DRTtools Documentation

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1. Introduction

DRTtools is a MATLAB GUI for the analysis of electrochemical impedance spectroscopy (EIS) data using the distribution of relaxation time (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.

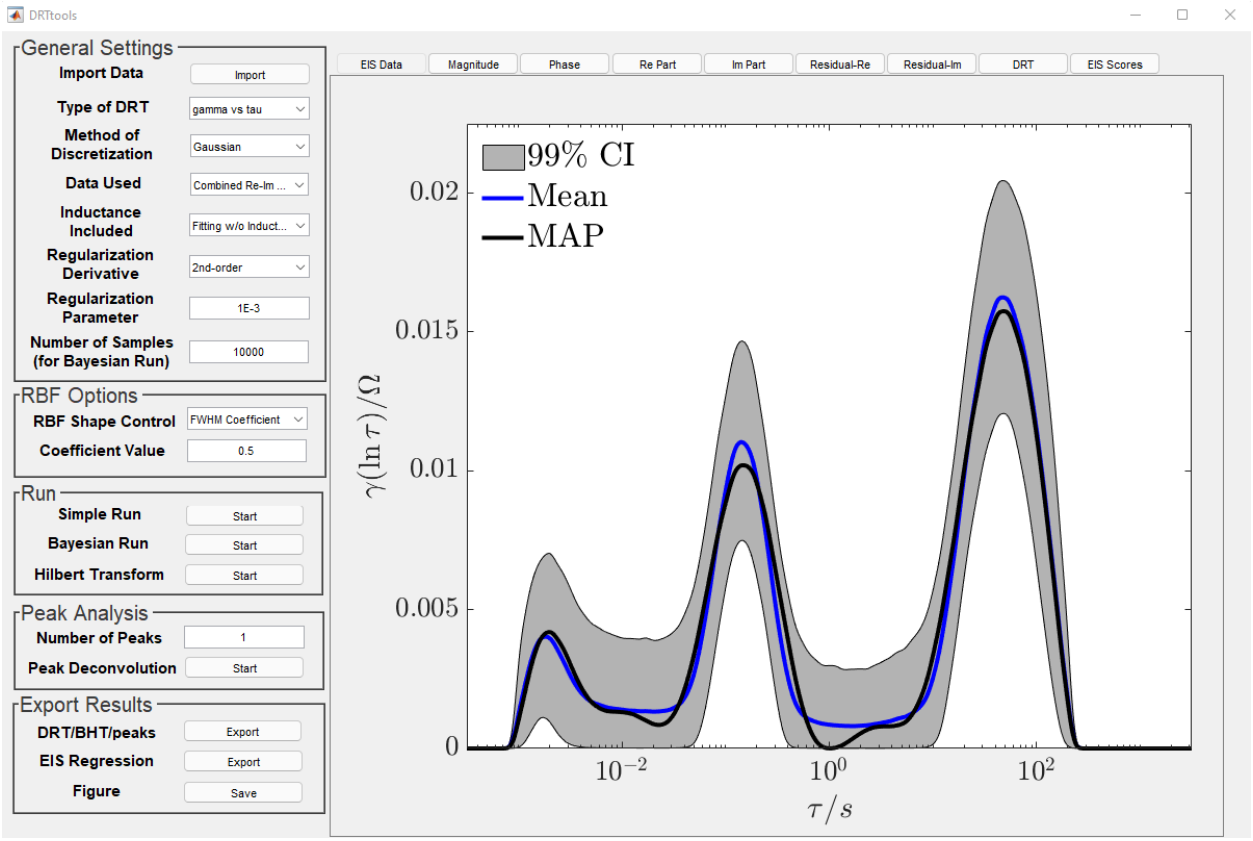


Figure 1 – A snapshot of the DRTtools GUI.

To launch DRTtools, users should **run the DRTtools.m file** in MATLAB. In addition, users should note that the Optimization Toolbox is needed for executing DRTtools.

When results generated by DRTtools are used in journal/conference articles, users should cite the following reference:

[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**)**

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

[2] 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**)**

[3] 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:

[4] 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 and cite other related articles from our group. A list of related references is included in section 7 of this document. Users can also refer to the Github of our group:

https://github.com/ciuccislab

for other codes developed for analyzing data from electrochemical experiments.

2. General Settings

In the general setting panel, users can import EIS data and select their preferences for the computation of the DRT (Figure 2). The basic options include the discretization method, the inclusion of an inductor, the selection of a specific part of the spectrum, the regularization parameter, and the number of samples for the Bayesian run.

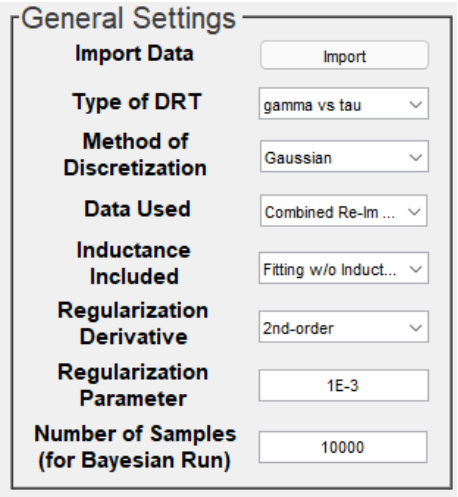


Figure 2 – General settings panel.

2.1 Importing Data

Data can be imported to DRTtools 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, you can find examples of .csv and .txt files.

(a)

A1 999.

	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 3 – Sample .csv and .txt file that can be imported.

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 4.

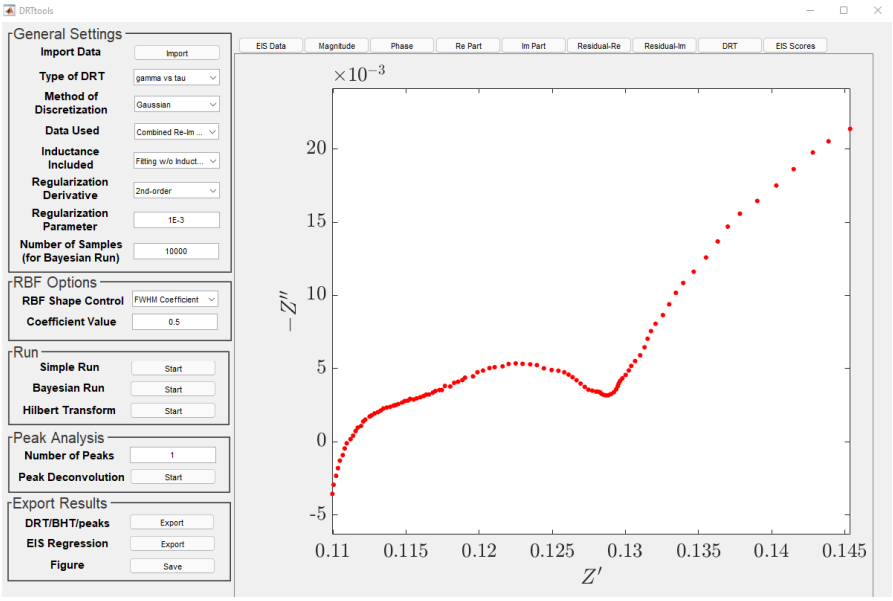


Figure 4 – The Nyquist plot of the imported experimental EIS data

2.2 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,

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

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 Table 1.

Table 1 –RBFs used by DRTtools 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	$1/(1+\lvert\mu x\rvert)$

2.3 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.

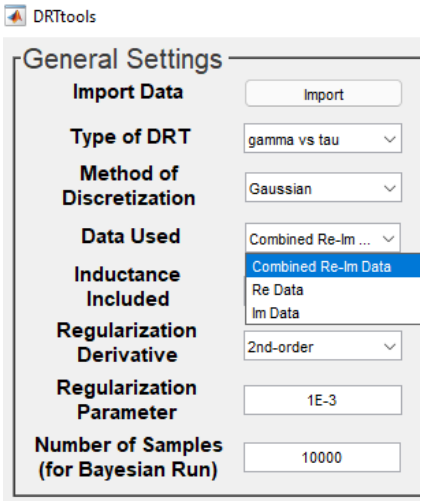


Figure 5 – "Data Used" option.

2.4 Inductance

DRTtools gives three options for treating the inductive features: 1) fitting without inductance; 2) fitting with inductance; and 3) discarding inductive data (*i.e.* discarding the part of the spectrum such that Im $Z>0$).

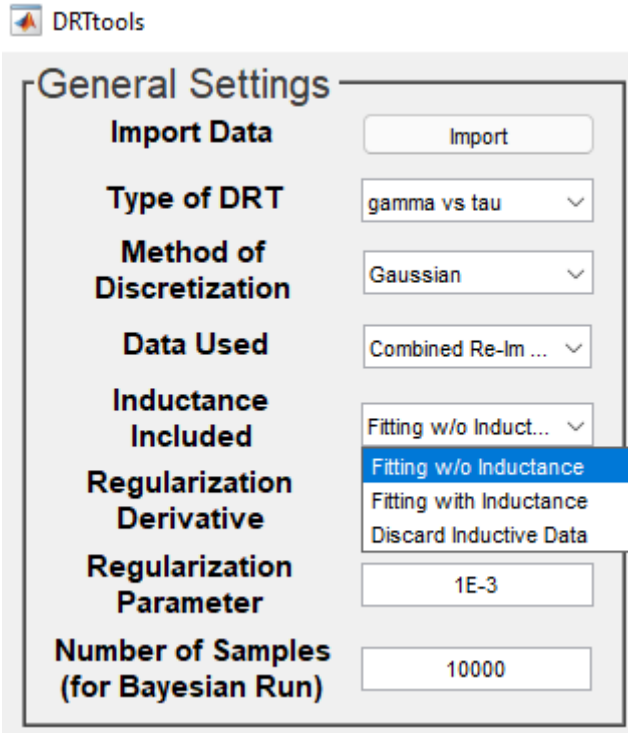


Figure 6 – "Inductance Included" option.

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

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

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:

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

where the additional term compared to (2), *i.e.*, $i2\pi fL$, denotes the contribution of an inductance L.

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

2.5 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 "1nd-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.

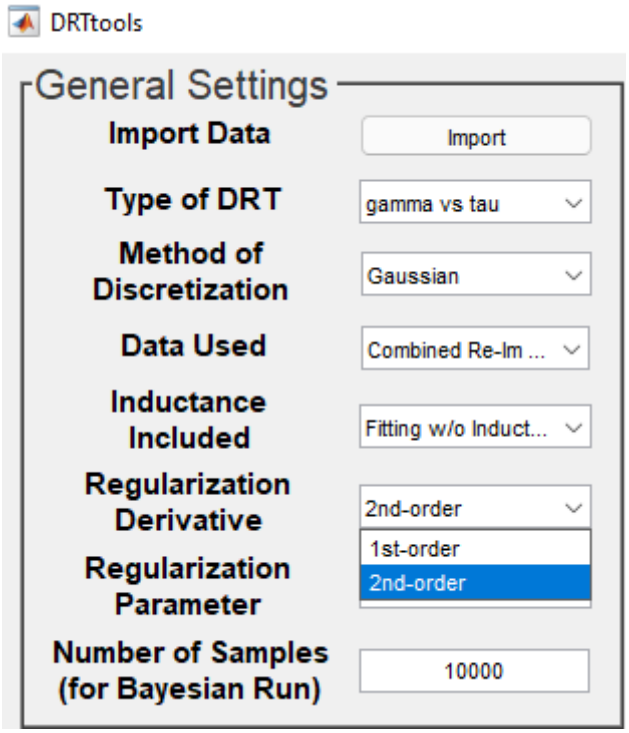


Figure 7 – The "Regularization Derivative" drop-down menu.

2.6 Regularization Parameter

The regularization parameter value can be selected using DRTtools as shown in Figure 8. Generally, the higher λ is, the smoother DRT profile will be. Conversely, the smaller λ is, the stronger the oscillation on the recovered DRT will be.

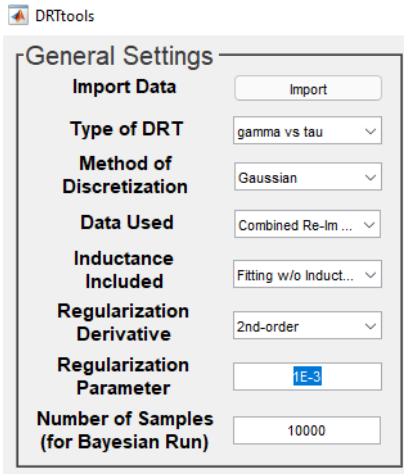


Figure 8 The "Regularization Parameter" drop-down menu option.

2.7 Number of Samples

During the Bayesian run, samples are drawn from a truncated multivariate normal distribution function. Doing so allows computing the credible interval (see section 4.2). Users can choose the total number of samples drawn during the Bayesian run. 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.

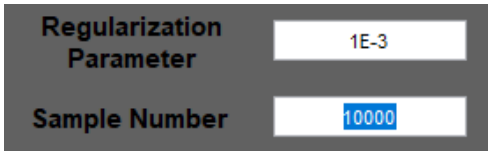


Figure 9 The "Sample Number" option

3. Options for Radial Basis Function Discretization

For all RBF discretizations, users can customize the shape of the RBF. In particular, there are two options provided for the shape control of the RBF with respect to its: 1) "FWHM Coefficient" and 2) "Shape Factor". By choosing "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.*,

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

where m is the FWHM coefficient. The m value can be entered at the editable space next to the "FWHM Control" label.

Alternatively, users may select the "Shape Factor" option, such that they may specify the shape factor μ in the discretization function directly (see Table 1). The μ value can be entered at the

editable space next to the “FWHM Control” label. The higher μ value, the wider the discretization functions are.

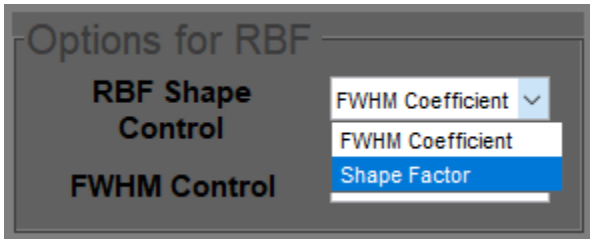


Figure 10 The options for radial basis function discretization

The shape control is set to be “FWHM coefficient” with the magnitude of 0.5 as default. In other words, the default FWHM of the discretization basis equals to two times to that of the average relaxation time spacing.

4. Result Display

Users can look at the imported EIS, fitting result and the estimated DRT for each computation by clicking the tabs above the figure panel (Figure 11). Particularly, the original EIS data and the fitting result are shown by clicking “EIS Data”. The corresponding magnitude, phase angle, real and imaginary part of the original and fitted EIS data at various frequencies are shown by clicking “Magnitude”, “Phase”, “Re Part”, and “Im Part” tab, respectively. The fitting residual with respect to the real and imaginary part are given in “Residual-Re” and “Residual-Im”, respectively. The DRT result and the EIS scores obtained from the Hilbert transform run are plotted when “DRT” and “EIS Scores” are clicked, respectively.

Figure 11 The tabs above the figure panel

5. Run

There are three types of computation for DRTtools: 1) Simple run, 2) Bayesian run, and 3) Hilbert transform (Figure 12). For simple run, the DRT is computed based on ridge regression. For the Bayesian run, in additional to the result from ridge regression, the credibility interval is also computed based on Bayesian statistics. As for the Hilbert transform, the Hilbert transformed EIS together with a set of EIS scores are computed, which can be utilized to quantify the quality of the EIS data.

5.1 Simple Run

The basic DRT computation starts when the “Start” button next to the “Simple Run” label is pressed. Generally, it takes a few second for the computation complete, which depends on the number of data point of the EIS, and whether the frequency data points are equally spaced in logarithm scale.

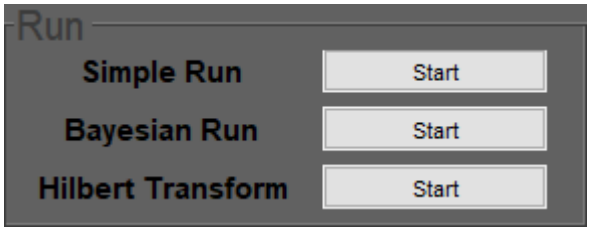


Figure 12 The buttons for the three types of computation

DRTtools provides a flag in the top right corner of the figure panel indicating that the computation is running (Figure 13)

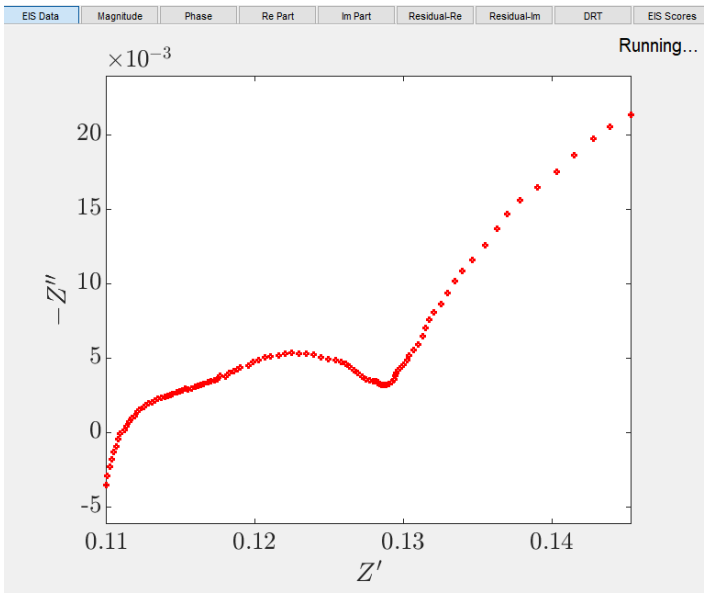


Figure 13 The “Running” flag during computation

When the computation is finished, the graphic panel on the right of the panel will be updated as shown in the panel (a) of Figure 14.

(a) (b)

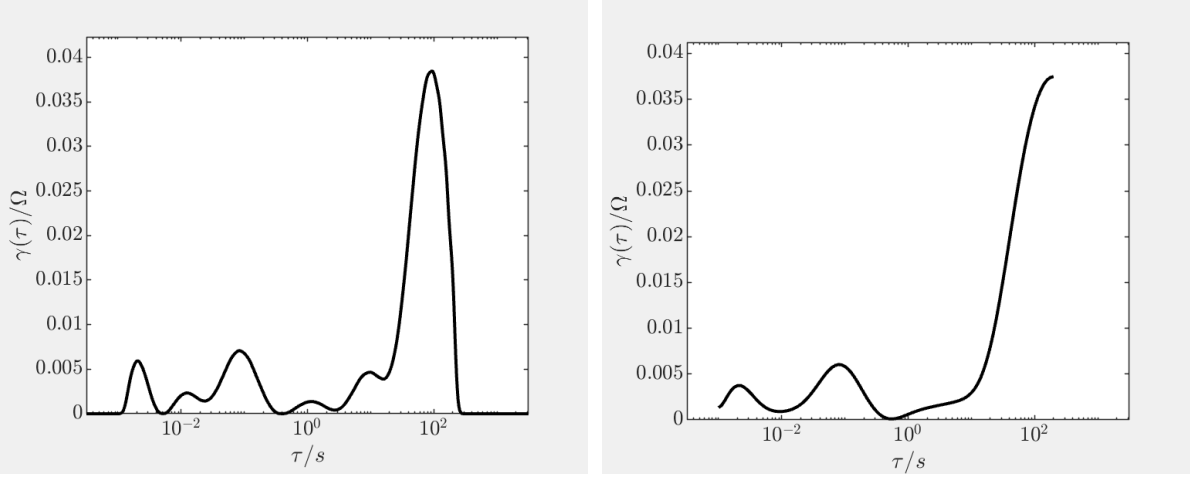


Figure 14 Sample DRT result of the simple run using (a) RBF and (b) piecewise linear discretization

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 time and will not extrapolate out of the range, as that of the RBF based discretization does. This is shown in panel (b) of Figure 14.

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 15.

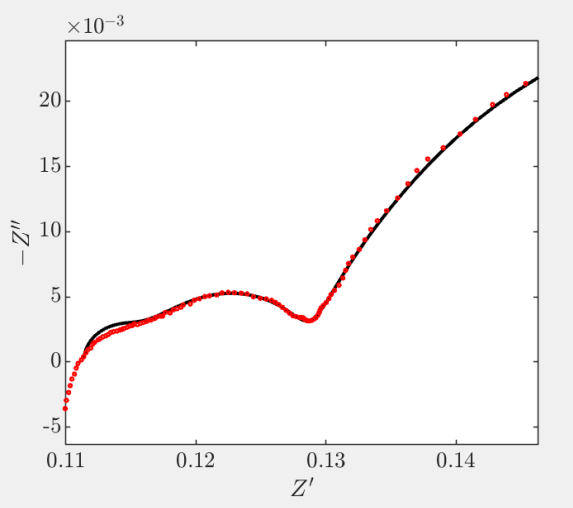


Figure 15 Sample EIS fitting result

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

5.2 Bayesian Run

Alternatively, if users would like to compute the credibility interval of the DRT, they may click the "Start" button next to the "Bayesian Run" label. 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:

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

where $\boldsymbol{x}$ is the vector of $\gamma(\tau)$, $\boldsymbol{\mu}$ is the mean, and $\boldsymbol{\Sigma}$ 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 the credibility interval function is used, users should also cite the following two paper:

[2] 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**)**

[3] 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**)**

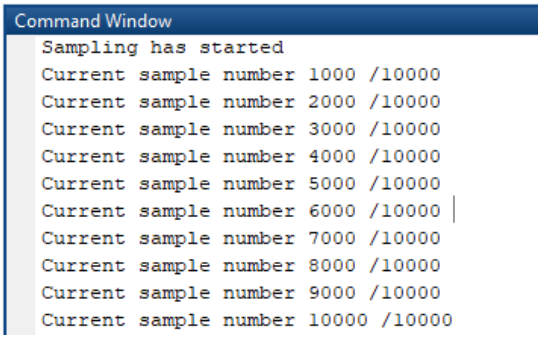


Figure 16 Sample output of the command window during sampling

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 and a larger regularization parameter for regularization. Users can also track the sampling progress on the MATLAB command window, as shown in Figure 16.

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

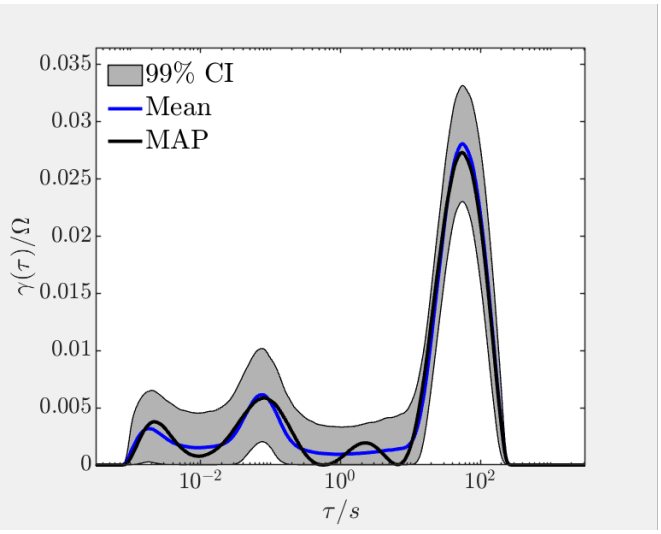


Figure 17 DRT output sample of the Bayesian run

In Figure 17, the black line is the Maximum-a-Posteriori (MAP) DRT, blue line is the mean DRT and the gray region denote the 99% credibility interval. The credibility interval reflects the confidence of the MAP obtained. Narrower the credibility interval implies a higher confidence of the MAP estimated.

5.3 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 "Start" 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 considered 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:

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

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

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

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

One should note that $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ depends on three hyperparameters, *i.e.*, σ_n, σ_β, and σ_λ. These hyperparameters are selected by the optimization of the hyperprior. Furthermore, the BHT applies both the real part and the 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 Parameter" inputs** as described in section 2.3 and 2.6 of this manual. For further details regarding the theory, interested users may refer to ref [4].

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 interval for the Hilbert transformed EIS are also shown for the real and imaginary part of the result. Moreover, the mean DRTs are calculated with both the real and imaginary part of the EIS data. The result is shown in the "DRT" panel as illustrated in Figure 18.

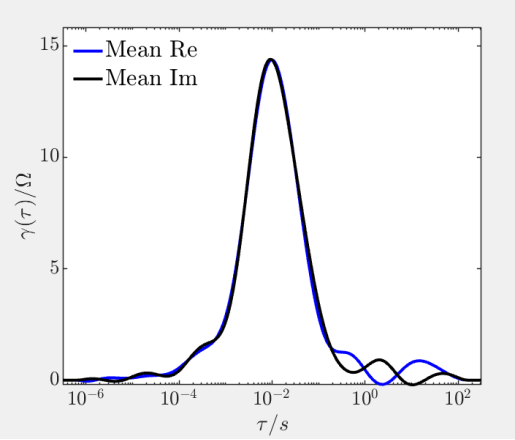


Figure 18 Sample DRT output of the Hilbert transform run

Users can assess the quality of the EIS data by checking the residual distribution of the real part and imaginary part of the Hilbert transformed impedance. The residual of the real part and imaginary part of the Hilbert transformed impedance are plotted with the corresponding 3σ credible band in the "Residual-Re" and "Residual-Im" panel, respectively, as illustrated in Figure 19.

(a) (b)

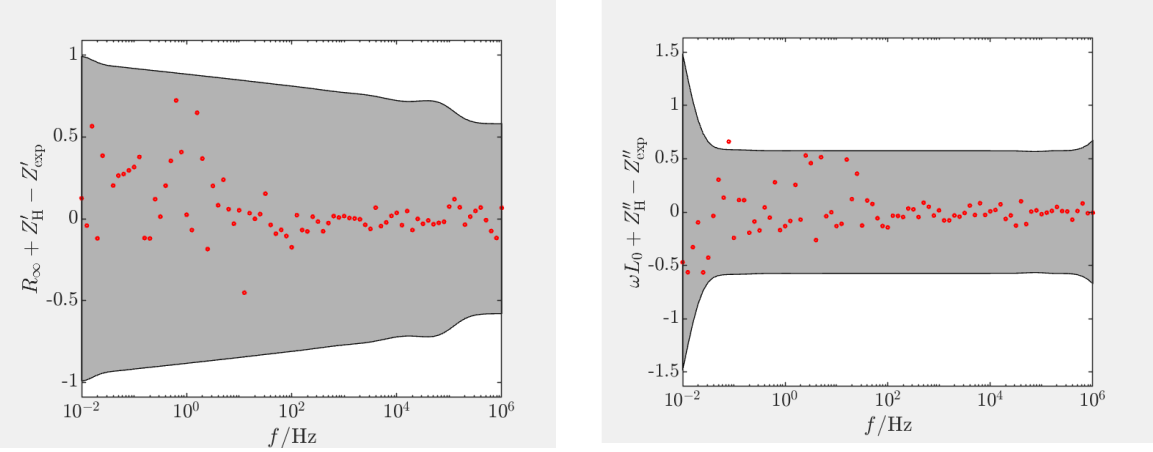


Figure 19 Sample residual plot of the real part and imaginary part of the Hilbert transformed impedance

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

Table 2 Notation of the EIS scores

Scores	Symbols in the Figure and ref [4]	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 part of the EIS data, respectively. The result is also given in the “EIS Scores” panel as a bar chart as shown in Figure 20.

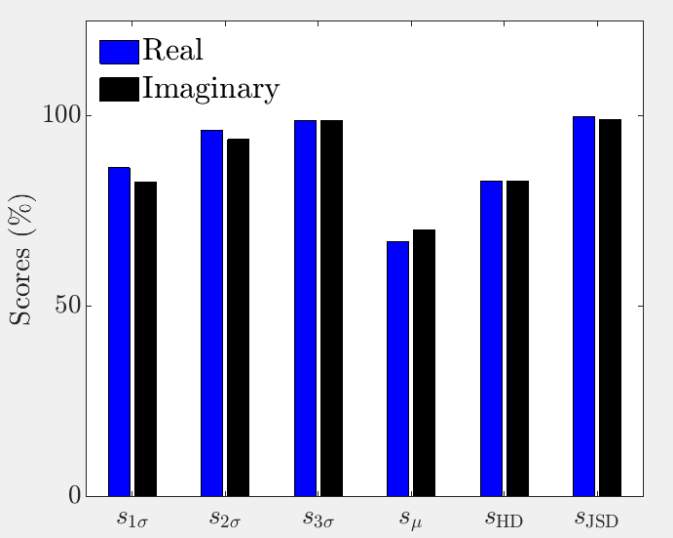


Figure 20 The EIS scores bar chart

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 100 %. The detail description of the scores are given in ref [4].

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

[4] 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**)**

6. Exporting the Results

6.1 DRT

Users can export the DRT data by clicking the export button next to "DRT". One may select the file type, either .csv file or .txt file.

Figure 21 The "Export Results" panel

Upon selecting the file type, the file management panel opens. Users can find his/her preference saving directory.

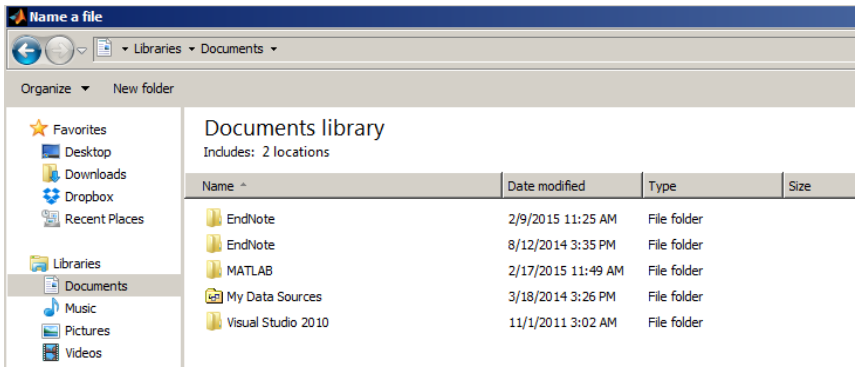


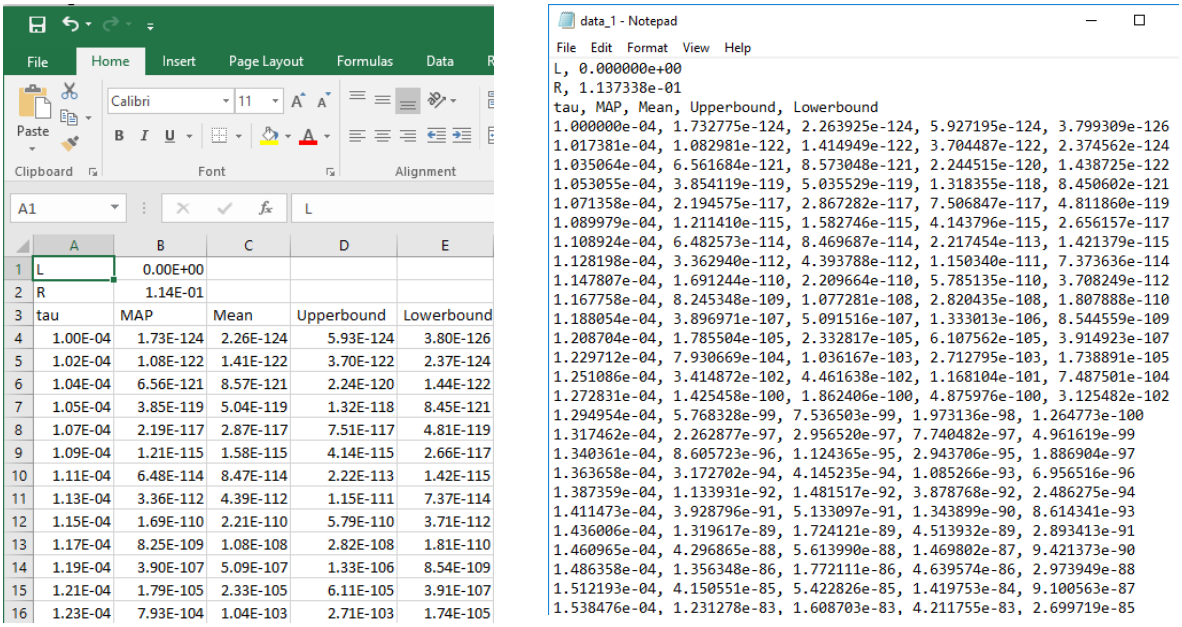
Figure 22 The file management panel

The first two rows of the saved set correspond to the fitted value of Ohmic resistance R_∞ and inductance L. 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 3rd and 4th column corresponds to the upper bound and the lower bound of the 99% credibility interval.

If the Hilbert transform is computed, the 2nd and 3th column corresponds to the $\gamma(\tau)$ computed with the real part and imaginary part, 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 23 Sample DRT .csv and .txt output file for the Bayesian run

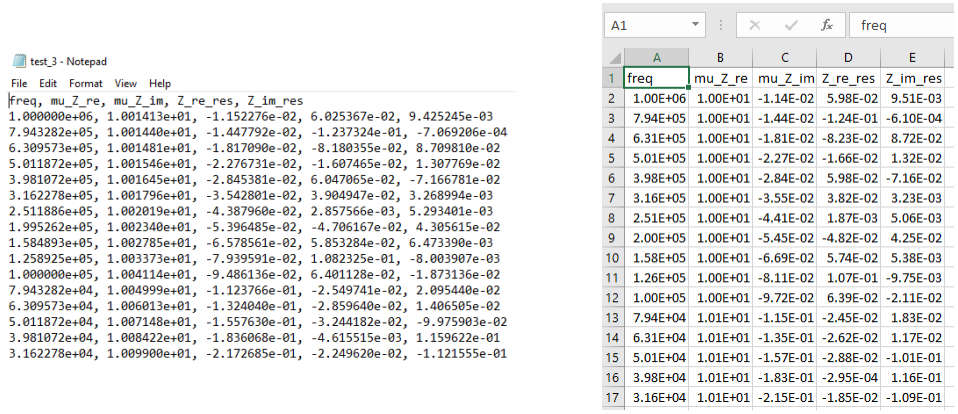
One should note that when the piecewise linear discretization is used, the total number of computed $\gamma(\tau)$ data points is equal to the number of EIS frequencies. On the other hand, when the RBF discretization is used, the total number of computed $\gamma(\tau)$ data points is 10 times the number 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 $1/f_{\max}$.

6.2 EIS Regression

Users can also save the fitted result of the EIS by clicking the "Export" button next to the "EIS". 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 column have the real and imaginary parts of the regressed impedance, respectively. The 4th and the 5th column correspond to the fitting residual of the real and imaginary part, respectively.

(a)

(b)



test_3 - Notepad

File Edit Format View Help

```
freq, mu_Z_re, mu_Z_im, Z_re_res, Z_im_res
1.000000e+06, 1.001413e+01, -1.152276e-02, 6.025367e-02, 9.425245e-03
7.943282e+05, 1.001440e+01, -1.447792e-02, -1.237324e-01, -7.069206e-04
6.309573e+05, 1.001481e+01, -1.817090e-02, -8.180355e-02, 8.709810e-02
5.011872e+05, 1.001546e+01, -2.276731e-02, -1.607465e-02, 1.307769e-02
3.981072e+05, 1.001645e+01, -2.845381e-02, 6.047065e-02, -7.166781e-02
3.162278e+05, 1.001796e+01, -3.542801e-02, 3.904947e-02, 3.268994e-03
2.511886e+05, 1.002019e+01, -4.387960e-02, 2.857566e-03, 5.293401e-03
1.995262e+05, 1.002340e+01, -5.396485e-02, -4.706167e-02, 4.305615e-02
1.584893e+05, 1.002785e+01, -6.578561e-02, 5.853284e-02, 6.473390e-03
1.258925e+05, 1.003373e+01, -7.939591e-02, 1.082325e-01, -8.003907e-03
1.000000e+05, 1.004114e+01, -9.486136e-02, 6.401128e-02, -1.873136e-02
7.943282e+04, 1.004999e+01, -1.123766e-01, -2.549741e-02, 2.095440e-02
6.309573e+04, 1.006013e+01, -1.324040e-01, -2.859640e-02, 1.406505e-02
5.011872e+04, 1.007148e+01, -1.557630e-01, -3.244182e-02, -9.975903e-02
3.981072e+04, 1.008422e+01, -1.836068e-01, -4.615515e-03, 1.159622e-01
3.162278e+04, 1.009900e+01, -2.172685e-01, -2.249620e-02, -1.121555e-01
```

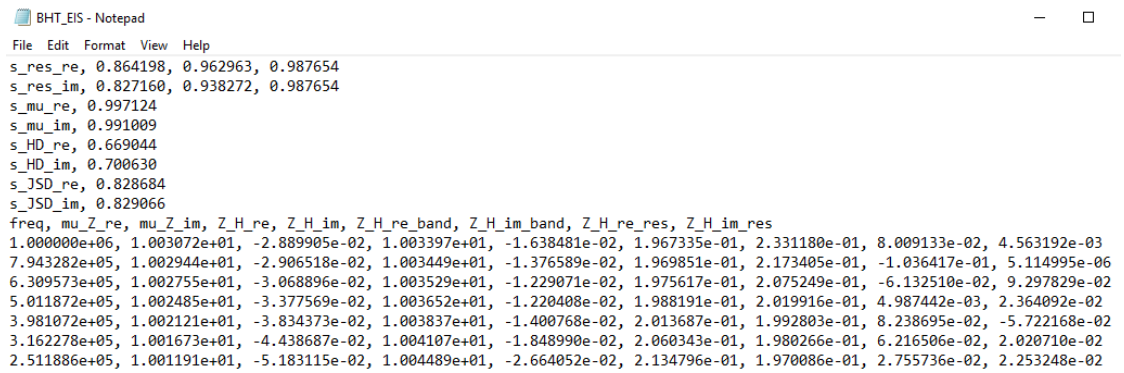
A1 freq

	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 24 Panel (a) and (b), .csv and .txt output file for simple run.

For the Hilbert transform, the first eight rows of the data file store the eight EIS scores, *i.e.*, $s_{k\sigma,\mathrm{re}}$, $s_{k\sigma,\mathrm{im}}$, $s_{\mu,\mathrm{re}}$, $s_{\mu,\mathrm{im}}$, $s_{\mathrm{HD,re}}$, $s_{\mathrm{HD,im}}$, $s_{\mathrm{JSD,re}}$, and $s_{\mathrm{JSD,im}}$. Following the EIS scores are nine columns of data. The 1st column corresponds to the frequency data. The 2nd and 3rd columns are real and imaginary parts of the Bayesian regressed impedance data, respectively. The 4th and 5th columns are real and imaginary parts of the Bayesian regressed impedance data, respectively. The 6th and 7th columns correspond to the standard deviation of real and imaginary parts of the Hilbert transform estimates. The 8th and 9th columns store the residual of the real and imaginary parts of the Hilbert transform estimates. (see Figure 25)

(a)



BHT_EIS - Notepad

File Edit Format View Help

```
s_res_re, 0.864198, 0.962963, 0.987654
s_res_im, 0.827160, 0.938272, 0.987654
s_mu_re, 0.997124
s_mu_im, 0.991009
s_HD_re, 0.669044
s_HD_im, 0.700630
s_JSD_re, 0.828684
s_JSD_im, 0.829066
freq, mu_Z_re, mu_Z_im, Z_H_re, Z_H_im, Z_H_re_band, Z_H_im_band, Z_H_re_res, Z_H_im_res
1.000000e+06, 1.003072e+01, -2.889905e-02, 1.003397e+01, -1.638481e-02, 1.967335e-01, 2.331180e-01, 8.009133e-02, 4.563192e-03
7.943282e+05, 1.002944e+01, -2.906518e-02, 1.003449e+01, -1.376589e-02, 1.969851e-01, 2.173405e-01, -1.036417e-01, 5.114995e-06
6.309573e+05, 1.002755e+01, -3.068896e-02, 1.003529e+01, -1.229071e-02, 1.975617e-01, 2.075249e-01, -6.132510e-02, 9.297829e-02
5.011872e+05, 1.002485e+01, -3.377569e-02, 1.003652e+01, -1.220408e-02, 1.988191e-01, 2.019916e-01, 4.987442e-03, 2.364092e-02
3.981072e+05, 1.002121e+01, -3.834373e-02, 1.003837e+01, -1.400768e-02, 2.013687e-01, 1.992803e-01, 8.238695e-02, -5.722168e-02
3.162278e+05, 1.001673e+01, -4.438687e-02, 1.004107e+01, -1.848990e-02, 2.060343e-01, 1.980266e-01, 6.216506e-02, 2.020710e-02
2.511886e+05, 1.001191e+01, -5.183115e-02, 1.004489e+01, -2.664052e-02, 2.134796e-01, 1.970086e-01, 2.755736e-02, 2.253248e-02
```

(b)

	A	B	C	D	E	F	G	H	I
1	s_res_re	0.864198	0.962963	0.987654					
2	s_res_im	0.82716	0.938272	0.987654					
3	s_mu_re	0.997124							
4	s_mu_im	0.991009							
5	s_HD_re	0.669044							
6	s_HD_im	0.70063							
7	s_JSD_re	0.828684							
8	s_JSD_im	0.829066							
9	freq	mu_Z_re	mu_Z_im	Z_H_re	Z_H_im	Z_H_re_b	Z_H_im_b	Z_H_re_r	Z_H_im_res
10	1.00E+06	1.00E+01	-2.89E-02	1.00E+01	-1.64E-02	1.97E-01	2.33E-01	8.01E-02	4.56E-03
11	7.94E+05	1.00E+01	-2.91E-02	1.00E+01	-1.38E-02	1.97E-01	2.17E-01	-1.04E-01	5.11E-06
12	6.31E+05	1.00E+01	-3.07E-02	1.00E+01	-1.23E-02	1.98E-01	2.08E-01	-6.13E-02	9.30E-02
13	5.01E+05	1.00E+01	-3.38E-02	1.00E+01	-1.22E-02	1.99E-01	2.02E-01	4.99E-03	2.36E-02
14	3.98E+05	1.00E+01	-3.83E-02	1.00E+01	-1.40E-02	2.01E-01	1.99E-01	8.24E-02	-5.72E-02
15	3.16E+05	1.00E+01	-4.44E-02	1.00E+01	-1.85E-02	2.06E-01	1.98E-01	6.22E-02	2.02E-02
16	2.51E+05	1.00E+01	-5.18E-02	1.00E+01	-2.66E-02	2.13E-01	1.97E-01	2.76E-02	2.25E-02

Figure 25 Panel (a) and (b), .csv and .txt output file for Hilbert transform run

6.3 Figures

Users can also save the figures of the result. Particularly, users should first select the figure they decided to save by clicking the tabs above the figure panel (see section 4). After that users can press the “Save” button next to the “Figure” label to save the figure. Upon pressing the button, the file management panel will open allowing users to select their preferred directory.

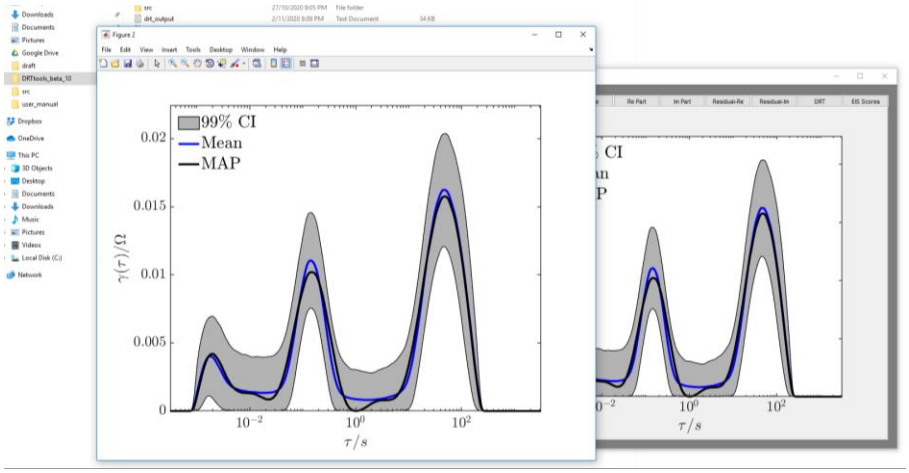


Figure 26 Sample MATLAB .fig file being exported

7. References

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