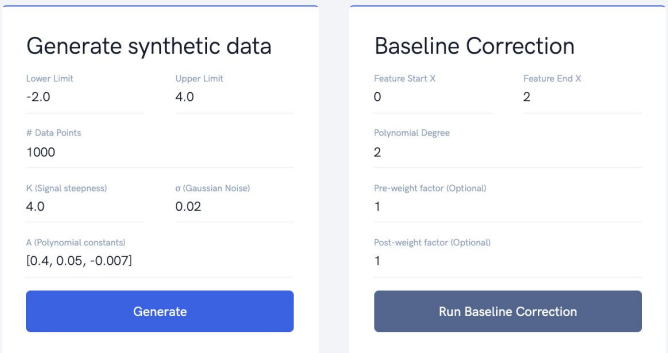
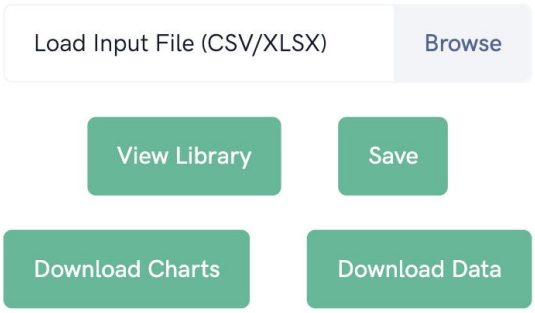
Logistic Baseline Correction

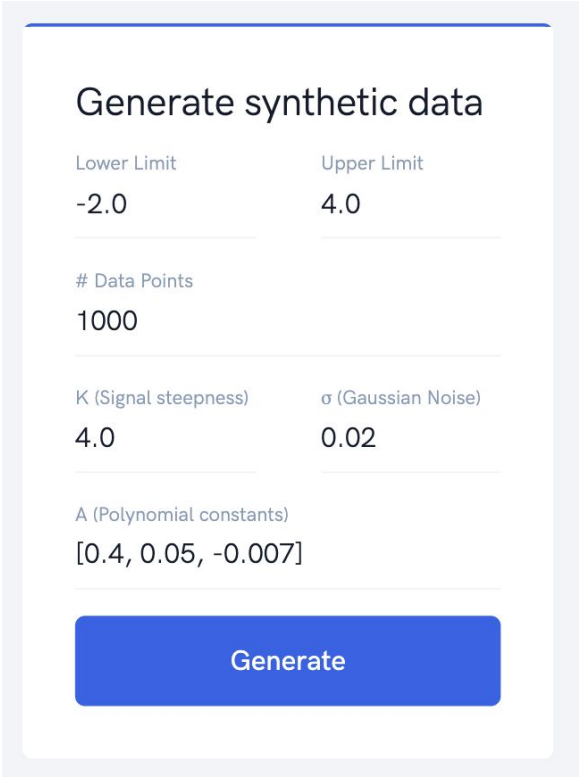
SUMMARY

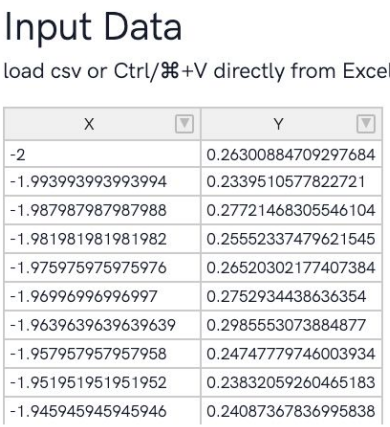
Welcome to the accompanying tool for Logistic baseline correction! LBC is a baseline correction method for features which do not return to the baseline, such as step or saturation features. It works by fitting a polynomial function together with a logistic function to data points before and after the feature. The polynomial function models the baseline while the logistic function compensates for the effect of the feature on the baseline. At the end, the polynomial function is subtracted from the raw data and the baseline corrected signal is obtained, with flat pre- and post-feature regions.

Below, you can find instructions for loading data, performing LBC, downloading your results and interacting with the tool.









Input Data

load csv or Ctrl/⌘+V directly from Excel

X	Y
-2	0.26300884709297684
-1.993993993993994	0.2339510577822721
-1.987987987987988	0.27721468305546104
-1.981981981981982	0.25552337479621545
-1.975975975975976	0.26520302177407384
-1.96996996996997	0.2752934438636354
-1.9639639639639639	0.2985553073884877
-1.957957957957958	0.24747779746003934
-1.951951951951952	0.23832059260465183
-1.945945945945946	0.24087367836995838

Step 1: Load Data

There are three ways to load data into the tool:

Load Data from the library

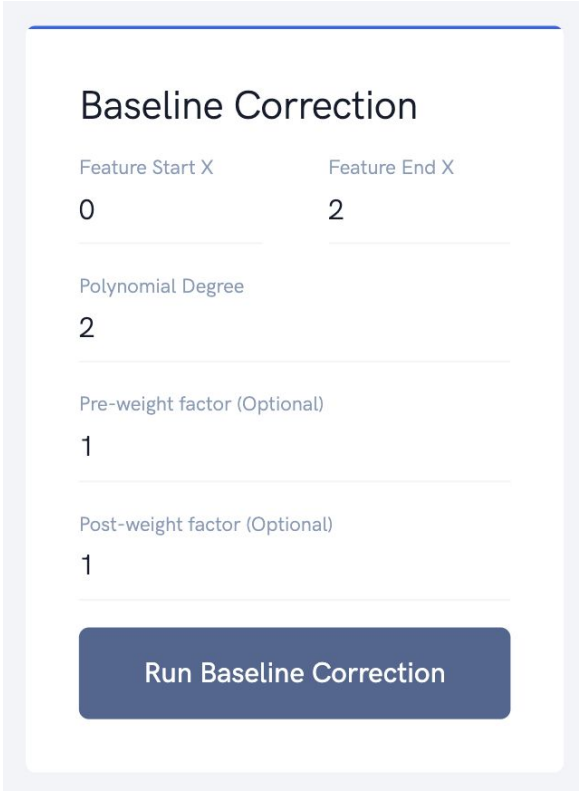
This is the easiest. To load data from the library, click on 'View Library', and click on a dataset. Please allow large datasets some time to load. You can also save your dataset back to the library if you'd like to share it with others later!

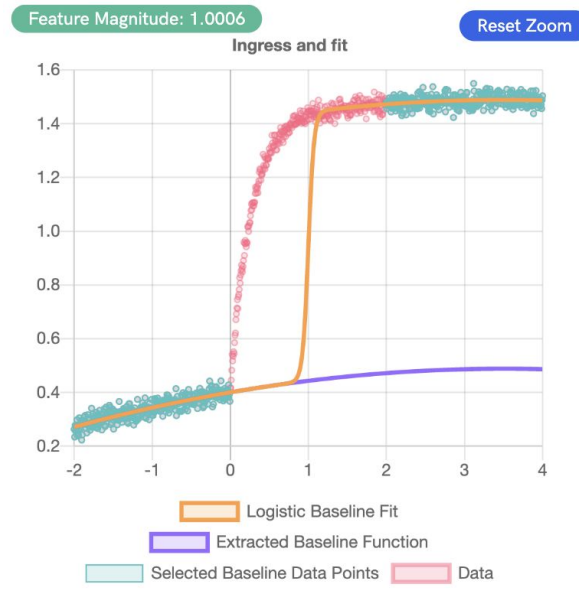
Generate Synthetic Data

Use the synthetic data section to the left to generate synthetic data. The data generated resembles a chemical reaction signal. The feature starts at $X = 0$ and goes from $Y = 0$ to $Y = 1$. k adjusts the signal steepness, σ the amount of gaussian noise. You can also adjust the number of data points, the lower and upper limits (in the x-axis) of the signal, and the polynomial constants of the baseline. A describes the polynomial constants and is entered as an array with square brackets on either side. The position of an array value translates to the polynomial constant in the following way: $f(x) = a + bx + cx^2 + dx^3 + \ldots$ from the array [a, b, c, d].

Import your own

There's two ways of loading your data. You can load csv, tsv or excel files using the 'Load Input File' tool. You can also Ctrl/⌘+V directly from Excel into the spreadsheet at the bottom left. The spreadsheet will let you edit your values directly once they're loaded.





Step 2: Perform LBC

Once your data is loaded, adjust the parameters for baseline correction in the right-hand side dialog.

Select the Feature start and end X values first. To find these values, look at the plot of your data and, if necessary, zoom into the regions where the data starts and ends to significantly deviate from the baseline. If it proves difficult to determine precise start and end points due to a gradual change from baseline to feature, it is better to choose an earlier start/later end value. While this reduces the number of considered data points, it ensures that the feature does not affect the baseline determination.

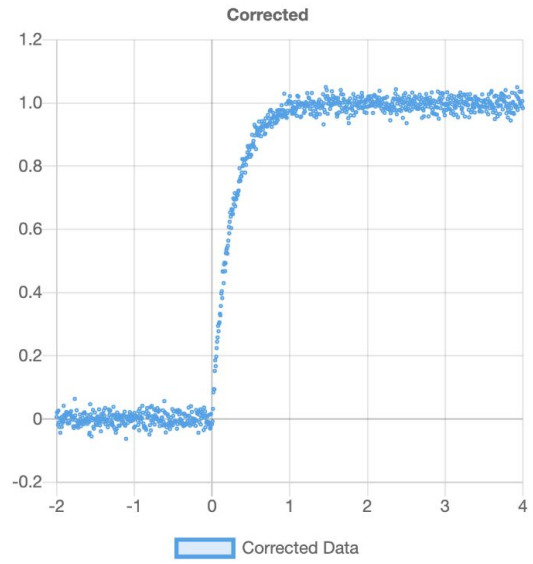
Next, select the polynomial degree for the function approximating the baseline. Here it is best to start with a lower degree and, if the result is not satisfactory, to slowly increase it. High polynomial degrees (> 8) are usually not required.

Optionally, you can assign weight factors that give more weight in the optimization to either pre- or post-feature data points.

Running LBC

Click ‘Run Baseline Correction’ to see the results. When successful, the plots will show the extracted baseline, estimated fit, and the corrected signal which ideally now highlights your features of interest. The estimated feature magnitude is also shown.

The output numerical data is also shown in the output data spreadsheet.



Load Input File (CSV/XLSX) Browse

View Library Save

Download Charts Download Data

Output Data

(Cannot be edited) Clear Data

X	Y	Cc
-2	0.27521482382631146	0.0064021
-1.993993993993994	0.28962682590900934	0.0203338
-1.987987987987988	0.2918302138055201	0.0220575
-1.981981981981982	0.2525345758146487	-0.017717
-1.975975975975976	0.2972567673185613	0.0265261
-1.96996996996997	0.25966057714956664	-0.011548
-1.9639639639639639	0.2464502567855357	-0.025236
-1.957957957957958	0.2748967029682558	0.0027330
-1.951951951951952	0.22918164924837878	-0.043458
-1.945945945945946	0.27437545113820466	0.0012590

Step 3: Experiment!

Download or Save your output

The ‘Download Charts’ and ‘Download Data’ buttons let you download the plots and data points in csv format. Click ‘Save’ to add your dataset and LBC parameters to the library, so you can share it with future users. We don’t collect any of your information unless you choose to save it, so none of it will be retained without saving.

Troubleshooting

In case you do not obtain a good logistic baseline fit or your corrected data is not flat before and after the feature, try the following:

1. Increase the degree of the polynomial to describe more complicated baseline shapes.

2. Select earlier feature start and/or later feature end values to remove influence from the feature on baseline correction.