

Hysteresis Loop Analysis Box:
Advanced processing and analysis of hysteresis data
v1.1.2

May 2022

Contents HystLab v1.1.2

# Contents

1	Introduction	2	
2	Version history		
3	System Requirements		
4	Quick Start Guide4.1 Installation4.2 The main window4.3 Loading and quick processing	5 6 7	
5	Loading Hysteresis Data5.1 Loading data5.2 Compatible data formats5.3 Loading a HystLab session	8 8 9 10	
6	Processing Hysteresis Loops           6.1         Processing control         6.1.1         Trim field data         6.1.2         Loop offset correction         6.1.3         Data regularization         6.1.4         Drift correction         6.1.5         Saturation slope correction           6.2         Default processing         6.3         Hysteresis loop fitting	11 11 11 12 12 14 16 16	
7	Hysteresis Statistics and Parameters	19	
8	Saving Data and Analyses  8.1 Saving the plots	23 23 23 23	
9 D	Customizing HystLab  9.1 Customizing plots	24 24 24 24 25	
$\mathbf{\pi}$	eierences	⊿၁	

1 Introduction HystLab v1.1.2

# 1 Introduction

Hysteresis loops are one of the most ubiquitous rock magnetic measurements and with the growing need for high resolution analyses of ever larger datasets, there is a need to rapidly, consistently, and accurately process and analyze these data.

To achieve this, we have developed HystLab (Hysteresis Loop analysis box), which is MATLAB based software for the advanced processing and analysis of magnetic hysteresis data. HystLab is an easy to use graphical interface that is compatible with a wide range of software platforms. The software can read a wide range of data formats and rapidly process the data. It includes functionality to re-center loops, correction for drift, and perform a range of slope saturation corrections.

If users encounter bugs or problems using HystLab, or have any suggestions for improving the software, we would really like to hear from you, as all input is welcome. If you use HystLab in your work, please make it clear what version was used and the what processing steps used. We would also be grateful if you cited the publications relevant to HystLab:

- 1. Paterson, G. A., Zhao, X., Jackson, M., & Heslop, D. (2018). Measuring, processing, and analyzing hysteresis data. *Geochemistry, Geophysics, Geosystems*, 19. doi: 10.1029/2018GC007620.
- 2. Jackson, M., Solheid, P., 2010. On the quantitative analysis and evaluation of magnetic hysteresis data. Geochem. Geophys. Geosyst., 11, Q04Z15, doi: 10.1029/2009GC002932.

Greig A. Paterson University of Liverpool, Liverpool, UK.

Xiang Zhao and David Heslop Australian National University, Canberra, Australia.

Mike Jackson Institute for Rock Magnetism, University of Minnesota, Minnesota, USA. 2 Version history HystLab v1.1.2

# 2 Version history

Only minor and major updates are documented here. Patch updates will only be reported on the GitHub releases page: https://github.com/greigpaterson/HystLab/releases

**v1.0.0** – July, 2018

The first finalized version of HystLab, published along side Paterson, G. A., Zhao, X., Jackson, M., & Heslop, D. (2018). Measuring, processing, and analyzing hysteresis data. *Geochemistry*, *Geophysics*, *Geosystems*, 19. doi: 10.1029/2018GC007620..

**v1.1.0** – June, 2021 Changes:

- 1. Improved reading of MPMS files and addition of coercivity meter data file support
- 2. Improved loop fitting, including testing for and fitting simple linear models
- 3. New separate function for regularizing the loops to ensure consistent behavior
- 4. New separate function for splitting the loops into upper and lower branches to ensure consistent behavior
- 5. New separate function for removing initial moment acquisition from data to ensure consistent behavior
- 6. Improved error reporting
- 7. Various bug fixes and minor updates

# 3 System Requirements

HystLab is written in MATLAB 2014a (now maintained in MATLAB 2018a), and requires MATLAB v8, or higher, to run. HystLab is self-contained and does not require any additional MATLAB Toolboxes. HystLab will run on Windows, Mac, and Linux platforms capable of running MATLAB. Processing time of hysteresis loops are CPU dependent and will vary from system to system, but the basic requirements to operate HystLab are the same as those required for MATLAB. The graphical elements of HystLab require a minimum screen resolution of  $1024 \times 720$ . Users that experience any difficulties should contact the authors for assistance.

HystLab may function with MATLAB versions older than 8, but users may encounter issues. Those who have older versions of MATLAB who have problems running HystLab should contact the authors as we are more than happy to help improve backward compatibility as best as we can.

HystLab was primarily written in MATLAB 2014a (version 8.3). The MathWorks introduced a major update to MATLAB graphics in the 2014b release (version 8.4). This completely changed the interface for manipulating figures, removing some features, while adding others (and sadly introducing some bugs). We have tried to make HystLab as compatible as possible with both preand post-2014b releases, but we may have missed some issues with newer versions of MATLAB. Anyone who encounters problems exporting graphics from HystLab, or have suggestions for improvements should contact the authors for further support.

# 4 Quick Start Guide

#### 4.1 Installation

All of the files required for HystLab are available from https://github.com/greigpaterson/HystLab. We recommend downloading the latest release of HystLab, which can be found on the GitHub page (https://github.com/greigpaterson/HystLab/releases).

Once downloaded, the files should be put in a HystLab folder and moved to your desired destination (e.g., your MATLAB user directory).

From the "Home" tab in the main MATLAB window, select "Set Path". This will bring up a window that lists all of the directories that are currently set in the MATLAB path. Click "Add Folder..." and navigate to the location of the HystLab folder. Click on the folder name, then click "Open". The HystLab folder should now appear at the top of the directory list. Now click "Save" and then "Close".

The HystLab program can now be called from any directory by typing "HystLab" in the MATLAB command window.

#### Useful Note...

GitHub provides a very useful piece of software call GitHub Desktop (https://desktop.github.com/). This allows user to watch key repositories and allows them to easily synchronize with the main GitHub website. This makes it extremely easy to keep your code up-to-date with the latest releases. We strongly recommend HystLab users to use this approach to keep their software fully up-to-date.

#### 4.2 The main window

When HystLab is launched the main window is opened (Figure 1). From here, all of the HystLab functions can be accessed.

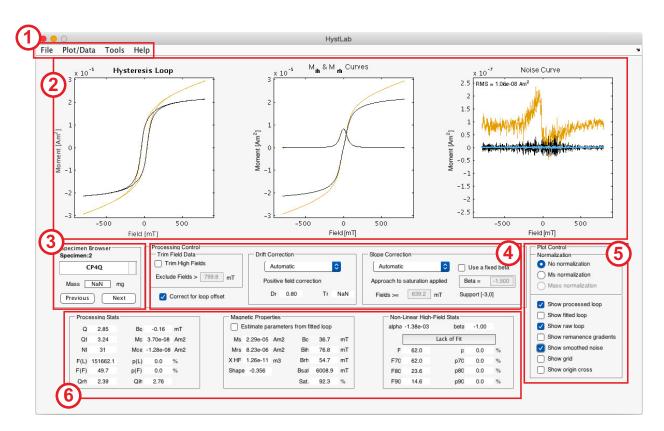


Figure 1: The main HystLab window.

#### 1. Menu bar

The main menu bar contains access to all the main function in HystLab.

File: Contains functions for loading data into HystLab. It also includes functions for

saving and loading a HystLab session.

Plot/Data: Contains functions for saving the main window plots and exporting data.

Tools: Contains functions for setting up and customizing HystLab. A function to

removed a selected specimen from the loaded data can also be found here.

Help: About HystLab and access to the PDF manual.

#### 2. Data plots

The hysteresis,  $M_{ih}$ ,  $M_{rh}$ , and noise plots. Here, the raw data and processed data can be plotted together with the fitted data. Colors can be customized from the "Tools" menu.

### 3. Specimen browser

Controls to browse through the loaded specimens and to manually assign a mass to each specimen.

### 4. Processing control

These buttons provide quick access to the main functions for processing the hysteresis data.

#### 5. Plot control

The interface for choosing which data to plot as well as plotting grid-lines etc.

#### 6. Processing and analysis results

The processing parameters and hysteresis statistics.

### 4.3 Loading and quick processing

From the "File" menu, select "Load Data". Using the browser window that appears, browse to your hysteresis files and select them. After reading the hysteresis files, the data will be automatically processed using the default settings (see Section 6).

#### Useful Note...

The default processing makes use of the automatic drift and saturation slope corrections. These are generally good for most specimens, but may not be suitable for all. After default processing it is recommended to manually check all data and re-process where necessary. See Section 6 for full details of the processing options.

# 5 Loading Hysteresis Data

# 5.1 Loading data

HystLab supports a wide range of data formats. Data can be loaded by selecting "Load Data" from the "File" pulldown menu. This will open up a file browser window, similar to that shown below (Figure 2), which allows the user to select their data files. Multiple files can be selected.

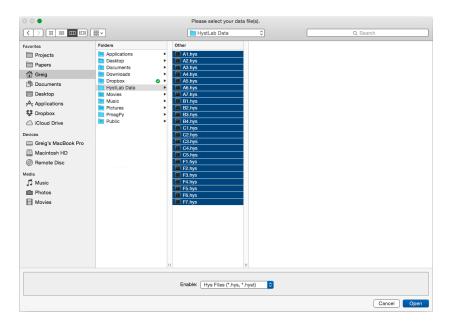


Figure 2: File browser window for loading data.

Once the data files have been selected the window in Figure 3 will open. This allows users to select the type of file they have selected. The most commonly used data formats are selectable with radio buttons, but additional formats are available in the pulldown menu after selecting "Other". **Note:** Only a single data format can loaded at a time.



Figure 3: Load options window for data files.

#### Useful Note...

When HystLab loads in the data measurement units are automatically convert to hybrid SI units. Moments are given as Am<sup>2</sup> and fields as mT.

If data are already loaded into HystLab, when "Load Data" is selected a prompt will appear asking if you wish to append new data, overwrite the existing data, or to cancel. Overwriting will clear all current data and load in the new data. Appending data will retain the currently loaded data and add the newly loaded data to the current session. This allows multiple data from different file formats to be loaded into the same HystLab session.

### 5.2 Compatible data formats

The currently supported data formats are:

$MicroMag\ VSM/AGM$	Princeton Measurements Corporation (PMC) MicroMag 3900
	VSM and 2900 AGM. The data format for these files is highly
	variable. HystLab is known to work with file versions 6, 8, 9, 15,

16, 16.001, and 16.002. If you have a different file version please contact the authors.

Note: Very early versions of PMC data files contain no data file version numbering. These files start with either '"Model 2900 ASCII Data File",0,...' for a VSM configuration, or '"Model 2900 ASCII Data File",-1,...' for an AGM configuration. HystLab will read these files, but users should carefully check the data are parsed correctly. If you encounter problems with these data files

please contact the authors.

Quantum Designs MPMS data files. Compatible with MPMS

MultiVu Application (Rev. 1.60, Build 081; Release 2.2.1.73). This may also be compatible with Quantum Designs PPMS data

file formats, but if issues occur, please contact the authors.

VFTB data files from a range of manufacturers.

Lake Shore VSMs Exported data from Lake Shore 7400 and 8600 VSMs.

Generic 2 Column This is a simple 2 column tab/space delimited file with fields and

moments, respectively, and 1 header line. Units must be mT and

 $Am^2$ .

MicroSense VSM data files (EasyVSM Software version 9.01p).

MolSpin VSM MolSpin VSM data files (N.B. this is based on only a single exam-

ple and may not work with all files. If issues occur please contact

the authors).

Coercivity Meter

Coercivity Meter data files (N.B. this is based on limited examples and may not work with all files. If issues occur please contact the authors).

Important Note: Since these data files record only the upper branch data, the lower branch is taken as direct inversion of the upper branch. This means offset and drift corrections are invalid and should not be performed. The noise curve and noise measurements parameters carry no information.

#### Useful Note...

The Quantum Designs MPMS data formats are highly flexible and can include multiple types of data measurements in a single file. Since information on the measurement sequence is not included in the data files, this makes it very difficult to consistently read in all possible data files. HystLab can read files that include the initial magnetization curve, but identifies the onset of the loop data by looking at the gradient of the field steps. Other data type present in these files will result in incorrectly read data.

We strongly recommend saving MPMS and PPMS measured hysteresis loops in a separate file.

#### Useful Note...

We have tried to incorporate as many data formats as possible, which includes variations in data files from the the same hardware. So, some unlisted file format version may be compatible with HystLab. If a data file that you commonly use is not currently supported, please contact the authors with an example of your data format and it will be added to HystLab.

#### 5.3 Loading a HystLab session

A previously saved HystLab analysis session can be loaded by selecting "Load Session" from the "File" pulldown menu.

# 6 Processing Hysteresis Loops

### 6.1 Processing control

In HystLab, the processing of hysteresis data closely follows the recommendations of *Jackson and Solheid* (2010). The main processing control is shown in panel 4 of the main window (Figure 1) and is expanded below in Figure 4.



Figure 4: The HystLab processing control options.

#### 6.1.1 Trim field data

This option allows users to remove data at high fields, which might be affected by artifacts, such a pole saturation effects. Users can enter a field value in the text box and all fields with an absolute value greater or equal to the user specified field will be excluded.

**Warning:** If too many data points are excluded this can inhibit the analysis and fitting of the hysteresis loops.

#### 6.1.2 Loop offset correction

When selected, this option will correct for undesirable loop offset (i.e., not a material characteristic) in both the vertical and horizontal directions. The correction follows  $Jackson\ and\ Solheid\ (2010)$ , whereby the lower hysteresis branch  $(M^-(B))$  is inverted  $(M^-_{inv}(B) = -M^-(-B))$  and the fields shifted by an offset  $-2B_{off}$ . When  $2B_{off}$  is an accurate measure of the horizontal shift, the upper hysteresis branch  $(M^+(B))$  and  $M^-_{inv}(B-2B_{off})$  are linearly correlated. HystLab uses a Nelder-Mead Simplex algorithm to find the  $B_{off}$  value that maximizes the squared Pearson correlation between  $M^+(B)$  and  $M^-_{inv}(B-2B_{off})$  – this optimized value is  $B_0$ .

The vertical offest  $(M_0)$ , is half of the intercept of the best fit linear line  $M^+(B)$  and  $M^-_{inv}(B-2B_0)$ . Jackson and Solheid (2010) use ordinary least squares to determine this line fit. Given that there is no obvious choice of dependent and independent variables and that the error variance on  $M^+(B)$  and  $M^-_{inv}(B-2B_0)$  should be near identical, in HystLab we use major axis regression, which minimized the perpendicular residual. In most cases, however, the differences are small.

The horizontal (field) offest,  $B_0$ , and vertical (magnetization) offset,  $M_0$ , are recorded in the "Processing Stats" panel (panel 6 in Figure 4; see also Section 7).

Figure 5a is the noise estimate of a hysteresis loop before offsetset correction - the noise is peaked close to zero field due to small field and magnetization offsets (-0.22 mT and  $9.49 \times 10^{-9}$  Am<sup>2</sup>, respectively). Correction for loop offset removes this peak (Figure 5b).

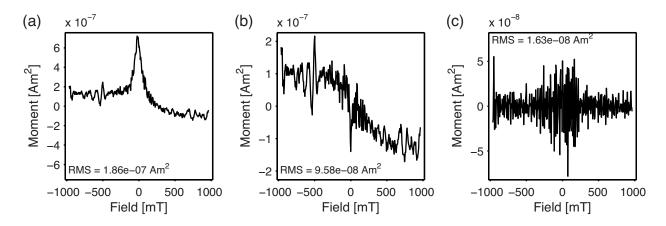


Figure 5: The effects of correcting for loop offset and drift of hysteresis loop noise. (a) The noise curve before correction. (b) The noise curve after offset correction. (c) The noise curve after both offset and drift correction. Positive field drift correction was applied.

#### 6.1.3 Data regularization

To be able to process hysteresis data and calculate many of the desirable statistics, is is necessary that both the upper and lower branches be measured at exactly the same field steps. In practice, however, real data measurements are rarely on the same grid of field values. Therefore, all hysteresis data are placed onto a interpolated field grid - this is not an optional step. Data regularization happens after data trimming and loop offset corrections.

#### $Useful\ Note...$

As of version 1.0.4, HystLab no longer interpolates to a grid of regularly spaced field step. HystLab interpolates fields of the lower branch to those of the upper branch, after the upper branch fields have been made symmetric about zero. This is more appropriate for loops with sparse and irregular field steps.

To avoid extrapolation beyond the measured fields the smallest peak field is used as the maximum for the regular field grid. To avoid oversampling with respect to the number of measured data, the number of points used to generate a regular field grid is taken to be the smallest number of points used to measure either the upper or lower branch of the loop.

#### 6.1.4 Drift correction

Drift may be caused by number of different factors and appear in different ways, but the most common manifestation is failure of a hysteresis loop close. A detailed discussion on the causes and manifestation of drift is given in *Jackson and Solheid* (2010).

Following the above regularization of the upper and lower hysteresis branches, the difference between the upper and inverted lower branch is a measure of the noise associated with the data. This error, or noise, curve, err(B), is defined as:

$$err(B) = M^{+}(B) - M_{inv}^{-}(B).$$

err(B) can be used to correct the drift. Where required, HystLab smooths err(B) using a LOESS smoothing algorithm with a span of 7–15 data points (dependent on the field spacing).

HystLab supports the following drift corrections:

**None** No drift correction is applied.

**Positive Field** Drift is corrected by subtracting the smoothed err(B) curve from the

positive field segments of the hysteresis loops. err(B > 0) is subtracted from the positive field half of the upper branch,  $M^+(B > 0)$ ; and -err(-B > 0) (the negative field err(B) reflected to positive fields) is subtracted from positive field half of the lower branch,  $M^-(B > 0)$ .

**Upper Branch** This drift correction subtracts the smoothed err(B) curve from the upper

branch  $(M^+(B))$  of the hysteresis loop only.

**Symmetric** This follows the method of *von Dobeneck* (1996), whereby the positive and inverted lower branches are averaged and vertically shifting each loop

sure.

Paramagnetic This follows the method of *Paterson et al.* (2018), whereby a param-

agnetic thermal drift model is fitted the noise curve. This estimate of paramagnetic drift is then subtracted from the hysteresis loop to correct for this component of drift. Then the automatic drift correction described below is applied to correct for any remaining drift that is unrelated to

branch by half their inter-tip distance, thereby ensuring perfect loop clo-

paramagnetic thermal drift.

Automatic HystLab supports an automated drift correction routine that decides be-

tween applying the positive field or upper branch corrections. The decision is based on the ratio of drift in the high-field range ( $\geq 75\%$  of the peak field) to the low-field range – a term called the drift ratio (see Section 7). When the drift ratio is  $\geq 0.75$ , then the positive field correction is applied, otherwise the upper branch correction is applied. This approach tends to favor applying the positive field correction, which, from experience, tends to be the most generally applicable correction (*Jackson* 

and Solheid, 2010).

**Note:** The automatic correction may not yield the most appropriate correction method for every specimen and users should carefully inspect

all automatic processing.

Figure 5b is an example of a noise curve exhibiting the effects of linear measurement drift. Following a positive field drift correction the noise estimate becomes flat and independent of the applied field (Figure 5c), which indicates successful drift correction. After correction, hysteresis noise is reduced by an order of magnitude.

### 6.1.5 Saturation slope correction

In sufficiently high magnetic fields, the moment of ferro- and ferrimagnetic materials saturates, while the moments of para- and diamagnetic materials continually increase or decrease, respectively. Therefore, when exploring the remanence capability of complex natural samples that are a mixture of magnetic carriers, it is necessary to correct the high-field portion for non-saturating components. HystLab supports the following correction methods.

None No slope correction is applied.

Linear High-Field This option allows for a simple high-field linear slope correction. Users can enter the field at which the specimen is saturated.

Approach to Saturation

This option applies an approach to saturation slope correction (Fabian, 2006; Jackson and Solheid, 2010). It follows the method outlined by Jackson and Solheid (2010), whereby 100  $\beta$  values evenly distributed as [-2, -1] are tested to find the optimal value to fit the data. Users can enter the field above which the specimen is assumed to be approaching saturation. Users can also specify a fixed value of  $\beta$  to be used, but  $\beta$  must be within the range [-3, 0].

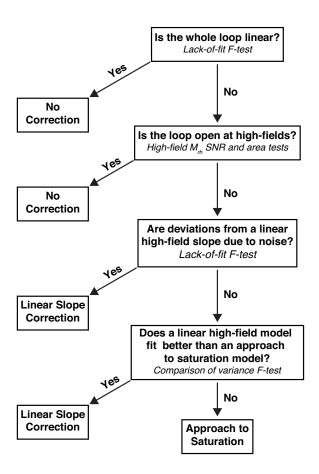


Figure 6: Schematic of the decision process for the automated slope correction routine.

#### Automatic

The automatic slope correction routine in HystLab follows a similar approach to that outlined by *Jackson and Solheid* (2010). A schematic of the decision process is shown in Figure 6.

The first step is to perform a lack-of-fit F-test for whole loop linearity using the uncorrected data. This test assesses if the lack-of-fit between the data and a linear model fit to the whole loop is significant. If the p-value of this test is < 0.05 (5% significance level) then we can reject the null hypothesis that the misfit between the data a linear loop is due to a lack of fit (i.e., the loop is not linear and has some coercivity and remanence). If the null hypothesis cannot be rejected (i.e., the whole loop appears linear) then no high-field slope correction is applied.

If a linear loop is rejected, HystLab assess if the loop is closed at high-fields. At a given field above which closure is to be tested, the signal-to-noise ratio (SNR) of the high-field  $M_{rh}$  curve to high-field noise is assessed. Similarly, the ratio of the positive area under the high-field  $M_{rh}$  to the area under the entire  $M_{rh}$  is determined (termed the high-field area ratio; HAR). Both SNAR and HAR are calculated in dB following  $20 \times \log_{10} (signal/noise)$ . The automatic correction determines that a loop is closed if the SNR is less than 8 dB or the HAR is the less than -48 dB. An 8 dB SNR corresponds to an average Mrh signal 2.5 times stronger than the noise, while an HAR of -48 dB corresponds to a high-field area 1/250th of the total Mrh area. These thresholds tend to prefer loop closure, for which high-field slope correction methods are viable. For loops where closure is rejected, no correction is applied and the user should manually consider the appropriateness of high-field slope corrections.

If an open loop is rejected, HystLab further tests the linearity of the high-field portion of the loop to test if a loop is saturated or approaching saturation. At a given field above which the specimen is assumed to be saturated or approaching saturation, two styles of F-test are performed to assess which mode of slope correction should be applied.

Firstly, a linear model is fitted to the high-field data. Using the negative high-field data as replicates of the positive high-field data, we perform an F-test lack-of-fit test, to test the null hypothesis that the misfit between the data and the model can be explained by the noise of the data. If the p-value of this test is < 0.05 (5% significance level), then we reject the null hypothesis. That is, the poor fit of a linear model to the high-field data cannot be explained by noise and may be better explained by an alternative model (i.e., approach to saturation).

The second test, is an F-test comparison between the variance accounted for by a linear model (with 2 free parameters) and the variance accounted for by an approach to saturation model (with 4 free parameters). If the p-value of this test is < 0.05 (5% significance level), then we reject the null hypothesis that the simpler linear model fits that data better than the more complex approach to saturation model.

If one or both of these test come out in favor of a liner high-field slope, a linear high-field correction is applied. Only if both test reject linearity, an approach to saturation correction applied.

This automated approach tends to favor applying a linear high-field slope correction. HystLab tests the suitability of slope adjustments at 70, 80, and 90% of the peak field, as well as the any field specified by the user.

**Note:** The automatic slope adjustment may not yield the most appropriate correction method for every specimen and users should carefully inspect all automatic processing.

### 6.2 Default processing

When new data are loaded, HystLab performs default processing to provide the user a starting point for their analyses. From our experience, this default processing is fairly general, but may not be suitable for all specimens. We therefore strongly recommend users manually check all data to ensure the processing is appropriate. The default processing does not trim any field, but corrects for loop offset, and applies the automatic drift and saturation slope corrections.

### Useful Note...

The default processing, which incorporates automatic corrections, may not be the most appropriate precessing for every specimen. This default processing is generally good for most specimens and is provided to give users a starting point for more in-depth analysis. Users should carefully inspect all automatic processing results.

#### 6.3 Hysteresis loop fitting

During the processing, HystLab also fits the hysteresis loops following similar procedures to *von Dobeneck* (1996) and *Jackson and Solheid* (2010). These fitted loops can be used to estimate the hysteresis parameters from noisy data, but are not appropriate for extremely noisy data. How well the model fits the observed data is assessed by a lack-of-fit F-test (*Jackson and Solheid*, 2010).

Firstly, the remanent  $(M_{rh})$  and induced  $(M_{ih})$  hysteresis curves are calculated  $(von\ Dobeneck, 1996)$ . The negative field halves are inverted and averaged with the positive field halves to reduce noise – HystLab fits to these averaged half curves. Like  $Jackson\ and\ Solheid\ (2010)$ , HystLab fits a combination of hyperbolic and sigmoid logistic basis functions to the  $M_{rh}$  and  $M_{ih}$  curves. In HystLab, however, the basis functions are not a pre-defined set, but are defined for each specimen such that the median fields of the basis functions correspond to equally spaced moments on the  $M_{rh}$  and  $M_{ih}$  curves.

Prior to fitting the hyperbolic and sigmoid logistic functions, HystLab assess the lack-of-fit tests for loop linearity (p(L), see Section 7). If p(L)  $\geq 0.05$  then a simple linear model with no intercept is fitted to the  $M_{ih}$  curve. The  $M_{rh}$  curve is assumed to zero. If p(L) < 0.05 hyperbolic and sigmoid logistic functions are used.

For each curve, a maximum of 22 basis functions are fitted, for a total maximum of 44 per hysteresis loop. The  $M_{rh}$  curve is fitted with 10 hyperbolic secant functions, 10 sigmoid logistic functions, and 2 linear function with positive and negative slopes. The  $M_{ih}$  curve is fitted with 10

hyperbolic tangent functions, 10 sigmoid logistic functions, and 2 linear functions (to account of paramagnetic and diamagnetic components). Where insufficient data are available to perform the lack-of-fit F-test, HystLab reduces the number of hyperbolic and sigmoid functions to less than 10 each.

For the  $M_{rh}$  curve, sigmoid basis functions have the form:

$$1 - \frac{1}{1 + \exp\left(-a_i\left(B - \hat{B}_i\right)\right)},$$

where B is the applied field,  $a_i$  is the scaling parameter of the  $i^{th}$  sigmoid and  $\hat{B}_i$  is the median field of the  $i^{th}$  sigmoid, which are taken to be the fields of equally spaced magnetic moments of the  $M_{rh}$  curve.

 $M_{rh}$  hyperbolic functions take the form:

$$\frac{\operatorname{sech}(s_i B) - \operatorname{sech}(s_i B_{Max})}{1 - \operatorname{sech}(s_i B)},$$

where B is the applied field,  $B_{Max}$  is the maximum applied field, and  $s_i$  is the  $i^{th}$  coefficient hyperbolic secant and is related to the median field  $(\hat{B}_i)$  by:

$$s_i = \frac{\ln\left(2 + \sqrt{3}\right)}{\hat{B}_i}.$$

For the  $M_{ih}$  curve, sigmoid basis functions have the form:

$$\frac{1}{1 + \exp\left(-b_i\left(B - \hat{B}_i\right)\right)},$$

where B is the applied field,  $b_i$  is the scaling parameter of the  $i^{th}$  sigmoid and  $\hat{B}_i$  is the median field of the  $i^{th}$  sigmoid, which are taken to be the fields of equally spaced magnetic moments of the  $M_{ih}$  curve.

 $M_{ih}$  hyperbolic functions take the form:

$$\frac{\tanh(t_i B)}{\tanh(t_i B_{Max})},$$

where B is the applied field,  $B_{Max}$  is the maximum applied field, and  $t_i$  is the  $i^{th}$  coefficient hyperbolic tangent and is related to the median field  $(\hat{B}_i)$  by:

$$t_i = \frac{\ln(3)}{2\hat{B}_i}.$$

The relative contribution of the basis functions is estimated using the spectral unmixing by variable splitting and augmented Lagrangian (SUNSAL) algorithm of Bioucas-Dias and Figueiredo (2010). Basis functions with a relative contribution of < 0.01% are omitted from the final fit to minimize the total number of used functions.

The quality of the fit is assessed using the F-test for lack-of-fit ( $Jackson\ and\ Solheid$ , 2010). This lack-of-fit test, performed on the whole hysteresis loop, test the null hypothesis that the misfit between the model and the data can be attributed to noise. If the p-value of this test (p(F) in panel 6 in Figure 1; see also Section 7) is < 0.05 (5% significance level), then we can reject the null hypothesis. That is, the poor fit of the basis functions to the loop cannot be explained by noise.

# Useful Note...

Specimens with strong, uncorrected diamagnetic components cannot be modeled with this approach, which requires increasing moment with applied field.

In addition, loops with both Qrh and Qih  $\gtrsim 0.5$ , tend to be most appropriate for loop fitting. Specimens with lower values are typically too noisy for fitting.

# 7 Hysteresis Statistics and Parameters

#### **Processing Stats**

- Q A measure of the quality of the raw hysteresis loop determined by taking the linear correlation between the upper and inverted lower branches. See the "Numerical Tip..." below for details of the calculation.
- $Q_f$  A measure of the quality of the slope-corrected (ferromagnetic) hysteresis loop determined by taking the linear correlation between the upper and inverted lower branches. See the "Numerical Tip..." below for details of the calculation.
- $B_0$  Hysteresis loop offset along the field (horizontal) axis.
- $M_0$  Hysteresis loop offset along the moment/magnetization (vertical) axis.
- $M_{ce}$  Hysteresis loop closure error (Jackson and Solheid, 2010). This is calculated as the difference between the moment of the initial positive field and the moment in the final positive field. Negative values indicate that the upper branch lies below the lower branch, while positive values indicate the upper branch lies above the lower branch. Larger absolute values indicate that a loop is not closed and that drift correction may be needed. Failure of a loop to close may also be an indication that the loop is far from saturation.
- $N_f$  The number of basis functions used to fit the hysteresis loop.
- F(L) The F-value for the lack-of-fit test for whole loop linearity (*Jackson and Solheid*, 2010).
- The p-value for the lack-of-fit test for whole loop linearity ( $Jackson\ and\ Solheid$ , 2010). If p(L) is < 5% (0.05 significance level), then we can reject the null hypothesis that the misfit between the data a linear loop is due to a lack of fit (i.e., the loop is not linear and has some coercivity and remanence).
- F(F) The F-value for the lack-of-fit test for loop fitting (Jackson and Solheid, 2010).
- The p-value for the lack-of-fit test for loop fitting ( $Jackson\ and\ Solheid$ , 2010). If p(L) is  $\geq 5\%$  (0.05 significance level), then we cannot reject the null hypothesis that the misfit between the data the model fit is due to a lack of fit (i.e., the loop is sufficiently noisy that it may be more reasonable to estimate the hysteresis parameters from the model fit rather than the data).
- $Q_{rh}$  A measure of the quality of the processed  $M_{rh}$  curve determined by taking the linear correlation between the positive field half and the reflected negative field half. See the "Numerical Tip..." below for details of the calculation.
- $Q_{ih}$  A measure of the quality of the processed  $M_{ih}$  curve determined by taking the linear correlation between the positive field half and the inverted negative field half. See the "Numerical Tip..." below for details of the calculation.
- $D_r$  Drift Ratio The ratio of the median absolute noise in the high-field range ( $\geq 75\%$  of the peak field) to the median absolute noise in the low-field range(< 75% of the peak field).

 $T_r$  Temperature Ratio – The ratio of the specimen initial temperature  $(T_0)$  to the ambient temperature between the pole pieces  $(T_A)$ . Estimated for the paramagnetic drift correction.

# $Useful\ Note...$

If the loop has a large offset from the field-moment origin, the above-described F-test for whole loop linearity may be unreliable. This is because is relies on the assumed inverse symmetry of the hysteresis upper and lower branches.

### Numerical Tip...

In Jackson and Solheid (2010), all varieties of Q are defined as:

$$Q = \log_{10}\left(\frac{1}{1 - R^2}\right).$$

In HystLab we define Q as:

$$Q = \log_{10} \left( \frac{1}{\sqrt{1 - R^2}} \right).$$

This is consistent will the calculation of Q used the database management software developed at the Institute for Rock Magnetism, University of Minnesota

#### Magnetic Properties

 $M_s$  Saturation moment/magnetization.

 $M_{rs}$  Saturation remanent moment/magnetization.

 $B_c$  Hysteresis loop coercivity.

 $B_{ih}$  The median value of the induced hysteresis curve (von Dobeneck, 1996).

 $B_{rh}$  The median value of the remanent hysteresis curve (von Dobeneck, 1996).

XHF High-field susceptibility (determined from the high-field slope correction).

Shape Hysteresis loop shape factor,  $\sigma$  (Fabian, 2003).

 $B_{sat}$  An estimate of the saturation field. If a linear saturation slope correction is applied, this is the field above which saturation is assumed. If the approach to saturation method is used, this corresponds to the field for 99% saturation.  $B_{sat}$  is less reliable if approach to saturation is used.

Sat. The estimated saturation percentage in the peak measurement field. Sat. is less reliable if approach to saturation is used.

### Non-Linear High-Field Stats

alpha The alpha parameter for the applied approach to saturation high-field slope correction (Fabian, 2006; Jackson and Solheid, 2010).

beta The beta parameter for the applied approach to saturation high-field slope correction (Fabian, 2006; Jackson and Solheid, 2010).

### Lack of Fit Stats

- F The F-value for the lack-of-fit test for high field linearity at fields greater than the user selected value.
- The p-value for the lack-of-fit test for high field linearity at fields greater than the user selected value. If p is  $\geq 5\%$  (0.05 significance level), then we cannot reject the null hypothesis that the misfit between the data and high field linearity is due to a lack of fit (i.e., we cannot distinguish if the high field segment is significantly different from being linear a linear high-field correction should be applied).
- F70/p70 The above lack-of-fit test for high field linearity at fields greater than 70% of the peak field.
- F80/p80 The above lack-of-fit test for high field linearity at fields greater than 80% of the peak field.
- F90/p90 The above lack-of-fit test for high field linearity at fields greater than 90% of the peak field.

### Model Comparison Stats

- F The F-value for the model comparison F-test to compare high field linearity with approach to saturation (both at fields greater than the user selected value).
- The p-value for the model comparison F-test to compare high field linearity with approach to saturation (both at fields greater than the user selected value). If p is  $\geq 5\%$  (0.05 significance level), then we cannot reject the null hypothesis that a linear high field model fits the data better than an approach to saturation model (i.e., linear high-field correction should be applied).
- F70/p70 The above model comparison test for high field linearity at fields greater than 70% of the peak field.
- F80/p80 The above model comparison test for high field linearity at fields greater than 80% of the peak field.
- F90/p90 The above model comparison test for high field linearity at fields greater than 90% of the peak field.

# Loop Closure Stats

SNR	The signal-to-noise ratio (SNR; in dB) of the high-field $M_{rh}$ to the high-field noise.
HAR	The high-field area ratio (HAR). The ratio (in dB) of the area under the high-field $M_{rh}$ curve to the area under the entire $M_{rh}$ curve.
70	The above loop closure stats for high field greater than $70\%$ of the peak field.
80	The above loop closure stats for high field greater than $80\%$ of the peak field.
90	The above loop closure stats for high field greater than $90\%$ of the peak field.

# Useful Note...

Users can switch between displaying the Lack of Fit, Model Comparison, and Loop Cosure Stats using the the toggle button in the "Non-Linear High-Field Stats" panel (panel 6 in Figure 1).

# 8 Saving Data and Analyses

### 8.1 Saving the plots

HystLab plots can be save in two ways. First, users can select the "Save Plots" option from the "Plot/Data" pulldown menu. This will generate a single encapsulated post script (EPS) file containing all three plots in the main window (panel 2 in Figure 1). Another approach is to click on each individual plot in the main window, which will open up a new MATLAB figure window for the selected plot. Users can then save the plot using the standard MATLAB figure saving functions.

### 8.2 Saving hysteresis stats and processing parameters

Users can export the various hysteresis statistics and processing parameters that are generated in HystLab to a tab delimited text file. This can be accessed from the "Plot/Data" pulldown menu and select "Save Statistics".

### 8.3 Saving and loading a HystLab session

For large data sets, some analyses can be time consuming and users may need to stop a session or wish to save their session for future work. To facilitate this, HystLab includes a "Save Session" function (accessed from the "File" pulldown menu), which saves the current fitting session to a MATLAB data file. Users can then load this data file at a later time (using the "Load Session" function in the "File" menu) and continue their analyses where they left off. This also allows users transfer their results and data to other users or computers and maintain the integrity of their analyses without having to repeat the time consuming steps.

#### Useful Note...

When loading in a save session, HystLab does a version check for compatibility. Future updates to HystLab may mean that saved sessions from older version may not be compatible with the latest HystLab version. If users encounter problems loading older saved sessions, they should contact the authors for help.

# 9 Customizing HystLab

# 9.1 Customizing plots

# 9.1.1 HystLab functions

The plot colors in the main HystLab window (panel 2 in Figure 1) can be full customized by selecting the "Set Colors" option from the "Tools" menu. The window shown in Figure 7 allows users to define custom color schemes for each of the three main plots.

By selecting "Save Default", HystLab will save the choice of color to a user default configuration file, which allows HystLab to recall user preferences each time it is run. If this is not selected, the color scheme will only remain for the current session – once HystLab is restarted the default color scheme will be restored.

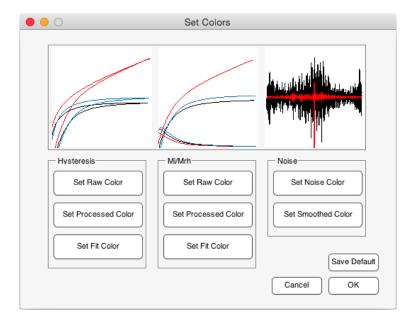


Figure 7: Options for customizing the HystLab plot colors.

#### 9.1.2 MATLAB functions

By clicking on an empty space on any plot in HystLab, the selected plot will open in a new MATLAB figure window. From here, users can use all of the inbuilt MATLAB functionality to fully customize HystLab plots.

**Note:** By using this method of customizing plots, user color choice and configuration cannot be saved to the HystLab default configuration.

References HystLab v1.1.2

# References

Bioucas-Dias, J. M., and M. A. T. Figueiredo (2010), Alternating direction algorithms for constrained sparse regression: Application to hyperspectral unmixing, in 2010 2nd Workshop on Hyperspectral Image and Signal Processing: Evolution in Remote Sensing, pp. 1–4, doi: 10.1109/WHISPERS.2010.5594963.

- Fabian, K. (2003), Some additional parameters to estimate domain state from isothermal magnetization measurements, *Earth Planet. Sci. Lett.*, 213, 337–345, doi:10.1016/S0012-821X(03)00329-7.
- Fabian, K. (2006), Approach to saturation analysis of hysteresis measurements in rock magnetism and evidence for stress dominated magnetic anisotropy in young mid-ocean ridge basalt, *Phys. Earth Planet. Inter.*, 154, 299–307, doi:10.1016/j.pepi.2005.06.016.
- Jackson, M., and P. Solheid (2010), On the quantitative analysis and evaluation of magnetic hysteresis data, *Geochem. Geophys. Geosyst.*, 11, Q04Z15, doi:10.1029/2009GC002932.
- Paterson, G. A., X. Zhao, M. Jackson, and D. Heslop (2018), Measuring, processing, and analyzing hysteresis data, *Geochem. Geophys. Geosyst.*, 19, doi:10.1029/2018GC007620.
- von Dobeneck, T. (1996), A systematic analysis of natural magnetic mineral assemblages based on modelling hysteresis loops with coercivity-related hyperbolic basis functions, *Geophys. J. Int.*, 124, 675–694, doi:10.1111/j.1365-246X.1996.tb05632.x.