-order derivative of $\gamma(\ln \tau)$, *i.e.*, $\left\| \frac{\mathrm{d}^2\gamma(\ln \tau)}{\mathrm{d} \ln \tau^2} \right\|^2$, is used as the penalty.

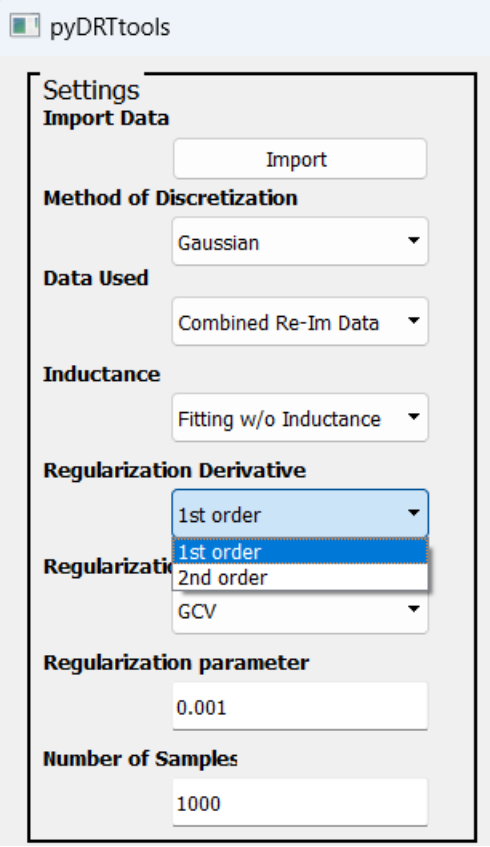


Figure 9– The "Regularization Derivative" drop-down menu.

3.6 Regularization Methods

The regularization methods can be used to optimally select the regularization parameter λ used in Tikhonov regularization. Generally, the higher λ is, the smoother the DRT profile will be. Conversely, the smaller λ is, the stronger the oscillations on the recovered DRT will be. As shown in Figure 10, pyDRTtools has different options for selecting λ.

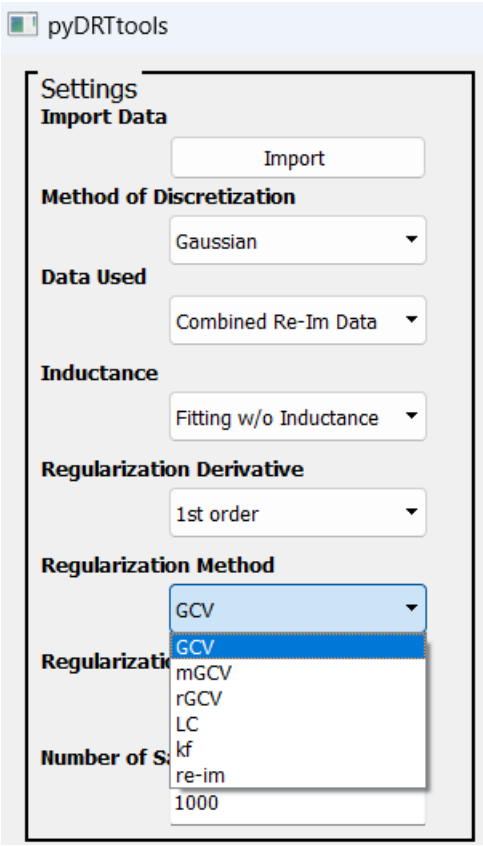


Figure 10 – The “Regularization Parameter” drop-down menu option.

3.7 Number of Samples

For the Bayesian run, samples are drawn from a truncated multivariate normal distribution. Doing so allows computing the credible interval (see section 4.2). Users can choose the total number of samples drawn. The larger this number, the more accurate the estimated credible interval will be. The sampling does not start if the number inputted is below 1000.

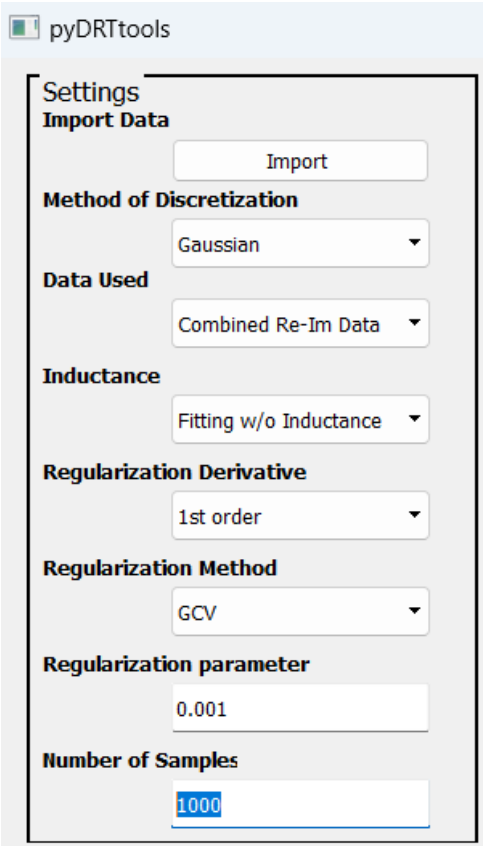


Figure 11 – The “Sample Number” option.

4. Options for Radial Basis Function Discretization

For all RBF discretizations, there are two options provided for the RBF shape control:

1) The full width at half maximum (FWHM) coefficient;
2) The shape factor.

The "FWHM Coefficient," the full width half maximum (FWHM) of the RBF is $1/m$ times the average relaxation time spacing in logarithm scale, *i.e.*,

$$\text{FWHM} = \frac{\Delta \ln \tau}{\text{coeff}} \tag{4}$$

where coeff is the FWHM coefficient that can be entered in the editable space next to the "Coefficient Value" label.

Alternatively, users may select the "Shape Factor" option. Doing so allows specifying the shape factor μ given in Table 1. The μ value can be entered in the editable space next to the "Coefficient Value" label. Users should note that, the higher the μ value is, the wider the discretization functions will be.

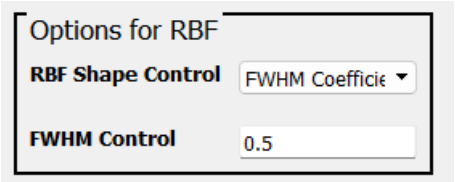


Figure 12 – The options for radial basis function discretization.

The default setting is "FWHM Coefficient" with a "Coefficient Value" of 0.5.

5. Plotting the Results

Users can visually inspect the imported EIS spectra as well as the results of regression by clicking on tabs above the figure panel (Figure 13). The original EIS spectra and the fitting result are shown by clicking “EIS Data.” The corresponding magnitude, phase angle, real and imaginary parts of the original and fitted EIS data at various frequencies are shown by clicking “Magnitude”, “Phase”, “Re Part”, and “Im Part” tabs, respectively. The residuals calculated with respect to the real and imaginary parts are shown under “Re Residual” and “Im Residual”, respectively. The deconvolved DRT is shown under the “DRT” tab. Finally, the EIS quality scores from the Hilbert transform analysis are shown if the “EIS Scores” tab is clicked.

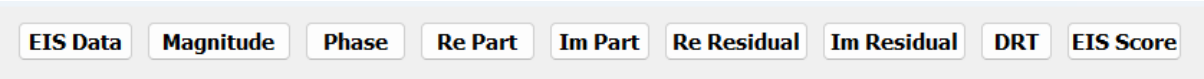


Figure 13 – The tabs above the figure panel.

6. Running pyDRTtools

DRTtools can carry out three types of computations (Figure 14):

1) Simple run – the DRT is computed based on ridge regression;
2) Bayesian run – ridge regression is used to obtain the maximum a posteriori probability (MAP) estimate of the DRT, and the credible intervals are computed using Hamiltonian Monte Carlo sampling;
3) Hilbert transform – the EIS scores are computed to quantify the quality of the EIS data.

6.1 Simple Run

The "Simple Run" starts when its corresponding button is pressed. It takes a few seconds to complete the computation. The exact duration depends on the number of data points and the discretization method.

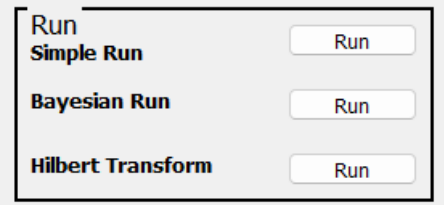


Figure 14 – The buttons for the three types of computation.

When the computation is finished, the graphic panel is updated as shown in Figure 15.

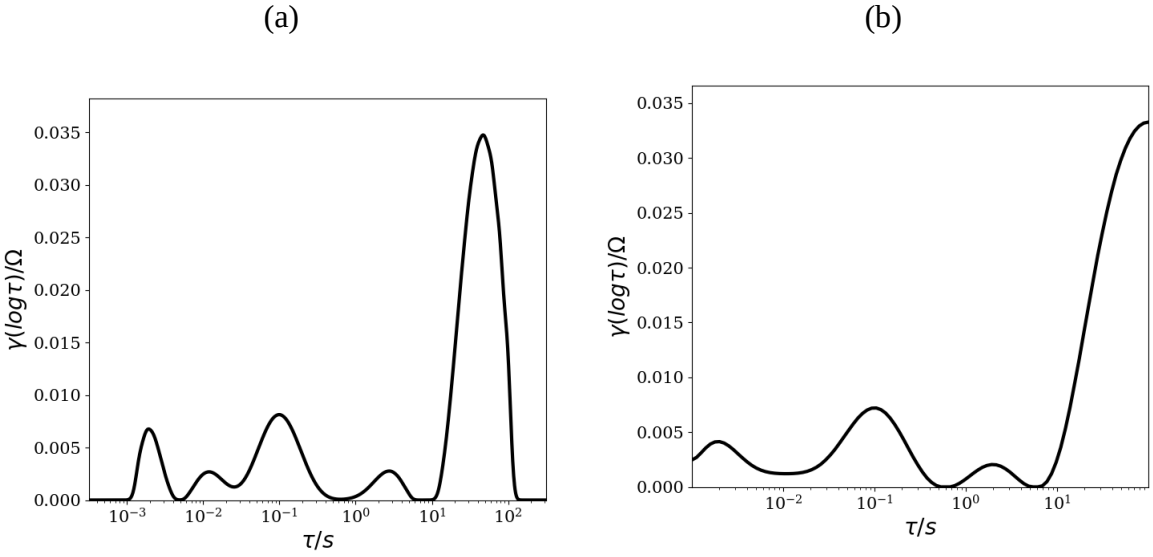


Figure 15 – Sample DRT result of the simple run using (a) RBF and (b) piecewise linear discretization.

Due to the property of the piecewise linear discretization, the $\gamma(\tau)$ is not interpolated between the collocation points. Also, the $\gamma(\tau)$ curve is truncated at the maximum and the minimum relaxation times, and will not be extrapolated out of the range, as that of the RBF based discretization does. This is shown in panel (b) of Figure 15.

In addition to the computed DRT, users can look at the fitted impedance by clicking the “EIS Data” tab above the figure panel. This is illustrated in Figure 16.

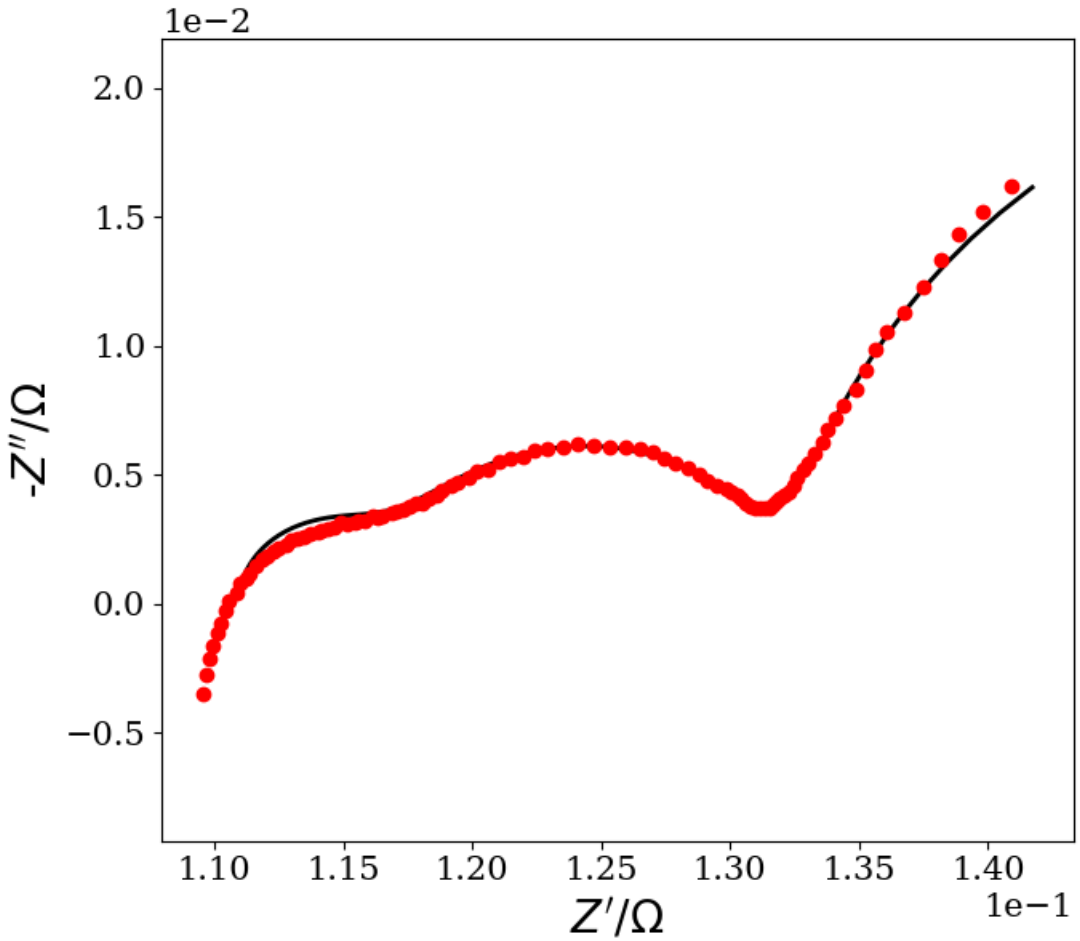


Figure 16 – Sample EIS fitting result.

The corresponding plots of the magnitude, the phase angle, the real and imaginary parts of the fitted impedance data are given in the “Magnitude”, “Phase”, “Re Part”, and “Im Part” tabs above the figure panel, respectively. Moreover, the fitting residual of the real and imaginary parts are given in the “Re Residual” and “Im Residual” tabs, respectively.

6.2 Bayesian Run

Alternatively, if users would like to compute the credibility interval of the DRT, they may click the “Bayesian Run” button. The computation of credibility interval is based on the work of Ciucci and Chen (2015) and Effat and Ciucci (2017). The credibility interval is computed by averaging the Bayesian DRT. Samples are drawn from a truncated Gaussian probability distribution function of the form of:

$$p(\mathbf{x}) \propto 1(\mathbf{x} \geq 0) \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{T}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right) \quad (5)$$

where $\boldsymbol{x}$ is the vector of $\gamma(\tau)$, $\boldsymbol{\mu}$ is the mean, and Σ is the covariance matrix. The sampling is done with a Hamiltonian Monte Carlo sampler. For more details, interested users can refer to the work of Effat and Ciucci (2017).

If credible intervals are used, users should also cite the following two articles:

[4] F. Ciucci, C. Chen, Analysis of Electrochemical Impedance Spectroscopy Data Using the Distribution of Relaxation Times: A Bayesian and Hierarchical Bayesian Approach, Electrochimica Acta, 167 (2015) 439-454.

(Link: doi.org/10.1016/j.electacta.2015.03.123**)**

[5] M.B. Effat, F. Ciucci, Bayesian and Hierarchical Bayesian Based Regularization for Deconvolving the Distribution of Relaxation Times from Electrochemical Impedance Spectroscopy Data, Electrochimica Acta, 247 (2017) 1117-1129.

(Link: doi.org/10.1016/j.electacta.2017.07.050**)**

```
-------------------------------------------------------------------------------
                                  Summary
-------------------------------------------------------------------------------
(CVXPY) Jun 13 02:01:25 PM: Problem status: optimal
(CVXPY) Jun 13 02:01:25 PM: Optimal value: -1.523e+00
(CVXPY) Jun 13 02:01:25 PM: Compilation took 1.500e-02 seconds
(CVXPY) Jun 13 02:01:25 PM: Solver (including time spent in interface) took 7.001e-03 seconds
Current sample number 1000 / 10000
Current sample number 2000 / 10000
Current sample number 3000 / 10000
Current sample number 4000 / 10000
Current sample number 5000 / 10000
Current sample number 6000 / 10000
Current sample number 7000 / 10000
Current sample number 8000 / 10000
Current sample number 9000 / 10000
Current sample number 10000 / 10000
```

Figure 17 – Sample output of the command window during sampling.

Users should note that sampling for the computation of the credibility interval takes extra time compared to the simple run. The time required for computation and the width of the credibility interval reduces if one chooses to use 2nd order derivatives. Users can also track the sampling progress on the spyder command interface, as shown in Figure 17.

When the computation is finished, the graphic panel on the right of the GUI will be updated as follow:

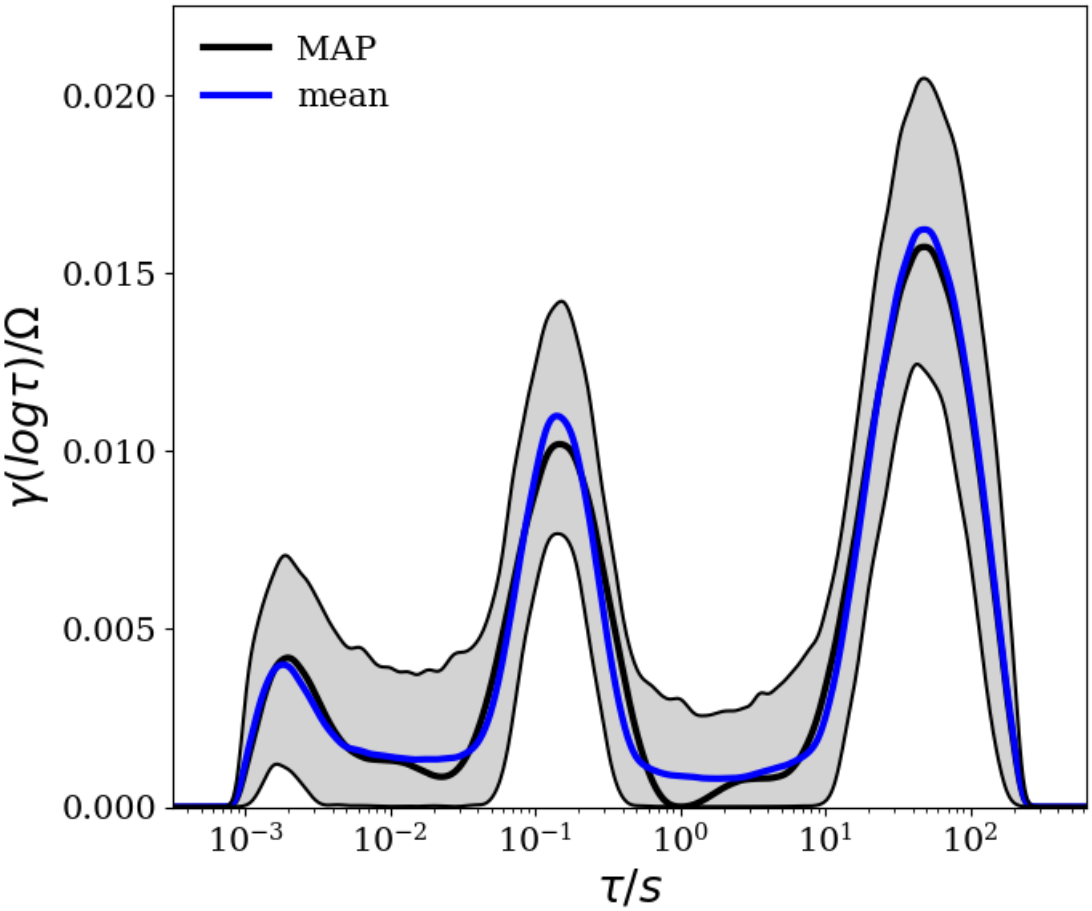


Figure 18 – DRT output sample of the Bayesian run.

In Figure 18, the black line is the Maximum-a-Posteriori (MAP) DRT, the blue line is the mean DRT, and the gray region denotes the 99% credibility interval. The credibility interval reflects the confidence of the MAP obtained. The narrower the credibility intervals, the higher the confidence of the MAP esimates.

6.3 Hilbert Transform

Moreover, users can assess the quality of their EIS data by carrying out the Bayesian Hilbert transform (BHT) computation. Users may click the "run" button next to the "Hilbert Transform" label. The BHT computation is based on Bayesian regression of the same posterior function as the Bayesian DRT, *i.e.*, (5), except that we did not considere the constraint of $\boldsymbol{x} \geq 0$. In other words, we considered that

$$p(\boldsymbol{x}) \propto \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right) \tag{6}$$

where $\boldsymbol{x}$ is the vector of $\gamma(\tau)$, and $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are the mean vector and the covariance matrix, respectively. The expressions of $\boldsymbol{\mu}$ is given as follow:

$$\boldsymbol{\mu}=\frac{1}{\sigma_n^2}\boldsymbol{\Sigma}\mathbf{A}^{\intercal}\mathbf{Z} \tag{7}$$

where $\boldsymbol{Z}$ is the impedance vector and $\boldsymbol{A}$ is the discretization matrix. The expression of $\boldsymbol{\Sigma}$ is given as follow:

$$\boldsymbol{\Sigma}=\left(\frac{1}{\sigma_n^2}\mathbf{A}^{\intercal}\mathbf{A}+\frac{1}{\sigma_\beta^2}\mathbf{I}+\frac{1}{\sigma_\lambda^2}\begin{pmatrix}0 & 0\\ 0 & \mathbf{D}_q^{\intercal}\mathbf{D}_q\end{pmatrix}\right)^{-1} \tag{8}$$

where $\mathbf{I}$ is the identity matrix and $\mathbf{D}_q$, is the q^{th} differentiation matrix.

One should note that $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ depend on three hyperparameters, *i.e.*, σ_n, σ_β, and σ_λ. These hyperparameters are selected by maximizing the experimental evidence. Furthermore, the BHT applies both the real and imaginary part of the EIS data for computation. Therefore, the computation result of the BHT **is not affected by the selection of the "Data Used" option and the "Regularization Methods" option,** as described in section 2.3 and 2.6 of this manual. For further details regarding the theory, interested users may refer to [2,6].

During the Hilbert Transform run, the Bayesian regressed and the Hilbert transformed EIS are plotted with the raw impedance data by clicking the "EIS Data" tab. In addition, the three standard deviation credible intervals for the Hilbert transformed EIS are also shown for the real and imaginary parts of the result. Moreover, the mean DRTs are calculated with both the real and imaginary parts of the EIS data. The result are shown in the "DRT" panel as illustrated in Figure 19.

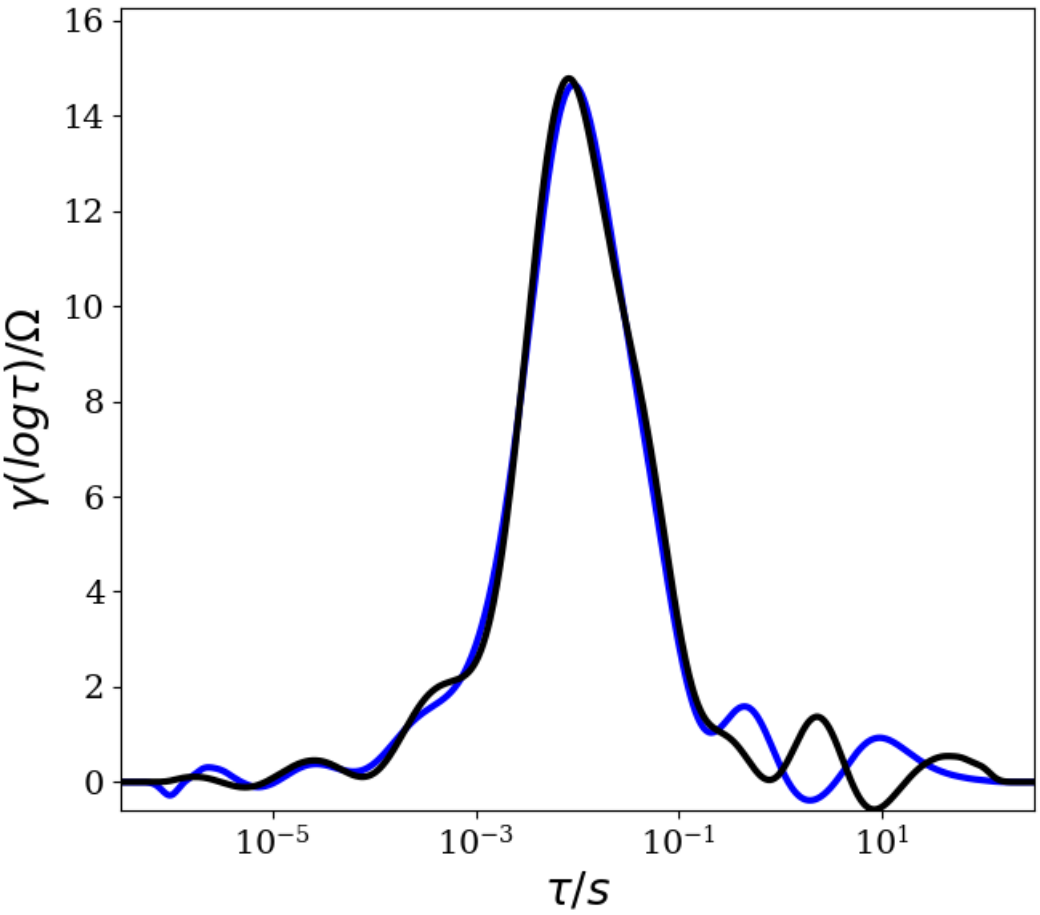


Figure 19 – Sample DRT output of the Hilbert transform run.

Users can assess the quality of the EIS data by checking the residual distribution of the real and imaginary parts of the Hilbert transformed impedance. The residual of the real and imaginary parts of the Hilbert transformed impedance are plotted with the corresponding 3σ credible band in the “Re Residual” and “Im Residual” panel, respectively, as illustrated in Figure 20.

(a) (b)

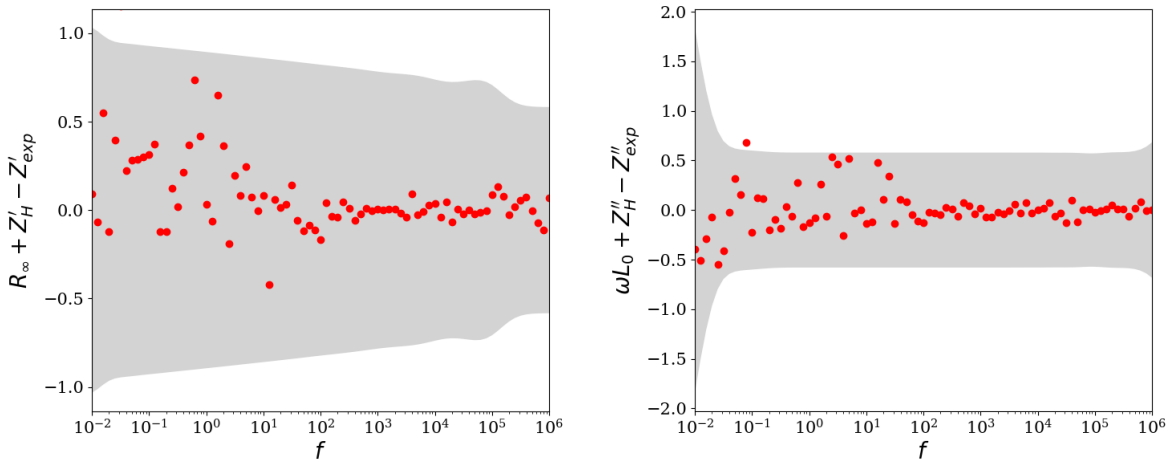


Figure 20 – Sample residual plot of the (a) real and (b) imaginary parts of the Hilbert transformed impedance.

Moreover, the Hilbert Transform run also outputs the EIS scores that quantify the quality of the EIS data. The eight EIS scores calculated are listed in Table 2.

Table 2 Notation of the EIS scores

Scores	Symbols in the Figure and [6]	Symbols in the output file
Residual	$s_{k\sigma,\mathrm{re}}, s_{k\sigma,\mathrm{im}}$	s_res_re, s_res_im
Mean	$s_{\mu,\mathrm{re}}, s_{\mu,\mathrm{im}}$	s_mu_re, s_mu_im
Hellinger Distance	$s_{\mathrm{HD,re}}, s_{\mathrm{HD,im}}$	s_HD_re, s_HD_im
Jensen-Shannon Discrepancy	$s_{\mathrm{JSD,re}}$, $s_{\mathrm{JSD,im}}$	s_JSD_re, s_JSD_im

where the subscript “re” and “im” denote the scores with respect to the real part and imaginary parts of the EIS data, respectively. The result is also given in the “EIS Score” panel as a bar chart as shown in Figure 21.

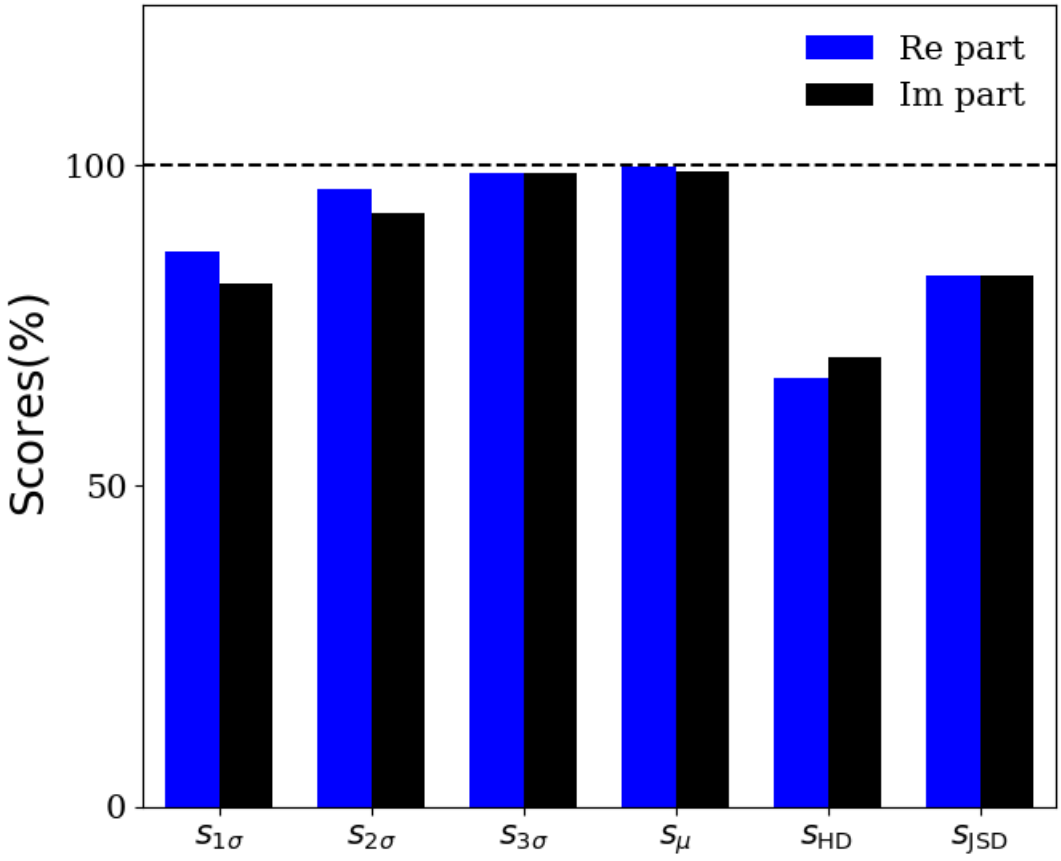


Figure 21 – The EIS scores bar chart.

All the scores were defined so that their outcomes are real numbers between 0 to 100 %. An HT-consistent EIS spectrum will score near 100 %. Instead, an HT-inconsistent EIS spectrum will score close to 0. The detail description of the scores are given in [6]. If the Hilbert Transform function is used, users should also cite the following paper:

[6] J. Liu, T.H. Wan, F. Ciucci, A Bayesian View on the Hilbert Transform and the Kramers-Kronig Transform of Electrochemical Impedance Data: Probabilistic Estimates and Quality Scores, Electrochimica Acta, 357 (2020) 136864.

(**Link:** doi.org/10.1016/j.electacta.2020.136864)

7. Peak Deconvolution

This contains functions to perform DRT peak deconvolution. Users can perform peak deconvolution by either 1) fitting separate Gaussians to the recovered DRT or 2) optimized the combined number of desired peaks, see Figure 23. To perform peak analysis, user should select the desired method (*i.e.*, separate or combine) using the "drop-down" list and input the desired number of peaks as shown in Figure 22.

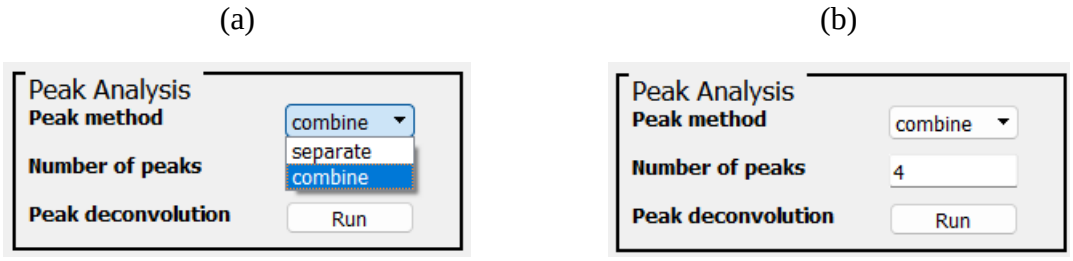


Figure 22 – Peak deconvolution

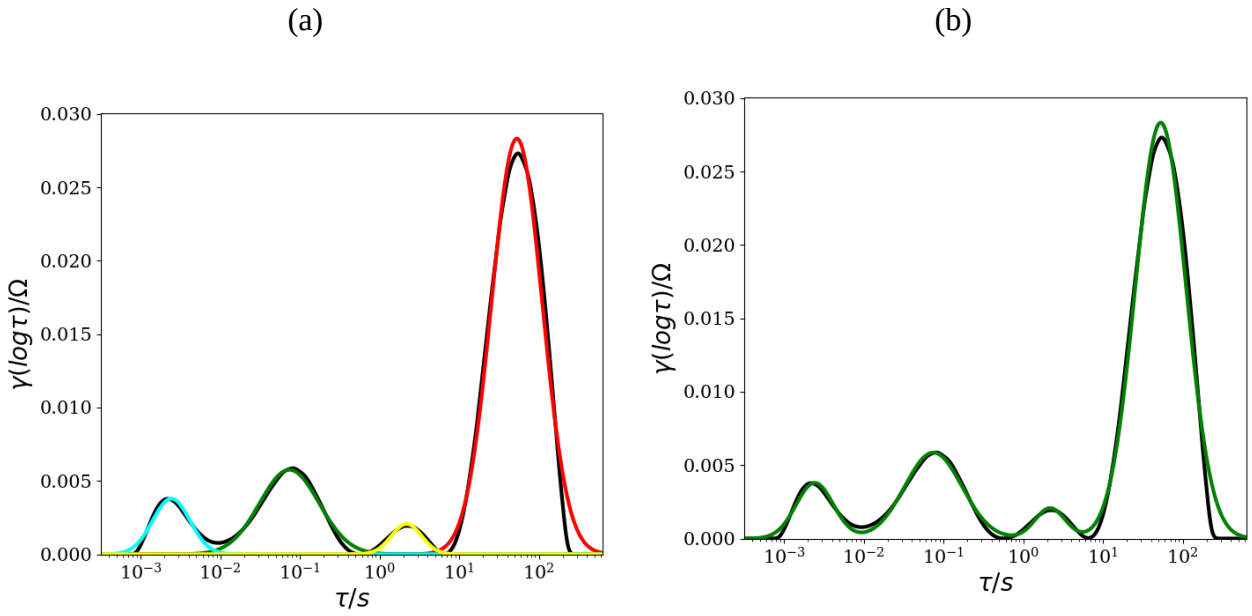


Figure 23 – Peak deconvolution by fitting (a) separate Gaussian, and (b) optimize the comnine number of peaks.

8. Exporting the Results

8.1 DRT

Users can export the DRT data by clicking the export button next to "DRT", see Figure 24. The file management panel opens and one may select the file type, either .csv file or .txt file.

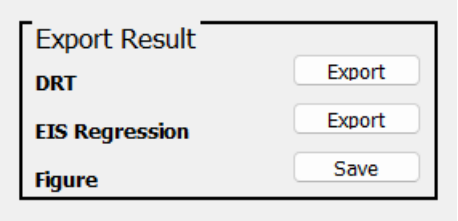


Figure 24 – The "Export Results" panel.

Users can navigate to his/her preference saving directory and click on the "save" button as shown in Figure 25.

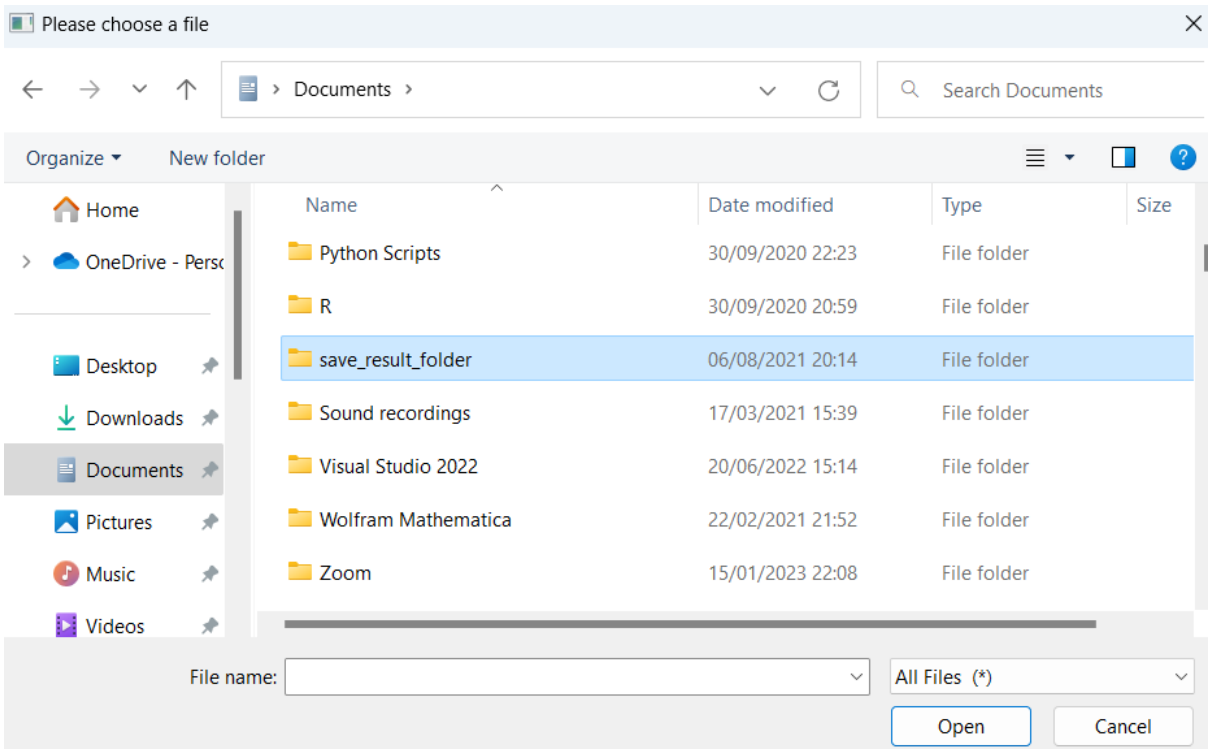


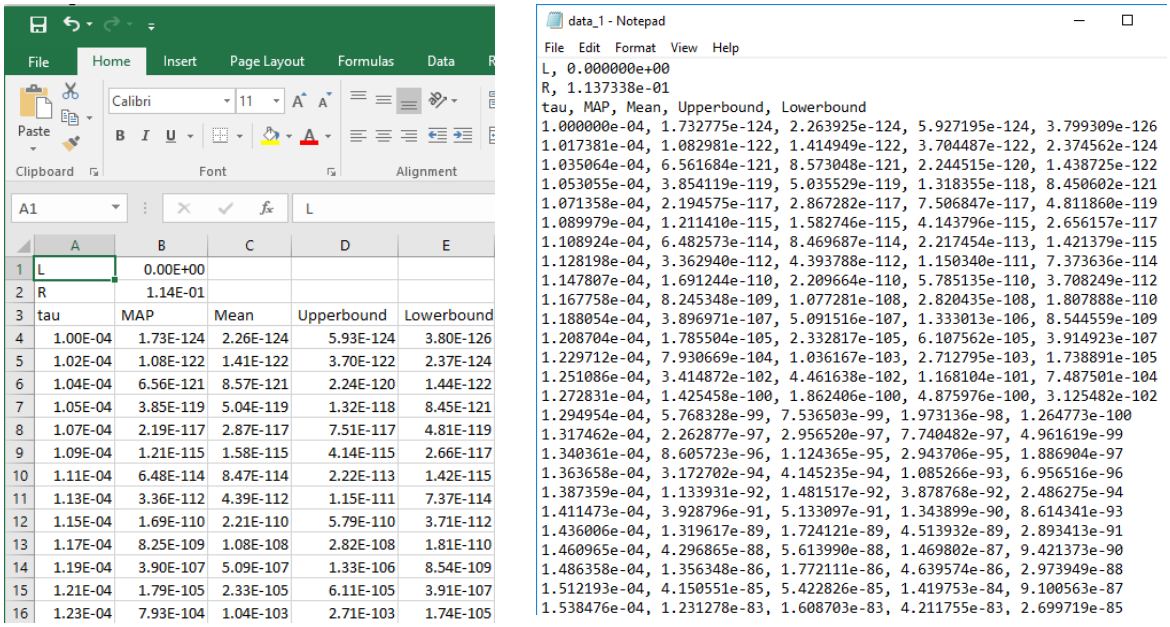
Figure 25 – The file management panel.

The first two rows of the saved set correspond to the fitted values of the Ohmic resistance R_∞ and inductance L_0. The rows under the resistance and inductance are the DRT results. The 1st column has the obtained τ values and the 2nd column corresponds to the computed $\gamma(\tau)$.

If the credibility interval is computed, the 2nd column has the MAP DRT result, the third column has the mean DRT, the 4rd and 5th columns correspond to the upper and lower bounds of the 99% credibility interval, respectively.

If the Hilbert transform is computed, the 2nd and 3th columns correspond to the $\gamma(\tau)$ computed with the real and imaginary parts, respectively.

(a) (b)



	A	B	C	D	E
1	L	0.00E+00			
2	R	1.14E-01			
3	tau	MAP	Mean	Upperbound	Lowerbound
4	1.00E-04	1.73E-124	2.26E-124	5.93E-124	3.80E-126
5	1.02E-04	1.08E-122	1.41E-122	3.70E-122	2.37E-124
6	1.04E-04	6.56E-121	8.57E-121	2.24E-120	1.44E-122
7	1.05E-04	3.85E-119	5.04E-119	1.32E-118	8.45E-121
8	1.07E-04	2.19E-117	2.87E-117	7.51E-117	4.81E-119
9	1.09E-04	1.21E-115	1.58E-115	4.14E-115	2.66E-117
10	1.11E-04	6.48E-114	8.47E-114	2.22E-113	1.42E-115
11	1.13E-04	3.36E-112	4.39E-112	1.15E-111	7.37E-114
12	1.15E-04	1.69E-110	2.21E-110	5.79E-110	3.71E-112
13	1.17E-04	8.25E-109	1.08E-108	2.82E-108	1.81E-110
14	1.19E-04	3.90E-107	5.09E-107	1.33E-106	8.54E-109
15	1.21E-04	1.79E-105	2.33E-105	6.11E-105	3.91E-107
16	1.23E-04	7.93E-104	1.04E-103	2.71E-103	1.74E-105

```
data_1 - Notepad
File  Edit  Format  View  Help
L, 0.000000e+00
R, 1.137338e-01
tau, MAP, Mean, Upperbound, Lowerbound
1.000000e-04, 1.732775e-124, 2.263925e-124, 5.927195e-124, 3.799309e-126
1.017381e-04, 1.082981e-122, 1.414949e-122, 3.704487e-122, 2.374562e-124
1.035064e-04, 6.561684e-121, 8.573048e-121, 2.244515e-120, 1.438725e-122
1.053055e-04, 3.854119e-119, 5.035529e-119, 1.318355e-118, 8.450602e-121
1.071358e-04, 2.194575e-117, 2.867282e-117, 7.506847e-117, 4.811860e-119
1.089979e-04, 1.211410e-115, 1.582746e-115, 4.143796e-115, 2.656157e-117
1.108924e-04, 6.482573e-114, 8.469687e-114, 2.217454e-113, 1.421379e-115
1.128198e-04, 3.362940e-112, 4.393788e-112, 1.150340e-111, 7.373636e-114
1.147807e-04, 1.691244e-110, 2.209664e-110, 5.785135e-110, 3.708249e-112
1.167758e-04, 8.245348e-109, 1.077281e-108, 2.820435e-108, 1.807888e-110
1.188054e-04, 3.896971e-107, 5.091516e-107, 1.333013e-106, 8.544559e-109
1.208704e-04, 1.785504e-105, 2.332817e-105, 6.107562e-105, 3.914923e-107
1.229712e-04, 7.930669e-104, 1.036167e-103, 2.712795e-103, 1.738891e-105
1.251086e-04, 3.414872e-102, 4.461638e-102, 1.168104e-101, 7.487501e-104
1.272831e-04, 1.425458e-100, 1.862406e-100, 4.875976e-100, 3.125482e-102
1.294954e-04, 5.768328e-99, 7.536503e-99, 1.973136e-98, 1.264773e-100
1.317462e-04, 2.262877e-97, 2.956520e-97, 7.740482e-97, 4.961619e-99
1.340361e-04, 8.605723e-96, 1.124365e-95, 2.943706e-95, 1.886904e-97
1.363658e-04, 3.172702e-94, 4.145235e-94, 1.085266e-93, 6.956516e-96
1.387359e-04, 1.133931e-92, 1.481517e-92, 3.878768e-92, 2.486275e-94
1.411473e-04, 3.928796e-91, 5.133097e-91, 1.343899e-90, 8.614341e-93
1.436006e-04, 1.319617e-89, 1.724121e-89, 4.513932e-89, 2.893413e-91
1.460965e-04, 4.296865e-88, 5.613990e-88, 1.469802e-87, 9.421373e-90
1.486358e-04, 1.356348e-86, 1.772111e-86, 4.639574e-86, 2.973949e-88
1.512193e-04, 4.150551e-85, 5.422826e-85, 1.419753e-84, 9.100563e-87
1.538476e-04, 1.231278e-83, 1.608703e-83, 4.211755e-83, 2.699719e-85
```

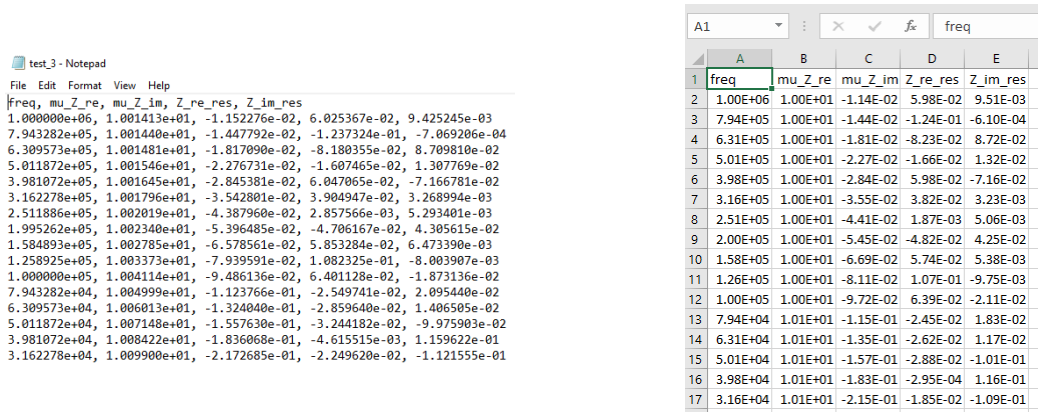
Figure 26 – Sample DRT (a) .csv and (b) .txt output files for the Bayesian run.

One should note that when the piecewise linear discretization is used, the total number of computed $\gamma(\tau)$ data points is equal to the number of EIS frequencies. On the other hand, when the RBF discretization is used, the total number of computed $\gamma(\tau)$ data points is 10 times the number of EIS data points used, with $\tau_{\max}$ being one order of magnitude larger than that of $1/f_{\min}$; $\tau_{\min}$ being one order of magnitude smaller than that of $1/f_{\max}$.

8.2 EIS Regression

Users can also save the fitted result of the EIS by clicking the "Export" button next to the "EIS Regression", see Figure 24. Upon clicking the button, the file management panel will open, allowing users to select the suitable directory. For the case of simple and Bayesian runs, the 1st column has frequencies. The 2nd and 3rd columns have the real and imaginary parts of the regressed impedance, respectively. The 4th and the 5th columns correspond to the fitting residual of the real and imaginary parts, respectively.

(a) (b)



	A	B	C	D	E
1	freq	mu_Z_re	mu_Z_im	Z_re_res	Z_im_res
2	1.00E+06	1.00E+01	-1.14E-02	5.98E-02	9.51E-03
3	7.94E+05	1.00E+01	-1.44E-02	-1.24E-01	-6.10E-04
4	6.31E+05	1.00E+01	-1.81E-02	-8.23E-02	8.72E-02
5	5.01E+05	1.00E+01	-2.27E-02	-1.66E-02	1.32E-02
6	3.98E+05	1.00E+01	-2.84E-02	5.98E-02	-7.16E-02
7	3.16E+05	1.00E+01	-3.55E-02	3.82E-02	3.23E-03
8	2.51E+05	1.00E+01	-4.41E-02	1.87E-03	5.06E-03
9	2.00E+05	1.00E+01	-5.45E-02	-4.82E-02	4.25E-02
10	1.58E+05	1.00E+01	-6.69E-02	5.74E-02	5.38E-03
11	1.26E+05	1.00E+01	-8.11E-02	1.07E-01	-9.75E-03
12	1.00E+05	1.00E+01	-9.72E-02	6.39E-02	-2.11E-02
13	7.94E+04	1.01E+01	-1.15E-01	-2.45E-02	1.83E-02
14	6.31E+04	1.01E+01	-1.35E-01	-2.62E-02	1.17E-02
15	5.01E+04	1.01E+01	-1.57E-01	-2.88E-02	-1.01E-01
16	3.98E+04	1.01E+01	-1.83E-01	-2.95E-04	1.16E-01
17	3.16E+04	1.01E+01	-2.15E-01	-1.85E-02	-1.09E-01

Figure 27 – (a) .csv and (b) .txt output files for simple run.

For the Hilbert transform, the first eight rows of the data file store the eight EIS scores, *i.e.*, $s_{k\sigma,re}$, $s_{k\sigma,im}$, $s_{\mu,re}$, $s_{\mu,im}$, $s_{HD,re}$, $s_{HD,im}$, $s_{JSD,re}$, and $s_{JSD,im}$. Following, the EIS scores are nine columns of data. The 1st column corresponds to the frequency data. The 2nd and 3rd columns are the real and imaginary parts of the Bayesian regressed impedance data, respectively. The 4th and 5th columns are the real and imaginary parts of the Bayesian regressed impedance data, respectively. The 6th and 7th columns correspond to the standard deviation of the real and imaginary parts of the Hilbert transform estimates, respectively. The 8th and 9th columns store the residual of the real and imaginary parts of the Hilbert transform estimates, respectively, see Figure 27.

(a)

EIS_RESULT.txt - Notepad

File Edit View

```
s_res_re,0.8641975308641975,0.9629629629629629,0.9876543209876543
s_res_im,0.8148148148148148,0.9259259259259259,0.9876543209876543
s_mu_re,0.9972169674312114
s_mu_im,0.9908294726766497
s_HD_re,0.6689403096743225
s_HD_im,0.6997447141533197
s_JSD_re,0.8266844706656269
s_JSD_im,0.8270413284966536
freq,mu_Z_re,mu_Z_im,mu_H_re,mu_H_im,Z_H_re_band,Z_H_im_band,Z_H_re_res,Z_H_im_res
1000000.0,10.02268859482722,-0.028348048595128777,-0.020337145190423542,0.194281192609983
794328.234724,10.022236234084486,-0.028927990940705674,-0.019106285095046926,0.1943970332
630957.34448,10.021570966014368,-0.030915764621666904,-0.019050683749270422,0.19466631154
501187.233627,10.0206323707483,-0.03430385523072299,-0.02029092956322161,0.19526757788142
398107.170553,10.019391057904597,-0.03907783601588673,-0.023086521507863837,0.1965344307
316227.766017,10.017911810162172,-0.04517869435702486,-0.027852432131710177,0.1989649736
251188.643151,10.016449009709559,-0.05247139052415379 6,-0.03513572956522333,0.20329410097
199526.231497,10.015543341148195,-0.06074635080480613,-0.04551411087521709,0.20984840470
158489.319246,10.01604658962598,-0.06978709048067788,-0.05940689156989315,0.2183698992945
```

(b)

	A	B	C	D	E	F	G	H	I
1	s_res_re	0.864198	0.962963	0.987654					
2	s_res_im	0.814815	0.925926	0.987654					
3	s_mu_re	0.997217							
4	s_mu_im	0.990829							
5	s_HD_re	0.66894							
6	s_HD_im	0.699745							
7	s_JSD_re	0.826684							
8	s_JSD_im	0.827041							
9	freq	mu_Z_re	mu_Z_im	mu_H_re	mu_H_im	Z_H_re_ba	Z_H_im_ba	Z_H_re_re	Z_H_im_res
10	1000000	10.02269	-0.02835	-0.02034	0.194281	0.227271	0.070794	0.000611	
11	794328.2	10.02224	-0.02893	-0.01911	0.194397	0.212734	-0.11281	-0.00534	
12	630957.3	10.02157	-0.03092	-0.01905	0.194666	0.203556	-0.0703	0.086218	
13	501187.2	10.02063	-0.0343	-0.02029	0.195268	0.198234	-0.00372	0.015554	
14	398107.2	10.01939	-0.03908	-0.02309	0.196534	0.195573	0.07404	-0.0663	
15	316227.8	10.01791	-0.04518	-0.02785	0.198996	0.194547	0.054257	0.010845	
16	251188.6	10.01645	-0.05247	-0.03514	0.203294	0.194203	0.020115	0.014037	

Figure 28 – (a) .csv and (b) .txt output files for Hilbert transform run.

8.3 Figures

Users can also save the figures of the results. Under Export result (Figure 24), users can click the “save” button corresponding to the label “Figure”. The file management panel will also open allowing users to select the preferred directory, see Figure 29. Users should give file name (e.g., DRT Plot) and click save.

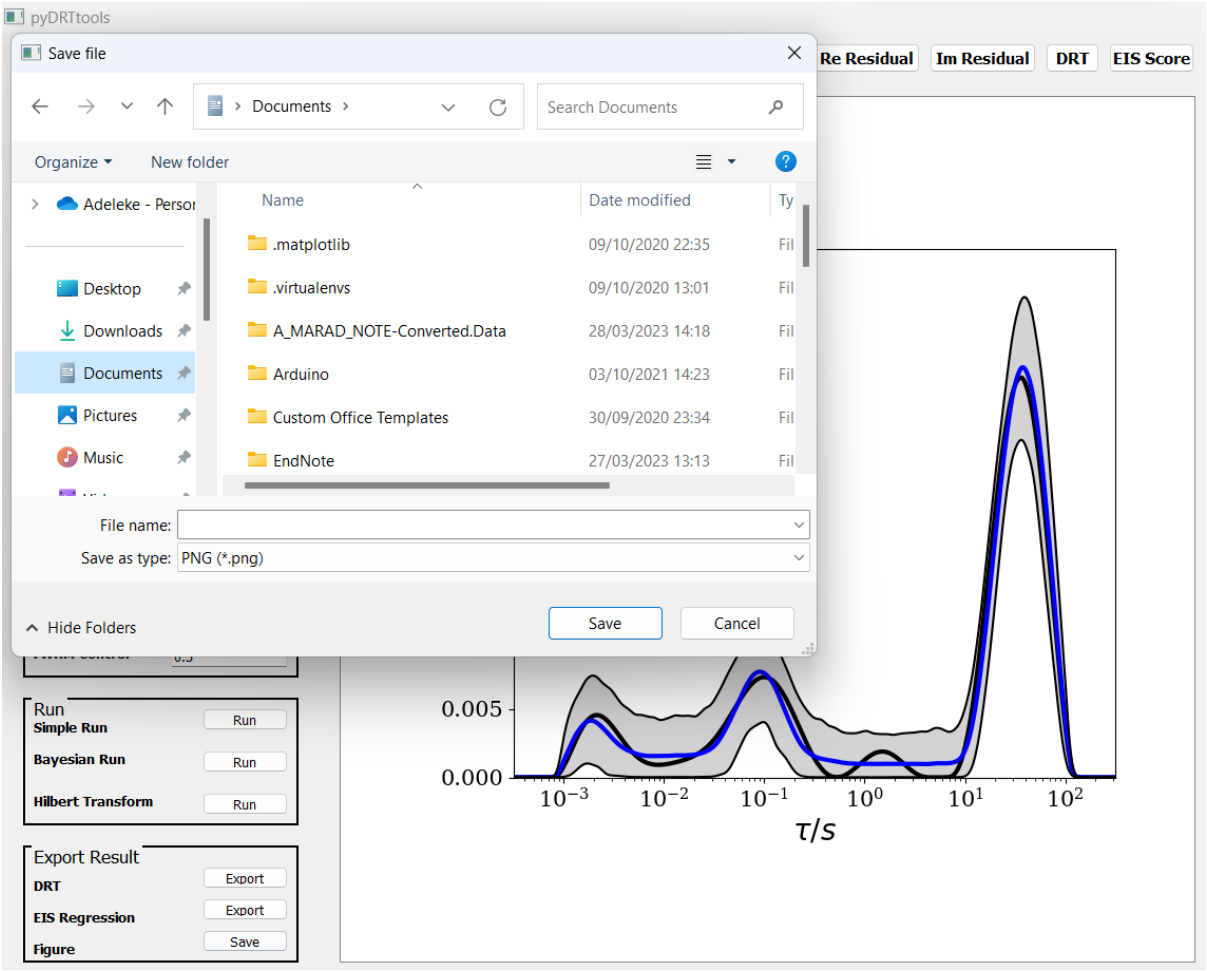


Figure 29 – Sample pyDRTtools .fig file being exported.

9. References

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