## Readme for the Tafel fitting procedure

Note: The following packages for running these scripts are required:

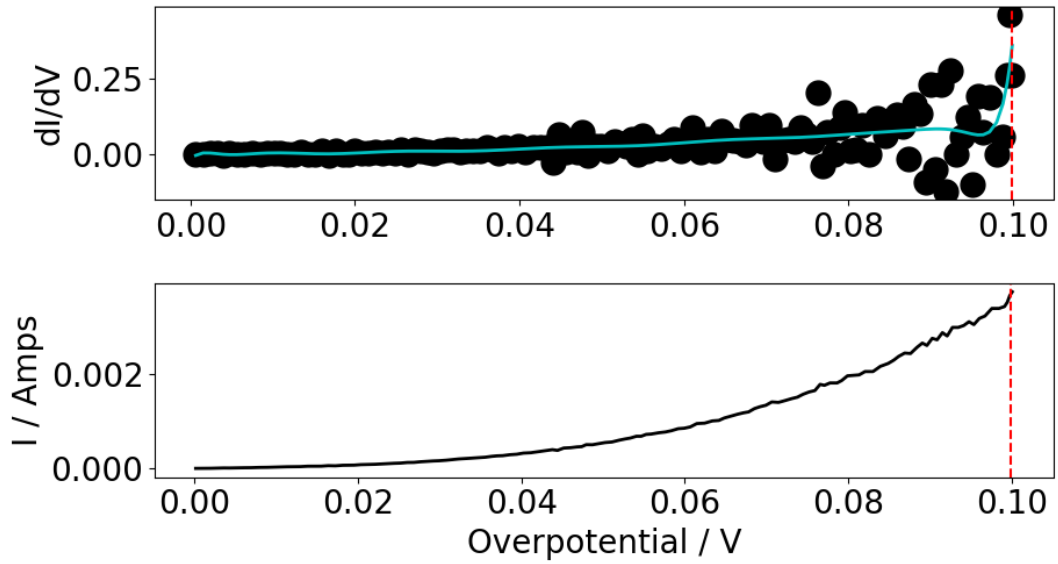
Directions on using the interactive prompt.
0. The file to be fit should be a .csv file located in the subdirectory '**Input_files**'. These input data should be files containing three columns: column 1 is the overpotential axis, column 2 is the current, in amperes, and column 3 is the logarithm of column 2 (or, equivalently, experimentally measured Tafel data acquired over the same overpotential range as the current data).
1. Start a python shell (ipython recommended) using either a client such as Anaconda, Jupyter or by starting a python shell from the command line. Ipython interpreters are highly recommended for this purpose.
2. Load the program into an ipython shell by entering '**from Tfit_beta1p5 import ***' from the command shell:
>>> from Tfit_beta1p5 import *
3. From here, call the Run() procedure from the shell:
>>>Run()
4. Calling Run() opens an interactive prompt that reads the data files provided in the 'Input_files' directory and presents them as a numbered list (Example 1). Enter the number (0, 1, etc.) for the file containing the data you wish to fit. Enter in the last line in the file containing header information (in the examples provided, the header information is only the first line of the file, so 1 is entered).

```
File  Edit  View  Terminal  Tabs  Help
In [5]: from Tfit_beta1p5 import *

In [6]: Run()
Files to be analyzed must be in the current working directory.
File number     Filename
0       /home/pcagbo/Desktop/Tafel_fit/Input_files/20181010Irhsa_perchloric_OER_02_CV_C01_cut2(baseline-a
djusted).csv
Which dataset do you want to inspect (enter file number)? 0
Enter the last line of the file header (enter "0" if none present): 1
Fit dLSV with a polynomial of order n = 1,2,3..? 15
voltage cutoff (blue dotted line) = 0.0997411 V
do you want to accept this fit (y/n)? y
Enter the range of overpotential window sizes (dV) to check, in volts (i.e., [0.01, 0.05] ): [0.01, 0.05]
Enter the dV increment to use, in volts (i.e., 0.001): 0.001
Enter the range of R-squared values over which to conduct the fits (i.e., [0.900, 1.000] ): [0.900, 1.000
]
Enter the increment for the R-squared value range (i.e., 0.001): 0.001
Enter the binning size to use for dV-span optimization, in millivolts (1 mV default): 1

Voltage cutoff = 0.0997411 V
Fit Interval / V        Exchange Current / A    Tafel slope (mV/decade) Tafel Residue
[0.0028484, 0.0128484]  4.394074368307124e-06   13.379586345528399      0.00333861691437

Actual Tafel R2:        0.9688432182344582 ; Actual LSV R2:     0.9787760118647355
For minimum R2 = 0.9, voltage interval width = 0.01


Voltage cutoff = 0.0997411 V
```

## Example 1

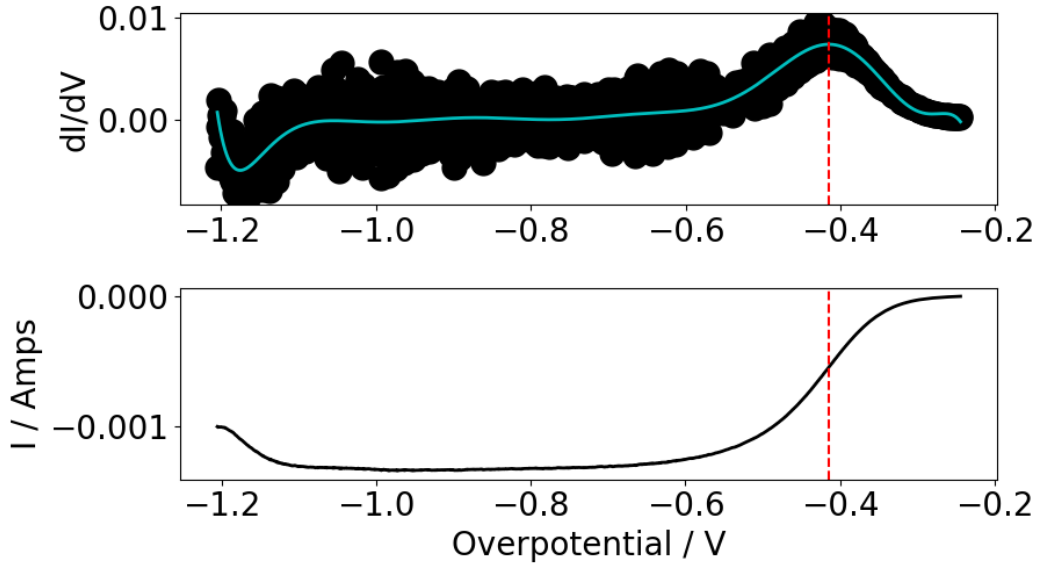
Typical interactive inputs for the program. Input data are read from the subfolder 'Input_files'. Potentials are in volts, binning values are in millivolts.

5. During the interactive prompt, the user is asked to provide a number for what order polynomial should be used to fit the first derivative of the linear sweep voltammogram. When a number is provided, the following plot is generated, which allows the user to check the suitability of the polynomial fit. A 15$^{th}$ order polynomial is used in the two fitting examples below.




## Example 2a

A polynomial fit of data featuring no diffusion-limited currents. Here, all data are accepted and used for fitting (data to the left of the red, dashed line).

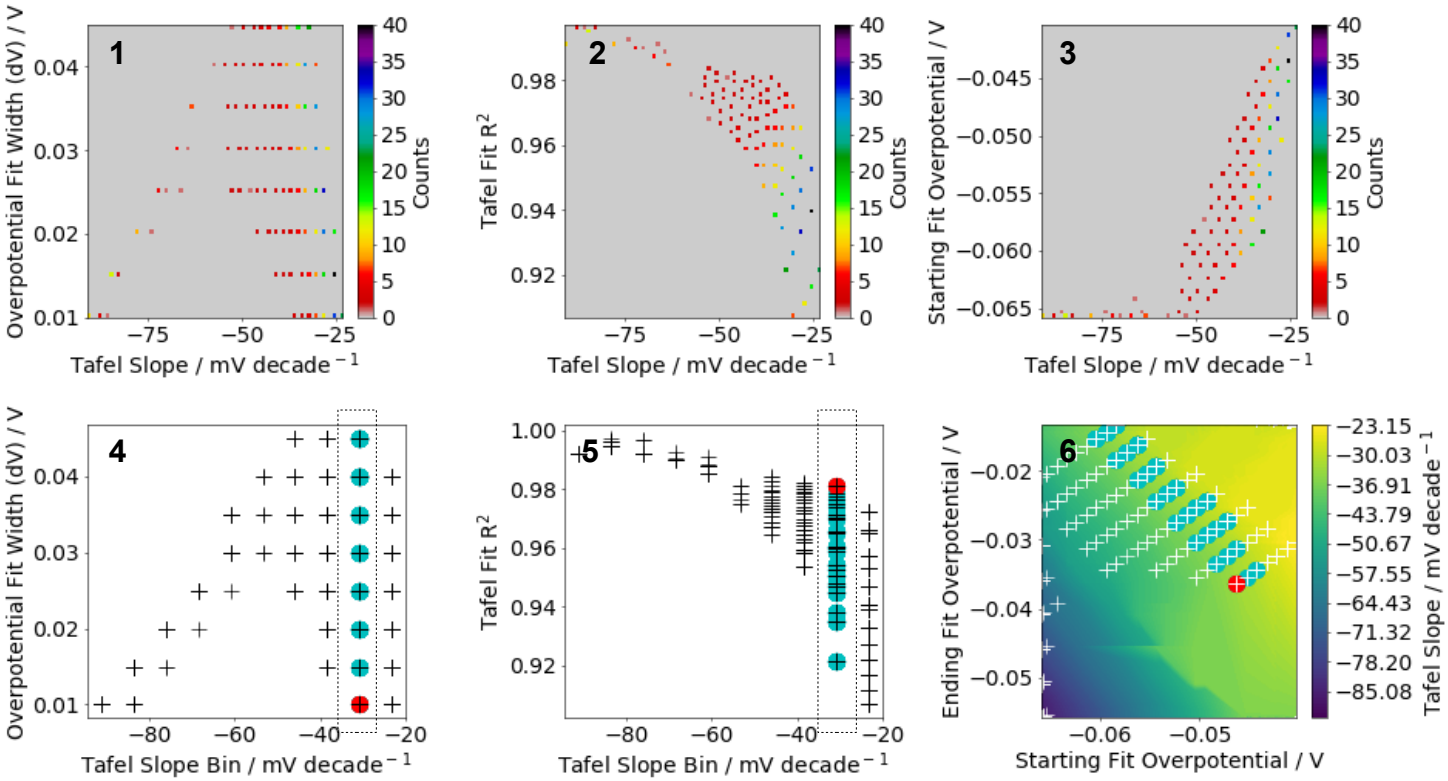



## Example 2b

A polynomial fit of data featuring diffusion limited current. Here, all data to the right of the dotted line form the kinetic region and are accepted for fitting. Data to the left of the dashed line represent diffusion-limited currents and are omitted from the fitting process.

6. When a suitable polynomial fit is accepted by the user, prompts for the overpotential fit widths and $R^2$ thresholds to be tested are provided. Intervals provided by the user are formatted as python lists (e.g., **[0.01, 0.05]** for an interval of 10-50 mV and **[0.900, 1.000]** for an $R^2$ threshold interval of 0.9-1.0). The increment sizes used for the overpotential fit widths to be tested should be no smaller than the resolution at which the experimental data were acquired. $R^2$ increments may be of any size, though a resolution of at least $\Delta R^2$=0.001 should be tested for coarse fits. In general, a $\Delta R^2$=0.001 to ensure high-fidelity fitting, is recommended.

7. Finally, enter a binning size to be used for generating the fully-optimized fits. In general, binning sizes should be small as possible, to reduce any data distortion. For data acquired at 1 mV resolution, binning should be set to anywhere between 1 mV decade$^{-1}$ to 10 mV decade$^{-1}$, with 1 mV decade$^{-1}$ representing the lowest degree of data distortion and so highest fit resolution. When the process has completed, a plot is generated similar to that found in Example 3, and all fitting results are saved as a subfolder in '**Fits**'.




## Example 3

Data visualization of the main program output. The data in these plots mark various representations of the space of residue-optimized fits generated through recursive Tafel fitting (dots in subplots 1-3, (+) in subplots 4-6). For plots 4-6, fully optimized fits are highlighted as red circles. Fits highlighted in cyan are only Tafel-residue and dV-span optimized.

*Top panels*: Subplot (1): Overpotential window (dV) dependence of the Tafel slope. Note that the residue-minimized fits cluster between the region of ca. -50 and -25 mV decade$^{-1}$ and span the widest range of dVs. (2) Tafel slope dependence on $R^2$. (3) Starting potential (position on curve) dependence of the extracted Tafel slope. In subplots 1-3, the color bar represents the number of times a particular fit is found to occur during the fit process.

*Bottom panels*: Subplot (4): Binned Tafel slopes plotted against dV. The Tafel slope spanning the maximum range of dVs is made apparent from binning (column with the most unique members) and is highlighted with a dotted box for clarity. (5) $R^2$ dependence of binned Tafel slopes. (6) Plot of the optimized Tafel fits and with respect to their location on the Tafel curve. Starting fit voltage is $\eta_0$ and ending fit voltage is the quantity ($\eta_0$ + dV) and gives the range of overpotentials defining a particular Tafel fit.

8. The residue-minimized fits generated from the main program recusion are all saved in the file *residue-minimized.csv in the same subdirectory as the individual fitting data. The plots generated by this process are located in a subdirectory named ‘Binned’ in the same sub directory as the individual fitting data.