Measuring, processing, and analyzing hysteresis data

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Key Points:

- Magnetic hysteresis loops are one of the most widely used rock magnetic data types in Earth sciences
- We outline a broad range of strategies to measure better data and more accurately analyze results
- We introduce *HystLab*, a new software package that incorporates these methods and the ability to produce publication ready figures

Abstract

Magnetic hysteresis loops are important in theoretical and applied rock magnetism with applications to paleointensities, paleoenvironmental analysis, and tectonic studies, among many others. Information derived from these data is amongst the most ubiquitous rock magnetic data used by the Earth science community. Despite their prevalence, there are no general guidelines to aid scientists in obtaining the best possible data and no widely available software to allow the efficient analysis of hysteresis loop data using the most advanced and appropriate methods. Here we outline detrimental factors and simple approaches to measuring better hysteresis data and introduce a new software package called *Hysteresis Loop analysis box* (*HystLab*) for processing and analyzing loop data. Capable of reading a wide range of data formats, *HystLab* provides an easy-to-use interface allowing users to visualize their data and perform advanced processing, including loop centering, drift correction, high-field slope corrections, as well as loop fitting to improve the results from noisy specimens. A large number of hysteresis loop properties and statistics are calculated by *HystLab* and can be exported to text files for further analysis. All plots generated by *HystLab* are customizable and user preferences can be saved for future use. In addition, all plots can be exported to encapsulated postscript files that are publication ready with little or no adjustment. *HystLab* is freely available for download at https://github.com/greigpaterson/HystLab and in combination with our simple measurement guide should help the paleo- and rock magnetic communities get the most from their hysteresis data.

Keywords: magnetic hysteresis; rock magnetism; paleomagnetism, software

1 Introduction

The use of magnetic hysteresis data is prevalent throughout paleomagnetic and Earth science studies. It has applications in fundamental rock magnetism (Krása et al., 2009; Williams et al.,

2010), analyzing paleointensity data (Haag et al., 1995; Carvallo et al., 2006; Kissel et al., 2011; Paterson et al., 2016; Paterson et al., 2017), paleoclimate and paleoenvironmental studies (Liu et al., 2015; Chang et al., 2016; Zhang et al., 2016; Hatfield et al., 2017), biomagnetism (Pan et al., 2005; Lin and Pan, 2009; Li et al., 2010), tectonics (Van Hinsbergen et al., 2008; Jackson and Swanson-Hysell, 2012; Li et al., 2017), pollution monitoring (Muxworthy et al., 2001; Zhang et al., 2013), and extraterrestrial magnetism (Muxworthy et al., 2017; Tikoo et al., 2017), among many others. Despite this widespread usage, the analysis of hysteresis data can be non-trivial and detrimental effects on the quality and accuracy of hysteresis data, such as off-center loops and drift are routinely unaccounted for (Jackson and Solheid, 2010).

Following a brief introduction to magnetic hysteresis, here we present some general guidelines for the improved measurement of magnetic hysteresis data and new graphical user interface software, *Hysteresis Loop analysis box* (*HystLab*), for the advanced processing and analysis of hysteresis loops. *HystLab* follows closely the recommendations proposed by von Dobeneck (1996) and in particular those of Jackson and Solheid (2010). In this introduction to *HystLab*, we briefly outline these procedures taking note of differences employed in our new software package.

Written in MATLAB, *HystLab* will run on all Windows, OS X, and Linux systems capable of running MATLAB v8 or above (no additional toolboxes are required). The *HystLab* package is available for download from https://github.com/greigpaterson/HystLab and installation and operating instructions are given in the provided documentation.

2 The basics of magnetic hysteresis

Measurement of a magnetic hysteresis loop begins by firstly saturating the magnetic moment (M) of a specimen in large positive (or negative) field (B). The intensity of the field is decreased to zero and increased in the opposite direction to negative (or positive) saturation (blue branch in Figure 1). Finally, the field is swept back to positive (or negative) saturation to complete the loop (red branch in Figure 1). The sweep from positive to negative saturation is termed the upper branch and the sweep from negative to positive saturation is termed the lower branch (Figure 1). Under

idealized conditions and for most specimens of natural material, the upper and lower branches are inverse (rotation) symmetric around the origin. That is, any point (B_i, M_i) on a loop can be inverted around the origin to (-B_i, -M_i), and lie exactly on the opposite branch. There are, of course, physical reasons why a hysteresis loop may not be centered and symmetric about the origin (e.g., Housen et al., 1996; Harrison et al., 2007), but for most geological materials it is reasonable to assume origin-centered symmetry, and deviations from symmetry can then be attributed to undesirable factors such as measurement noise, drift, and/or offsets.

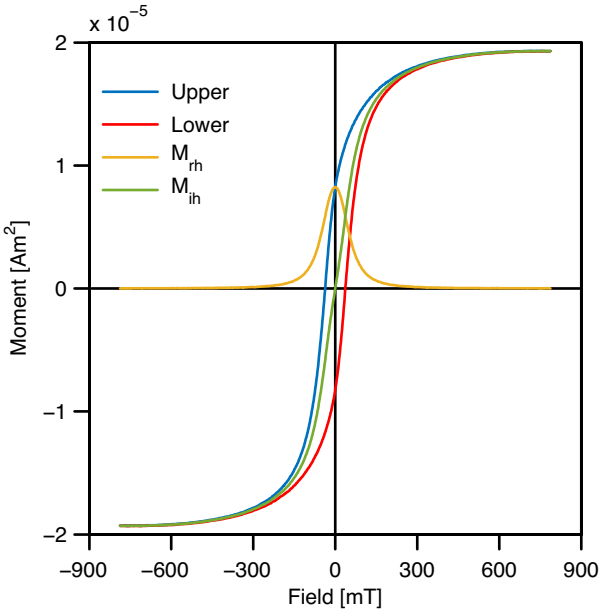

Figure 1. Example hysteresis loop. A basic hysteresis loop distinguishing the upper and lower branches as well as the remanent (M_{rh}) and induced (M_{ih}) hysteretic curves**.**

Given the inverse symmetry expected for geological materials, when the lower branch of a noise-free hysteresis loop is inverted about the origin it will lie exactly on the upper branch. In practice, however, the match is rarely exact and the difference between the upper and inverted lower branch can be viewed as an estimate of the noise of a hysteresis measurement. This is the err(H) curve of Jackson and Solheid (2010), herein simply called the noise curve.

A basic hysteresis loop can be further processed into remanence and induced hysteretic curves (Rivas et al., 1981; von Dobeneck, 1996; Figure 1). The remanence hysteretic curve, M_{rh}, is half the difference between the upper and lower hysteresis branches, while the induced hysteretic curve, M_{ih}, is half the sum of the upper and lower hysteresis branches. Like a basic hysteresis loop, both M_{rh} and M_{ih} have expected symmetries: reflection symmetry about the vertical axis and rotation symmetry about the origin, respectively.

3 Measuring a hysteresis loop

Regardless of the sophistication of data processing and analysis, low quality data will always yield low quality results. In this section, we briefly outline some common artifacts in hysteresis loop data and simple approaches for improving the measurement quality of a hysteresis loop. These guidelines are particularly aimed at Princeton Measurements Corporation MicroMag 3900 vibrating sample magnetometers (VSMs) (now owned by Lake Shore Cryotronics, Inc.) as these are the most widely used instruments in the rock magnetic community and are the ones with which we have most experience. Nevertheless, the basic ideas behind these recommendations are applicable to a wide range of equipment capable of measuring magnetic hysteresis loops. Similarly, many of these recommendations can be used to improve data for other measurements that can be performed on these types of instruments (e.g., isothermal remanent acquisition curves, or first-order reversal curves).

3.1 Improving signal-to-noise

Most VSMs have a number of settings that can be used to improve the signal-noise-ratio of a hysteresis loop. This includes the physical setup of the experiments such as the size of the specimen and the spacing between the sensing/pick-up coils (pole gap), as well as software and measurement protocol settings such as the measurement average time, the field sweep mode, field stabilization time, as well as averaging multiple loops. The trade-off for measuring a higher quality loop, however, is a longer measurement time per specimen, which may result in larger drift during measurement of a single loop.

One of the most obvious approaches to increase the moment signal of a hysteresis loop is to measure a larger specimen. For a specimen with uniformly concentrated magnetic particles, increasing the volume by a factor *n* increases the magnetic moment by a factor *n*. A typical VSM specimen is a small cylindrical core or gel capsule specimen with a diameter of 4–5 mm and height of 5–6 mm (volume ≈ 0.125 cm^3). For weakly magnetized materials (e.g., carbonate sediment or chert), however, this size may not be sufficient to obtain data of sufficient quality for analysis. To produce a moment increase of a factor 10 requires increasing specimen dimensions by a factor of ~2.15 $\left(\sqrt[3]{10}\right)$ to a size of ~11 mm (volume ≈ 1.3 cm^3). A limiting factor with increasing specimen size is the specimen mass. A typical VSM has a mass limitation on the order of ~10 g and specimens that are heavier than this may introduce noise to the vibration system and, ultimately, can lead to failure of the vibration mechanism or damage the system and introduce a permanent and undesirable source of noise. For a typical lithified sediment with a density of ~2.2–2.8 g/cm^3, this mass restriction corresponds to a maximum volume of ~3.5–4.5 cm^3, or an equidimensional size of ~15–17 mm – a factor ~40–50 increase in moment compared to the typical 4–5 mm specimen. For powdered specimens, larger volumes can be used (lower density material), or the powder can be more tightly compressed to increase the measurable mass, but packing too tightly may introduce unwanted magnetostatic interactions (Chen et al., 2005). A caveat to increasing specimen size is that this limits the minimum distance between the pick-up coils used to measure the specimen moment – a larger specimen requires a large spacing, which reduces the overall moment sensitivity of the system.

Most VSM systems have adjustable spacing between the pick-up coils used to detect the magnetic moment of a specimen, known as the pole or air gap. This adjustment not only allows for variable sizes of specimens to be measured, but offers higher moment sensitivity as well as higher applied fields for smaller pole gaps. Pole gaps can typically range from 3.5 mm to 25 mm, and although smaller and larger gaps are possible, they present problems in the form of physical interference with specimen holders and practical limits on moment sensitivity, respectively. In **Figure 2** we re-plot moment root mean square (RMS) noise as a function of pole gap spacing for the Lake Shore 7400 series VSMs (Dodrill, n. d.). Increasing the pole gap from ~7–8 mm (the minimum gap

suitable for a 4–5 mm specimen) to ~14 mm to accommodate a 10 times increase in volume would result in a 2–4 times increase in the moment noise, irrespective of the measurement averaging time. Although this source of noise can vary from system to system, increasing the size of the specimen can yield a stronger signal without an overly large loss of moment sensitivity due to a wider pole gap.

As a general rule of thumb, ~5 mm chips or cores are sufficient for most volcanic materials and ~10 mm diameter gel caps (~1.4 cm^3) hold enough material to measure many powdered sediments. For weaker materials, 4 cm^3 (~16 mm diameter) paleomagnetic cubes can be used. These are smaller than typical paleomagnetic cubes (8 cm^3), but allow the maximum possible material volume while not overloading the VSM drive system. In some cases, however, measuring a larger specimen may be not possible (e.g., insufficient material) and other methods of noise reduction may be needed.

An alternative way to improve hysteresis signal-to-noise is to increase the measurement averaging time, which is the duration over which each moment measurement is averaged. The MicroMag 3900 VSM has a sampling rate of 1 measurement per 10 ms and is capable of averaging over times of 10 ms to 10,000 s (averaging 1 to 10^6 measurements). In general, however, averaging times less than 1 s, most commonly less than 500 ms, are sufficient for measuring a hysteresis loop on a typical geological material. In Figure 3a we show a hysteresis loop measured in continuous field sweep mode (described below) with an averaging time of 100 ms and in Figure 3b, we show the same specimen measured in continuous mode with a 200 ms averaging time. By doubling the averaging time, we reduce the RMS noise curve by a factor of 1.66 (~$\sqrt{2}$). Thirty replicates of these measurements, confirm the $\sqrt{2}$ reduction in the average noise (average RMS noise ratio of 1.51), which is expected if measurement noise is approximately independent and identically distributed (i.i.d.) Gaussian noise. This level of noise reduction is a general feature of increasing averaging time, such that increasing the averaging time by a factor n corresponds to ~$\sqrt{n}$ reduction in noise, but increasing measurement time by a factor n. The slightly higher level of noise reduction we observe (1.51 versus 1.44) is likely a consequence of smoothing introduced during necessary interpolation of the hysteresis loop data (see Section 4).

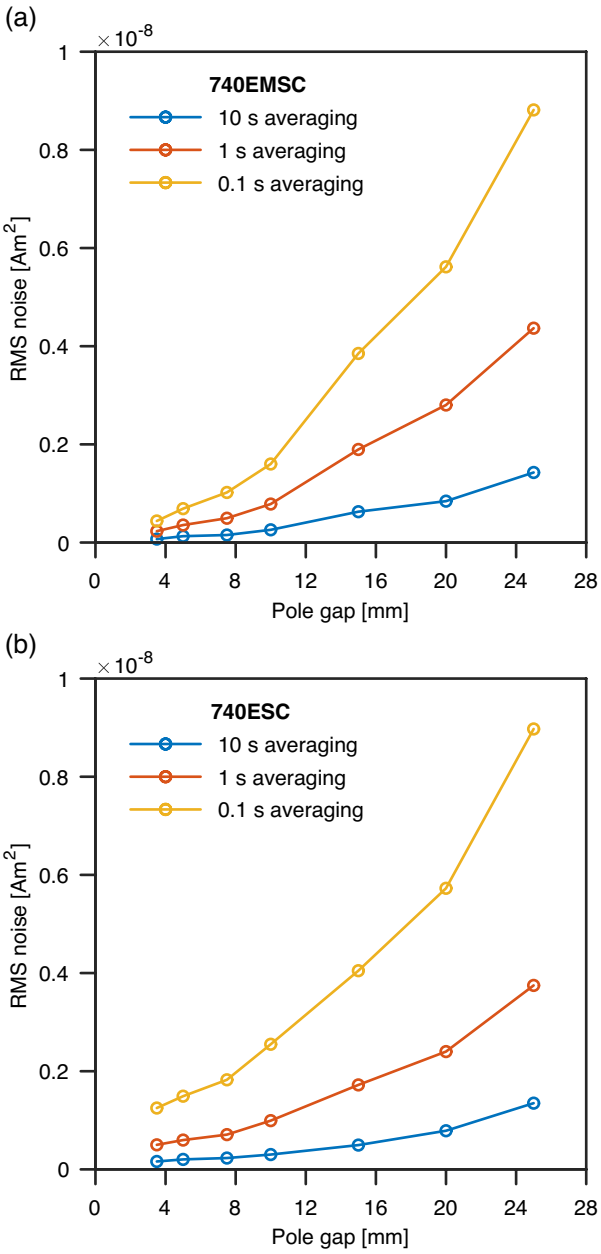

Figure 2. Moment root mean square (RMS) noise as a function of the gap between the pick-up coils of the Lake Shore 7400 series VSM when measured with different averaging times. (a) The 740EMSC VSM, which is optimized for small specimens. (b) The 740ESC VSM. Data are from Dodrill (n. d.).

Another measurement setting that can be adjusted is the field sweep mode, which offers two possible options: continuous or discrete. Using continuous sweep mode, the field is swept over the

186 measurement averaging time and the average field and moment are recorded. In discrete mode
187 (also known as point-by-point mode), the field sweep is paused for a specified time (called the
188 pause or settling time) to allow the field to stabilize before the measurement proceeds. Continuous
189 mode offers a rapid measurement option that works well for strong specimens or where the field
190 sweep rate is low. For weaker samples, discrete mode often offers a higher signal-to-noise, but
191 with a longer measurement time. In Figure 3c, we show an example of a loop measured in discrete
192 mode with an averaging time of 100 ms and a settling time of 300 ms (i.e., the field is paused for
193 300 ms before the field and moment are averaged over the proceeding 100 ms). Compared with
194 the equivalent loop measured in continuous mode (Figure 3a), we see a reduction of noise by a
195 factor of 4.9 (30 replicates yield an average RMS noise reduction by a factor ~5), but with a factor
196 ~4.6 increase in measurement time. For weak specimens, measurement in discrete mode often
197 offers a better trade-off between improved signal-to-noise and increased measurement time (factor
198 ~n increase in time yields a factor ~n decrease in noise) than simply increasing the averaging time
199 (factor ~n increase in time yields a factor ~$\sqrt{n}$ decrease in noise). The magnitude of noise
200 reduction switching from continuous to discrete field sweep depends not only on the choice of
201 averaging and settling times, but also on the exact shape of the loop – Hysteresis loops with large
202 gradient changes will benefit more from discrete sweep measurements.
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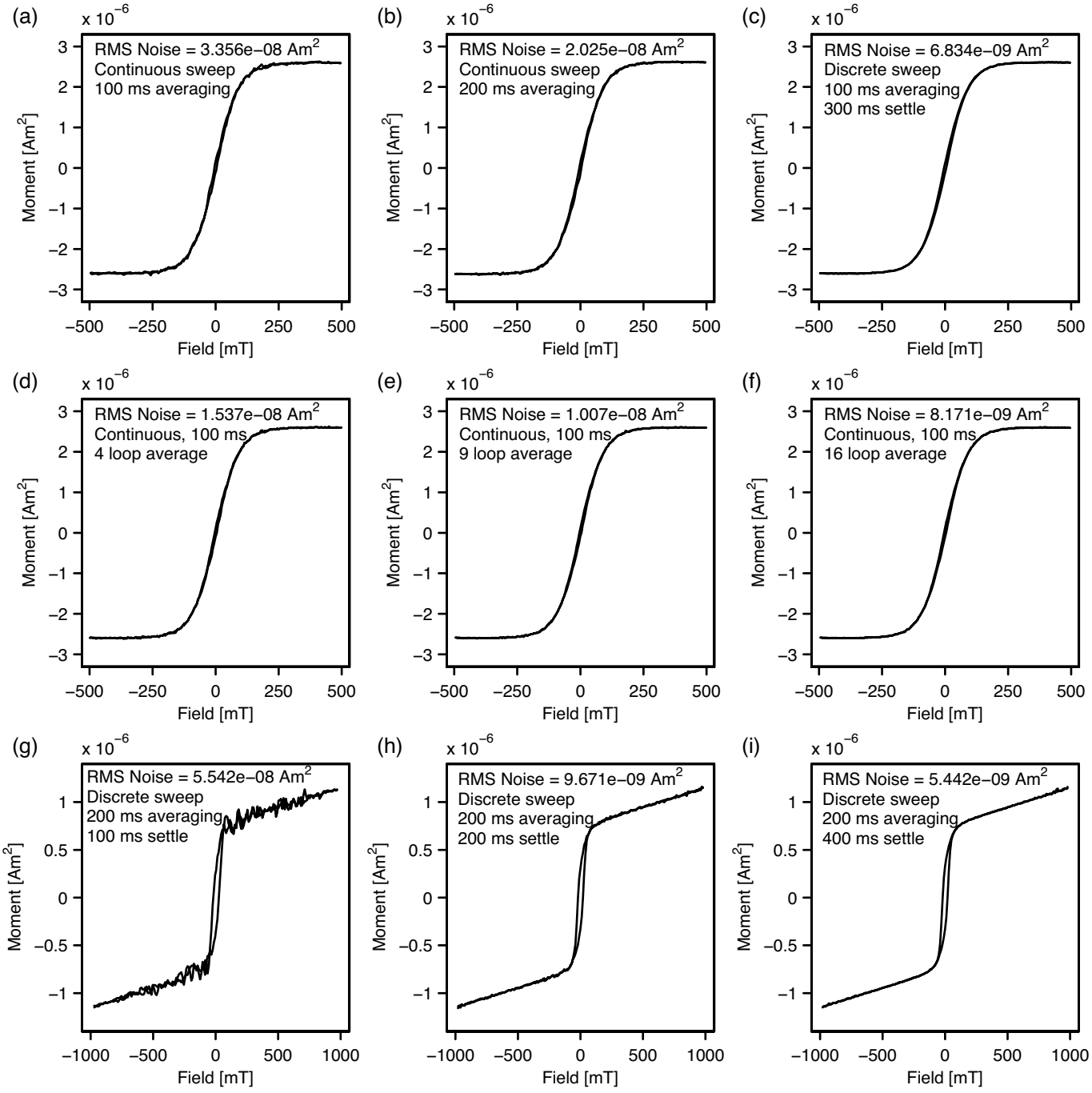


Figure 3. Examples of hysteresis loops with differing measurement parameters and the resultant noise levels. Hysteresis loops from a volcanic speck measured with a continuous field sweep with a (a) 100 ms averaging time and (b) a 200 ms averaging time. The hysteresis loops measured using a discrete field sweep with a 300 ms settling time before measuring with a 100 ms averaging time. The average of (d) 4, (e) 9, and (f) 16 loops measured in continuous mode with 100 ms averaging. A cultured magnetotactic bacteria specimen (Li et al., 2012) measured in discrete mode with 200 ms averaging time and (g) 100 ms, (h) 200 ms, and (i) 400 ms settling time.

Another approach to improving signal-to-noise ratio is to average multiple hysteresis loops. To do this, it is often, but not always, necessary to correct for measurement drift between each loop before averaging (for our example data it is necessary and the drift is described in Section 3.2). After correcting for inter-loop drift, we take the specimen shown in Figure 3a, and average it with a total of 4, 9, and 16 loops (Figure 3d–f). This averaging requires interpolation of all loop moments onto the same field spacing as the loop in Figure 3a. Although this interpolation adds a degree of smoothing, the noise reduction by averaging n loops broadly follows the expected $\sim\sqrt{n}$ factor reduction (noise is reduced by a factor 2.2, 3.3, and 4.1, for averaging 4, 9, and 16 loops, respectively). Like increasing the averaging time, averaging n loops comes with a factor n increase in the total measurement time. It should be noted, however, that to measure these 16 loops in continuous sweep mode with 100 ms averaging, took approximately 720 s (with 402 points per loop). A similar, or slightly lower noise can be achieved by using the discrete sweep mode with 100 ms averaging and 300 ms settling time, which requires just a single loop measurement time of only ~210 s (compare Figure 3c and Figure 3f). Again, measuring in discrete mode often offers a better trade-off between improved signal-to-noise and increased measurement time.

When measuring in discrete mode, the field settling time offers another means of reducing measurement noise. In Figure 3g–i, we compare three loops measured in discrete mode with an averaging time of 200 ms and settling times of 100, 200, and 400 ms. We observe that a factor n increase in settling time results in a factor $\sim n^2$ reduction in the loop RMS noise (confirmed by additional measurements at 100 and 300 ms averaging). This large reduction in noise rapidly approaches the manufacturer's nominal moment sensitivity of $\sim 0.5\times10^{-9}$ Am^2 (1000 ms averaging, pole gap unspecified), and in our collective experience, settling times of > 500 ms offer little improvement at the expense of considerably longer measurement times. Generally, settling times of 100-300 ms are sufficient for most measurements.

Overall, for weak and noisy hysteresis loops, measuring in discrete field sweep mode with averaging times of 100–300 ms and settling times of ~300 ms offers the best balance between maximizing signal-to-noise, while maintaining a reasonable measurement time (hence minimizing drift). Each specimen and instrument is, of course, unique, and each measurement should be

tailored appropriately. For example, chips of volcanic materials that are > ~2–3 mm in size are typically strong enough to be measured in continuous mode with short (~100 ms) averaging times – The example in Figure 1 is a such a chip, but has a RMS noise of ~1×10^{-8} Am^2, or < 0.05% of the saturation moment (M_s), while the example in Figure 3a has a RMS noise of ~1.3% of M_s. The above descriptions of loop noise and guidelines for reduction should serve as general starting point for the majority of specimens encountered by the rock and paleomagnetic community.

3.2 Minimizing drift

Although the sources of drift can be difficult to characterize and quantify, many can be related to temperature or mechanical effects. Thermal factors are relevant not only to the temperature of the specimens being measured, but also to the ambient temperature of the room and to temperature changes of the experimental apparatus as the experiments proceed. Mechanical factors can be related to the solidity/friability of the specimen, specimen position during measurement, or the physical mechanisms and electronics of the instrument being used.

Temperature changes in the specimen being measured are one potential source of thermal drift. Not only can this affect measurement of the temperature dependence of magnetic properties, but can also have an impact on measurements at room temperature due to the temperature between the pole pieces being influenced by the temperature of the magnets. This type of thermal drift can strongly influence specimens with large paramagnetic components such as sediment samples and is most likely the main cause of extreme drift and failure of loops close after return to the initial saturation field.

This drift type of thermal drift, which we term paramagnetic drift, can be described by a simple temperature model of paramagnetic moments (Jackson and Solheid, 2010). Curie's Law states that the paramagnetic magnetization (M_p) in an applied field, B, is inversely proportional to temperature, T:

$$M_p\left(B,T\right)=\frac{CB}{\mu_0 T}, \tag{1}$$

where C is the Curie constant and μ_0 is the permeability of free space. If the temperature of a specimen changes from an initial temperature of T_0 to temperature T_i, the paramagnetic magnetization at can be expressed as:

$$M_p\left(B,T_i\right) = M_p\left(B,T_0\right)\frac{T_0}{T_i}. \quad (2)$$

Here T_i follows Newton's Law of Cooling:

$$T_i = T\left(t_i\right) = T_A + (T_0 - T_A)\exp\left(-kt_i\right). \quad (3)$$

where T_A is the ambient temperature (temperature between the VSM pole pieces), k is a rate constant, and t_i is the time of the i^{th} measurement.

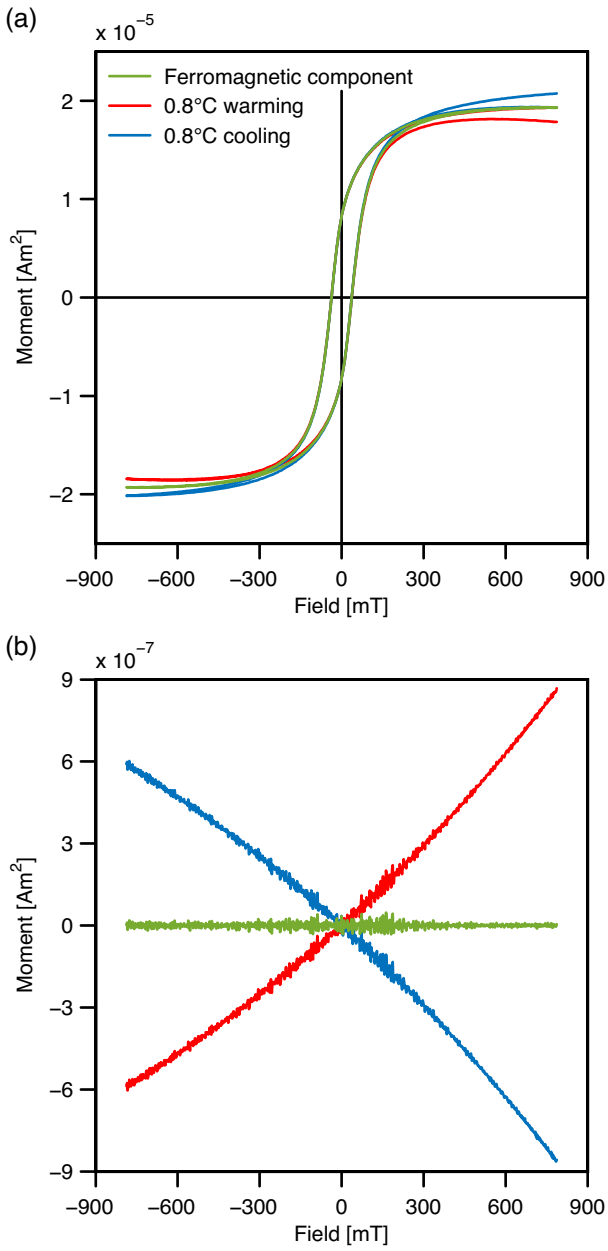
In **Figure 4** we show examples of hysteresis loops that experience drift due to a change in temperature inducing a change in paramagnetic magnetization. Here we take the ferromagnetic loop shown in Figure 1 and add in a paramagnetic contribution such that in a 1 T field the ratio of paramagnetic to ferromagnetic magnetization (M_p/M_f) is 35 (many natural sediments have ratios of ~1 to > 50). The initial specimen temperature is set to 20°C and we model two loops where the ambient temperature is initially 1.5°C above and below the specimen temperature, such that the specimen experiences warming and cooling, respectively. All loops, therefore, start at the same point (**Figure 4**). The rate constant in equation 3 is set such that the specimen does not reach thermal equilibrium, but experiences a 0.8°C temperature change over the measurement of each loop. All loops have been corrected for the paramagnetic contribution using the known high-field paramagnetic susceptibility.

The green loop in **Figure 4**a is the loop that would be measured if there is no change in the specimen temperature (i.e., specimen and ambient temperaures are the same). If the ambient temperature is intially above specimen temperature, then the specimen experiences warming towards ambient and the loop fails to close after returning to positive saturation with the lower branch lying well below the upper branch (red loop **Figure 4**a). The apparent M_s value after high-field slope correction is lower than the true value. If the specimen is intially above ambient temperature and experiences cooling towards ambient, the lower branch crosses the upper as the

293 loop returns to positive saturation and ends well above the upper branch (blue loop **Figure 4**a).
294 The apparent M_s value, however, is higher than the true value. This lack of closure can be
295 quantified by a closure error (M_{ce}), which is the difference between the moments of initial and final
296 peak positive field measurements. In both cases M_{ce} is ~7.5% of the true M_s value.

297 This type of drift always manifests as failure of the loop to close (**Figure 4**a) and a non-linear noise
298 curve (**Figure 4**b). These features, however, can be variable as they are dependent not only on
299 the relative strength/abundance of paramagnetic minerals with respect to the ferro-/ferrimagnetic
300 contribution, but also on the initial temperature of the specimen, ambient temperature, as well as
301 the thermal properties of the specimen, which control *k* in equation 3.

302 This kind of thermal drift can be minimized by a number of simple steps to control temperature
303 fluctuations. Among other measures, this can include regulating room temperature with the use of
304 air conditioning, ensuring laboratory doors are closed to prevent uneven temperatures, shading
305 windows to avoid heating by sun glare, and minimizing the temperature difference between room
306 temperature and the water used to cool the electromagnets (but maintaining appropriate operating
307 temperature). Similarly, allowing a specimen to thermally stabilize before measurement will reduce
308 drift, particularly if temperature dependent hysteresis loops are being measured. Even for room-
309 temperature measurements this effect can be important if the cooling-water temperature and
310 temperature in the magnet air gap differ significantly from the general room temperature. In such
311 cases it is beneficial to allow the samples to thermally equilibrate on the electromagnet base prior
312 to measurement. As noted before, thermal drift has the strongest influence on specimens that have
313 large paramagnetic contributions with respect to the ferromagnetic component. So, these
314 precautions may not be needed for all types of specimens.



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316 **Figure 4. Theoretical model of paramagnetic thermal drift.** (a) Example hysteresis loops of a
317 theoretical ferromagnetic component mixed with a strong paramagnetic component that
318 experiences thermal drift during measurement. The green loop is the expected loop if the
319 specimen experiences no temperature change during measurement. The red and blue loops are
320 for a specimen that experiences warming and cooling towards ambient temperature, respectively,
321 during measurement. All loops have been corrected for the known high-field paramagnetic
322 susceptibility. (b) The resultant noise curves. Colors are the same as in part (a).

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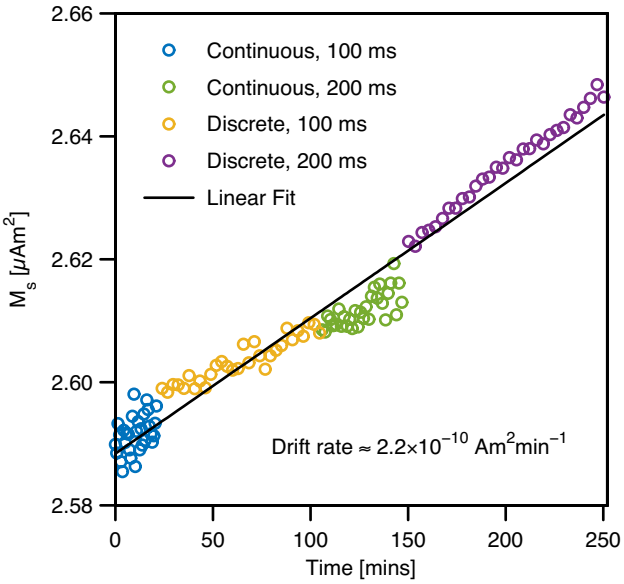
Drift can also be caused by non-thermal mechanisms. This can include instabilities in the vibration system, electronic drift, or physical movement of the specimen during measurement. Quantifying the manifestation of these types of drift is difficult and, depending on the source, may be a linear or non-linear function of time and/or field. Avoiding extremely heavy specimens, ≥ 10 g, which are at or beyond the specifications of the VSM system being used, can minimize vibrational drift and prevent long-term damage. Physical movement of the specimen during measurement can occur if it is not properly attached to the holder or if a powder is not properly compacted.

For the 30 replicates of each loop shown in **Figure 3**a–c (plus 30 replicates of the loop measured in discrete mode with 200 ms averaging and 300 ms settling time; a total of 120 loops), the total measurement time for these 120 loops was ~250 minutes. Over this time, we observe an approximately linear increase in M_s of ~6.3×10^{-8} Am^2 (~2.4% of the average M_s value), which corresponds to a drift rate of ~2.2×10^{-10} Am^2min^{-1} (

Figure 5). Drift for the longest individual loop measurements of ~210 s (discrete field sweep with 200 ms averaging) is on the order of 0.02% of M_s and can be neglected. This specimen was a speck of basalt (< 1 mg) mounted to the VSM sample holder using silicon grease and although this drift is small, this is an example of mechanical drift related to changes in the specimen's position during measurement. Such movement can be avoided by properly fixing the specimen to the holder.

For solid specimens, glue can be easily used to affix the specimen to the holder, but allow sufficient time for the glue to dry otherwise the specimen may fall off during measurement. We recommend the use of water-based polyvinyl acetate (PVA) glue (superglue can easily damage friable specimens and is harder to remove from the holder). For powdered specimens packed into gel caps or cubes, an additional top layer of cotton wool can help better compact the specimen and avoid particle movement. In extreme cases, the powder can be impregnated with glue to solidly bind the particles, but this is generally not needed.



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352 **Figure 5. Moment drift caused by specimen movement over time.** Change in saturation
353 moment over the ~250 mins needed to measure the 120 loops comparing averaging times and
354 continuous and discrete field sweep modes.

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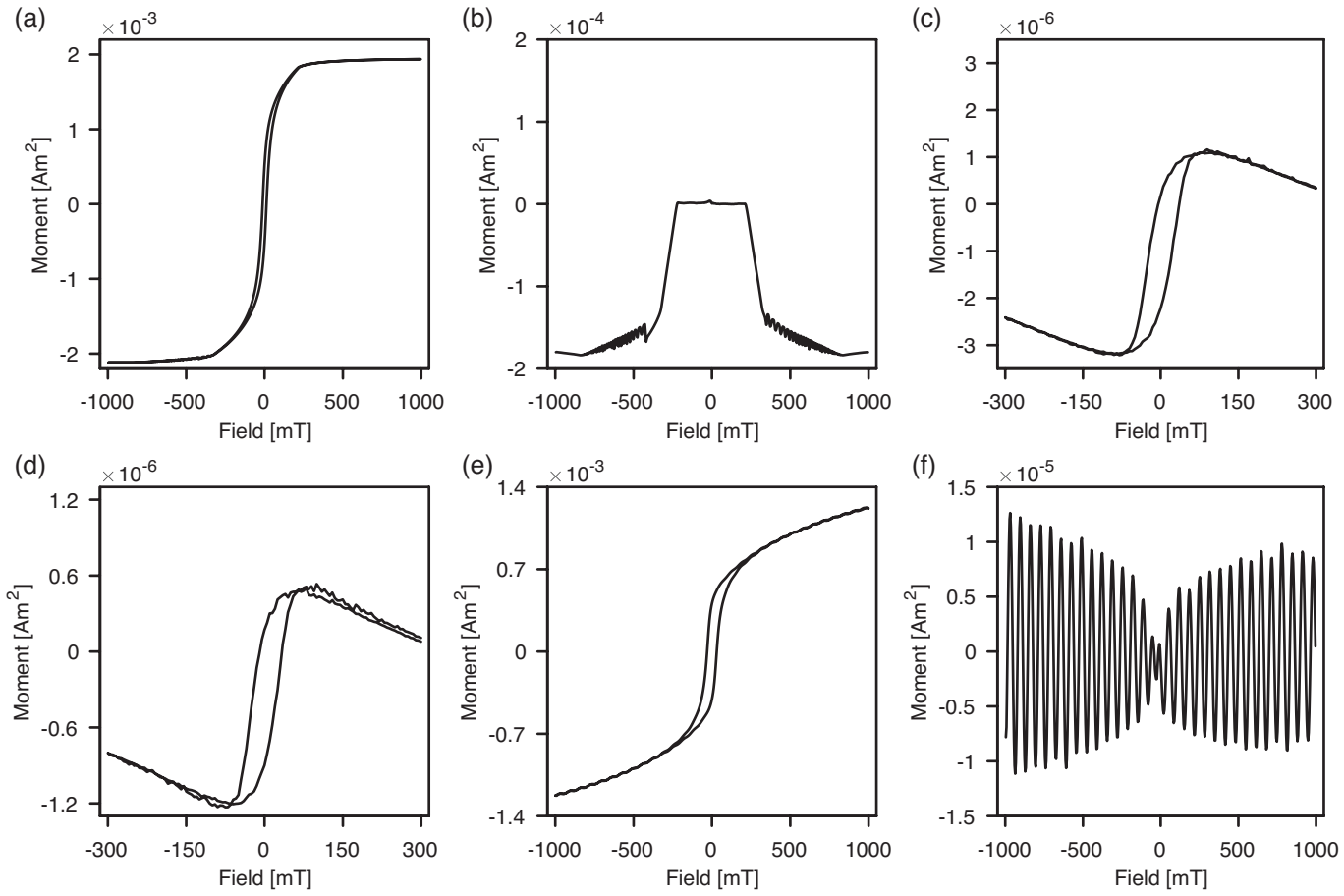
356 ***3.3 Other influences***

357 Instruments for measuring hysteresis loops typically have nominal moment ranges of ~10^{-11}–1 Am^2
358 and specimens weaker or stronger than this cannot be easily measured. For a MicroMag 3900
359 VSM (nominal moment range of 5×10^{-8}–1×10^{-2} Am^2), the moment range ("sensitivity" setting) has
360 to be selected manually. The VSM software warns if the range is set too low for the specimen
361 moment, but if missed incorrect moment range can have a detrimental impact on the loop
362 measurement. This can easily happen if the high-field slope is negative and the peak moment
363 occurs at low fields (cf. Figure 6c), or when the loops are measured as a function of temperature
364 and the specimen moment increases beyond the initially set range. Figure 6a is an example of a
365 loop measured with the moment range set too low. The high-field branches have a distinct change
366 in slope that does not follow the natural curvature of the loop. For other specimens, this effect may
367 occur subtly at higher fields and may give the impression of reaching saturation. The noise curve
368 (Figure 6b) has a distinct plateau shape that is characteristic of the moment range being too low
369 and can be diagnostic when the effects are subtle.



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371 **Figure 6. Examples of hysteresis loops suffering from other detrimental effects.** (a) A
372 hysteresis loop measured with the moment range set too low. (b) The noise curve of the loop
373 shown in part (a). (c) A hysteresis loop offset from the plot origin due to the presence of an
374 electrostatic charge on the specimen holder. (d) A specimen with an electrostatic charge that
375 partially dissipated during measurement. (e) A hysteresis loop that suffers from vibrational
376 instability. (f) The noise curve of the loop shown in part (e) reveals a clear periodicity to the noise.
377 The loop in parts (e) and (f) is a volcanic chip from Muxworthy et al. (2011).

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Some systems are capable of dynamically adjusting the moment range and such artifacts are not an issue. Where the range has to be set manually, the range should be set prior to measurement with the specimen in place and most commonly with the peak measurement field applied. In some cases, however, if the specimen is has a strong diamagnetic component and a negative high-field slope, the maximum moment in the loop measurement occurs at lower fields and a large portion of the loop will need to be measured before an incorrect moment range is detected. Data with the moment range set too low must be remeasured to obtain interpretable data.

Most VSMs will allow the vibration amplitude to be adjusted. Reducing the vibration amplitude reduces the magnitude of the voltage induced in the pick-up coils and allows the moment sensitivity to be adjusted to a higher range. If the moment range is set to the instrument maximum and this effect still occurs, the specimen is too strong and should be reduced in size then remeasured. Alternatively, if reducing sample size is undesirable, a wider pole gap may allow measurement (a wider pole-gap reduces the magnitude of the voltage induced in the pick-up coils; note that the system should be recalibrated if the gap is adjusted).

In Figure 6c we show an example of a hysteresis loop from a magnetotactic bacteria (MTB) specimen deposited in a plastic cube (Paterson et al., 2013). The loop is offset from the plot origin due to an electrostatic charge on the plastic cube. Such oscillating electrostatic charges are equivalent to time-varying currents, which generate changing magnetic fluxes that are additive to that from the specimen moment, and typically manifest as a large moment offset with negligible field offset. The electrostatic signal is independent of applied field, which preserves the size and shape of the loop and allows for correction of the offset (see Section 4.2).

Figure 6d is a hysteresis loop from another MTB specimen in a plastic cube with an electrostatic charge. In this example, the static charge partially dissipates during measurement causing the lower branch to lie above upper branch on returning to positive saturation. The various methods used to correct for loop drift (outlined in Section 4.4) perform poorly for this type of drift and such loops are best remeasured (the distribution of moment drift depends on when and how fast the charge dissipates). Anti-static sprays can help dissipate electrostatic fields before measurement. In

laboratories where electrostatic charges are a long term problem (e.g., locations with seasonal periods of low humidity), air ionizers can be used to reduce the build-up of static charges.

On VSMs, the vibration drive system can also be a source of noise. Figure 6e is an example of loop that suffers from vibrational drive instability. Examination of the noise curve (Figure 6f) reveals that the noise is highly periodic and a spectral analysis (not shown) indicates significant power at an angular frequency of 1.84 Hz, confirming that this is not random noise. The exact cause of this periodic noise is unknown, but is likely due to instability in the electronic feedback loop that controls the vibration drive system (H. Reichard, personal communication, 2018). Although observable, in this case, the magnitude of the instability is insufficient to greatly affect the interpretation of the loop statistics.

Other possible sources of vibrational drive instability include insecure drive rods, loose specimen holders or specimens not being fully secured to the holder, the specimen touching the pole pieces or Hall probe, or noise introduced by overloading the system with heavy (> 10 g) specimens. For mechanical sources of instability, simple fixes of securing drive rods and specimens, and ensuring vibrations are unimpeded will resolve any noise issues. Particular attention should be paid to ensure the specimen does not physically interact with Hall probe as this may damage the probe. For the case of periodic instability (Figure 6e, f), restarting the instrument, reseating the vibration drive system cables, and adjusting the orientation stage have been known to resolve this issue. If these simple approaches fail to remove vibrational drive instability, users should consult the instrument manufacturers for further advice.

4 Hysteresis processing

Following measurement of a hysteresis loop it is necessary to process the data appropriately to correct for unavoidable negative influences (e.g. unavoidable drift etc.) and isolate the desired components before extracting the parameters and statistics of interest for further analysis. To that end, we have developed new graphical software called *HystLab* to aid the paleo- and rock magnetic community in processing and analyzing hysteresis loop data. The remainder of this

paper will discuss the functionality of *HystLab* and the tools available to minimize the detrimental impact of measurement artifacts on the final interpretation of hysteresis data.

HystLab supports a number of advanced processing options that are combined with automated decision processes used by default for all specimens when they are first loaded. This includes automatic centering of hysteresis loops and automatic decisions on drift and saturation slope corrections (details outlined below). In general, this default processing performs well for most geological specimens and provides a quick starting point for users to analyze their data. The default processing, however, may not be suitable for every specimen. We therefore strongly encourage analysts to carefully consider the processing of each specimen to ensure appropriateness.

4.1 Loop interpolation

All hysteresis processing in *HystLab* is based around the assumed symmetry of the basic hysteresis loop and the remanence and induced hysteretic curves. When comparing the upper and lower branches it is necessary to interpolate to consistent field steps. When a "raw" hysteresis loop is initially processed and analyzed, the lower branch is inverted and linearly interpolated to the field steps of the upper branch. For all other processing, both the upper and lower branches are linearly interpolated on to a regularly spaced field grid. To avoid extrapolation of data where there are no measurements, the peak field of the grid is taken as the lowest of the four absolute peak fields (termed B_{max}). To avoid artificially oversampling the loop, the number of points used, n, is taken to be the minimum number of points used to measure either the upper or lower branches (after fields with absolute field values < B_{max} are removed). The interpolation field grid is n equally spaced field points in the range [B_{max}, -B_{max}]. These necessary interpolations inevitably introduce a degree of data smoothing and as a result, estimates of noise and loop quality statistics (described below) are likely to be slight underestimates and overestimates, respectively, of their true values.

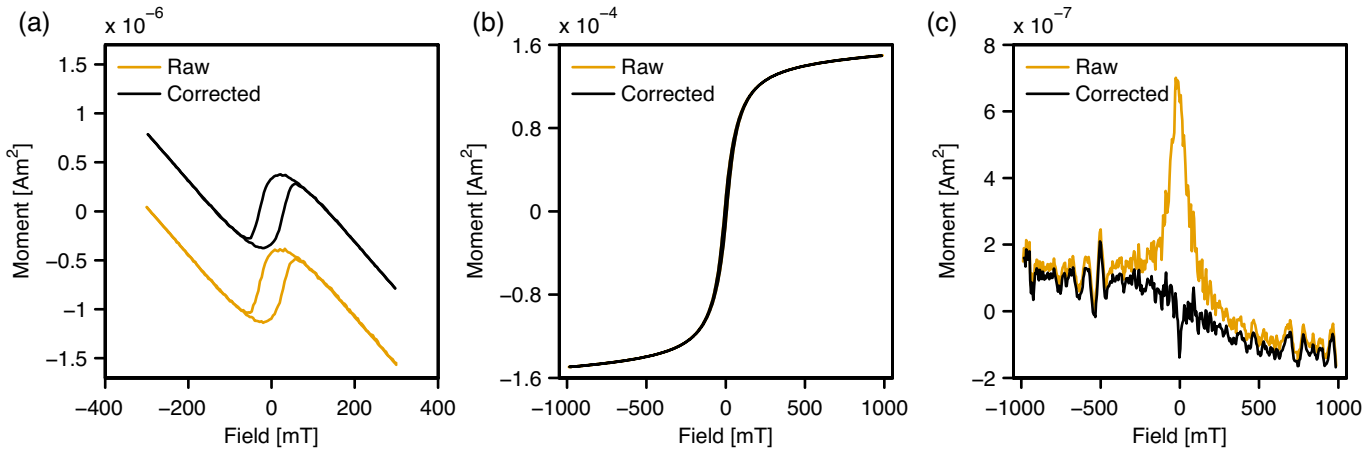
4.2 Loop centering

If uncorrected, asymmetry of a loop about the origin may lead to misestimating of hysteresis descriptive statistics (e.g., M_s, M_{rs}, B_c, etc.). In Figure 7a we show an example of extreme loop

offset of a magnetotactic bacteria specimen with a strong diamagnetic signal from the specimen holder (Paterson et al., 2013). This large moment offset (on the order of the specimen's M_s) is likely caused by an electrostatic charge on the specimen's plastic holder. A subtler example of loop offset is seen from a volcanic specimen from Paterson et al. (2010) (Figure 7b). This less visually obvious offset becomes evident in the noise curve where it manifests as a distinct peak around zero field (Figure 7c). This peak is removed and the root mean square noise level is reduced by a factor two after correctly centering the hysteresis loop (Figure 7c). Following loop centering, a systematic trend in the noise curve becomes more evident (Figure 7c) – This is due to measurement drift (drift corrections are discussed in Section 4.4).

Loop offset is corrected for following Jackson and Solheid (2010), whereby the offset along the field axis is found by maximizing the linear correlation between upper branch and inverted lower branch when the lower branch is shifted by the correct field offset (B_0). The intercept of a linear model fit to the B_0 shifted lower branch and upper branch corresponds to twice the offset along the moment axis (M_0).

In *HystLab*, a Nelder-Mead optimization routine (Lagarias et al., 1998) is used to find the correct field offset. For determining the moment offset, we employ a major axis regression model, which, given the lack of obvious choice of dependent and independent variables (upper versus lower branch moments) and the likely similar noise structure of the upper and inverted lower branches, is more appropriate than a standard linear regression model.



481

482 **Figure 7. Examples of specimens requiring loop centering.** (a) A magnetotactic bacteria
483 specimen with visually obvious loop offset (Paterson et al., 2013). (b) A volcanic specimen
484 (Paterson et al., 2010) with more subtle offset, which is evident as a zero-field spike in the noise
485 curve (c) that is removed after loop centering. RMS noise is 3.679×10^{-6} Am^2 before correction and
486 1.907×10^{-6} Am^2 after.

487

488

489 ### *4.3 Loop quality*

490 The squared linear correlation (R^2) between the upper and inverted lower branches can be used to
491 define a quantitative measure of the quality (Q) of a hysteresis loop (Jackson and Solheid, 2010).
492 The definition of Q used in *HystLab* is given by:

493 $$Q = \log_{10}\left(\frac{1}{\sqrt{1-R^2}}\right), \quad (4)$$

494 This differs from the definition of Jackson and Solheid (2010) who erroneously omitted the square
495 root in the denominator in their paper; although it was included in their calculations and internal
496 software at the Institute for Rock Magnetism, University of Minnesota, which has been used to
497 quantify numerous hysteresis loops. Q values in *HystLab* take the square root to maintain
498 consistency, and we view the above definition of Q as correcting that of Jackson and Solheid
499 (2010).

In addition to the quality of the raw loop (Q) and the fully processed loop (Q_f), *HystLab* also determines the quality of the remanent (Q_{rh}) and induced (Q_{ih}) hysteretic curves. These Q values are based on the expected reflection and rotational symmetries of the remanent and induced curves, respectively, and the correlations between the negative and positive field halves.

4.4 Drift correction

Given the diverse possible sources of hysteresis loop drift, a number of different approaches to drift correction have been proposed and *HystLab* supports many of these. In addition to the option of applying no drift correction, *HystLab* offers four types of correction: 1) positive field correction, 2) upper branch correction, 3) symmetric averaging, and 4) paramagnetic drift correction. The positive field correction subtracts the smoothed noise curve from the positive field segments of the hysteresis loops: The positive field half of the noise is subtracted from the positive field half of the upper branch and the negative field half of the noise curve (reflected to positive fields) is subtracted from positive field half of the lower branch (Jackson and Solheid, 2010). The upper branch correction subtracts the smoothed noise curve from the upper branch of the hysteresis loop only (Jackson and Solheid, 2010). Symmetric averaging follows von Dobeneck (1996), whereby the upper and inverted lower branches are averaged and vertically shifted by half their tip-to-tip separation to ensure loop closure; This results in a zero noise curve. The paramagnetic drift correction accounts for changes in paramagnetic moment due to changes in specimen temperature and is described in detail below.

An automatic correction option is available, which decides between positive field and upper branch corrections. The decision is based on the ratio of drift in the high-field range (≥ 75% of the peak field) to the low-field range. If drift tends to occur in the high-field range then the positive field correction is applied, otherwise the upper branch correction is applied. In most cases, the positive field correction tends to perform best and is therefore favored in the automatic correction approach. We note, however, that although these methods for drift correction generally recover many statistics with reasonable accuracy, the detailed shape of the loop may not always be accurately recovered for certain types of drift (e.g., paramagnetic thermal drift).

The paramagnetic drift correction is newly introduced here and is based on the thermal model of paramagnetic drift described in Section 3.2, which after expansion, describes the change in paramagnetic moment in terms of the ratio (T_r) of a specimen's initial absolute temperature (T_0) to ambient absolute temperature in the measurement space (T_A): $T_r = T_0/T_A$. The first step of this method is to correct drift using the positive field correction described above, and the user defined high-field slope correction (see Section 4.5) is applied to estimate the high-field/paramagnetic susceptibility (χ_{HF}). If no saturation slope correction is applied a linear fit is made to the data at fields ≥ 70% of the peak field (this slope correction is not applied to the final loop, but used only to estimate χ_{HF}). This estimate of χ_{HF} is used to estimate the paramagnetic magnetization $\left(M_p = \chi_{HF}\mu_0 B\right)$. The thermal rate constant, k, and the relative temperature ratio T_r are then optimized to fit the observed noise curve. Each point of the hysteresis loop is then corrected for the predicted change in the paramagnetic moment. Following this, the above described automatic drift correction routine is used to apply either a positive field or upper branch correction to account for any other drift not related to paramagnetic thermal instabilities.

An advantage of this correction over others is that it provides a justifiable means of distributing components of drift across all measurements and not just across a restricted range of data (e.g., positive fields only). Furthermore, for specimens that experience this type of thermal drift, the hysteresis loop shape is generally better recovered than with the other corrections.

An example of a specimen with extreme paramagnetic drift is shown in Figure 8a. This specimen is a relatively weak lake sediment with a ferromagnetic component dominated by detrital magnetite (Liu et al., 2015). This specimen is strongly paramagnetic with a 1 T para-to-ferromagnetic magnetization ratio (M_p/M_f) of ~35 (cf. the theoretical example in Section 3.2). After linear high-field slope correction, the lower branch crosses the upper branch and lies well above the upper branch resulting in a closure error of M_{ce} = -1.993×10^{-7} Am^2 (~65% of the estimated M_s). The noise curve is non-linear with an RMS of 5.570×10^{-8} Am^2 or ~18% of M_s (Figure 8b). A positive field drift correction reduces the closure error (M_{ce} = -6.390×10^{-10} Am^2; ~0.2% of M_s), yields more acceptable saturation behavior, and reduces the RMS noise (2.783×10^{-9} Am^2, ~1% of M_s). Although this loop looks more reasonable, the high-field portions are offset from each other and close only at the

555 peak fields, giving the impression of high coercivity “lobes” (Figure 8c). The shape factor (Fabian,
556 2003) of the loop is 1.47. This is indicative of extremely wasp-waited behavior and the presence of
557 a high coercivity component, which is not seen in isothermal remanent magnetization acquisition
558 data and does not fit with the geological context of the specimen (Liu et al., 2015; Liu et al., 2016).
559 An upper branch correction fails to reduce the loop closure error and symmetric averaging
560 exaggerates the high coercivity lobes yielding a loop shape factor of 1.67.

561 The paramagnetic drift model fit to the noise curve is shown in Figure 8b and the paramagnetic
562 drift corrected loop in Figure 8d. The loop is considerably more closed than before correction (post-
563 correction M_{ce} = -1.340×10^{-8} Am^2) and the high-coercivity “lobes” seen in positive field corrected
564 loop are absent. Although after applying only the paramagnetic drift correction RMS noise is
565 reduced (1.258×10^{-8} Am^2), considerable structure remains in the noise curve, which indicates that
566 not all drift has been corrected for and another source of drift it likely present (Figure 8e). After
567 applying the paramagnetic drift correction followed by the upper branch correction, the RMS is
568 further reduced and becomes flat, which should be expected from random measurement noise.
569 The fully corrected loop (Figure 8d) changes only slightly, but both RMS noise (2.702×10^{-9} Am^2)
570 and the closure error are reduced (M_{ce} = -6.700×10^{-9} Am^2), yielding a much more reasonable
571 hysteresis loop that can be more easily interpreted. The shape factor for the fully corrected loop,
572 0.06, indicates a constrained coercivity population, which is more consistent with the geological
573 context of the specimen (Liu et al., 2015; Liu et al., 2016).

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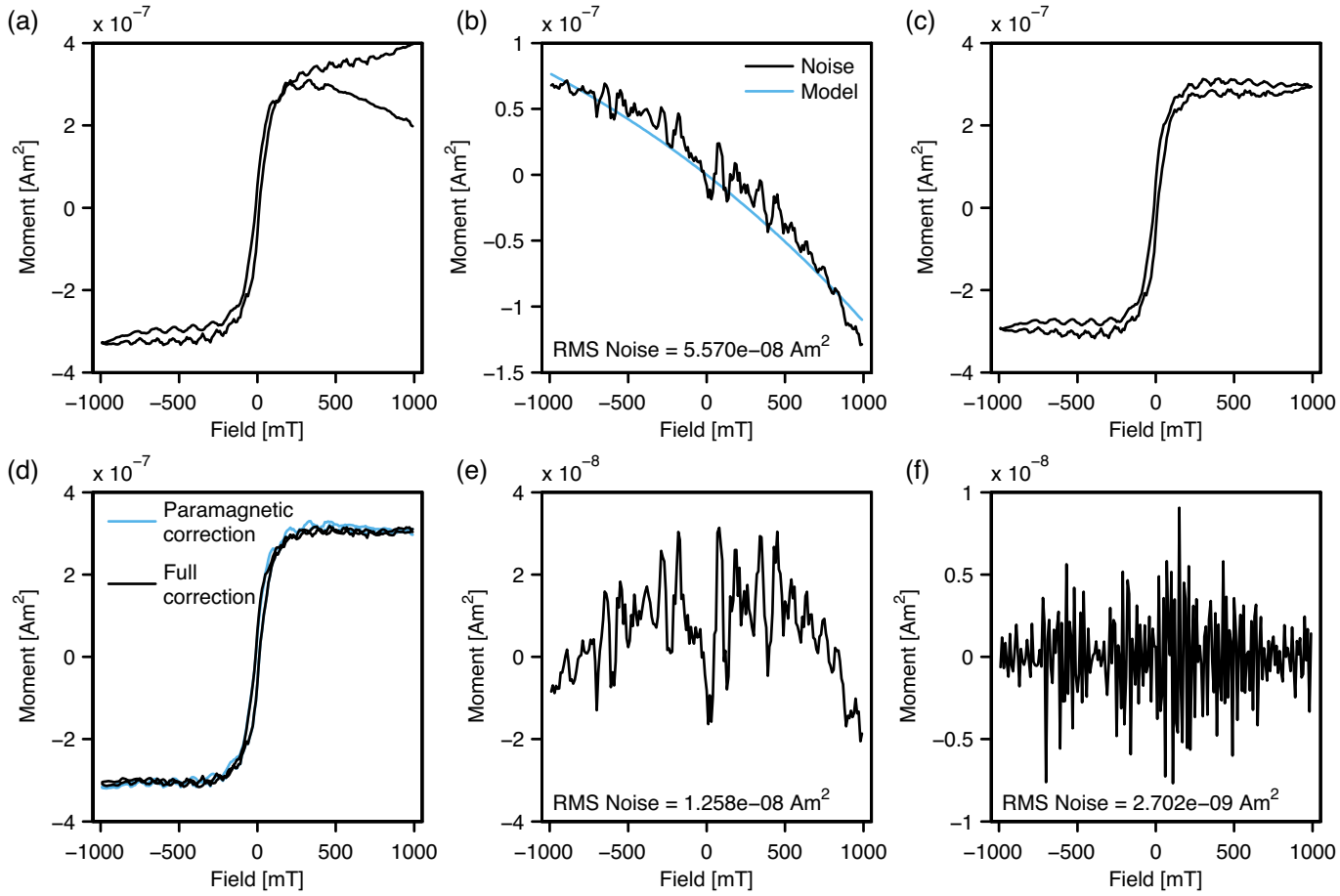

575

576 **Figure 8. Example of hysteresis loop drift and the paramagnetic drift correction.** (a) A weak
577 lake sediment sample from Liu et al. (2015) where the loop fails to close after returning to positive
578 saturation. (b) The noise curve (black line) exhibits a clear non-linear field dependent trend
579 indicative of drift. This trend can be well modeled by a paramagnetic thermal drift model (blue line).
580 (c) The hysteresis loop closes after positive field drift correction, but the overall shape of the high-
581 field regions is not satisfactory and does not match the geological context of the specimen. (d) The
582 hysteresis loop after paramagnetic drift correction only (blue loop) and after applying the combined
583 paramagnetic and positive field drift correction (black loop). (e) After paramagnetic drift correction
584 the RMS noise is reduced, but considerable structure remains in the noise curve, indicating other
585 drift sources are present. (f) The noise curve is flat after the full drift correction.

586

587 The paramagnetic thermal drift model estimates a temperature ratio of 1.036 for this hysteresis
588 loop. At the Institute of Geology and Geophysics, Chinese Academy of Sciences (IGGCAS), where
589 this measurement was performed, the VSM electromagnets are cooled with chilled water running
590 at ~17–19°C, which would yield an initial specimen temperature of ~27–29°C. Although high for the
591 time of measurement (mid-May with typical daytime ambient temperatures on the order of ~20–
592 26°C), it is still plausible. The exact room and specimen temperatures were not measured, so we
593 cannot exclude the possibility of unusual temperature conditions such as sun glare warming, which
594 can occur. Similarly, we cannot exclude the possibility that the model may be fitting other
595 components of drift not related to paramagnetic thermal effects and this may skew the estimated
596 temperature ratio.

597 This paramagnetic drift correction is not suitable for all specimens and works best for those with a
598 distinct lack of loop closure and strongly non-linear noise curve (e.g., Figure 8a, b). For example,
599 applying this correction to the loop shown in Figure 7b (noise curve is given in Figure 7c), yields a
600 temperature ratio of ~1.19. That is, the initial temperature of the specimen was ~20% higher than
601 ambient. For an ambient temperature of ~293 K (~20°C) this estimates a specimen temperature of
602 almost 80°C, which is physically unreasonable and indicates that the drift is unlikely to be related
603 to paramagnetic thermal effects. When applying this type of drift correction these factors should
604 always be considered when assessing the physical plausibility of the model and correction.

605 ### *4.5 Saturation slope correction*

606 In sufficiently high magnetic fields, the moment of ferro- and ferrimagnetic materials saturates,
607 while the moments of para- and diamagnetic materials continually increase or decrease,
608 respectively. Therefore, when exploring the remanence capability of complex natural samples that
609 are a mixture of magnetic carriers, it is necessary to correct the high-field portion for non-saturating
610 components. *HystLab* supports two standard approaches: a linear high-field slope correction, and
611 an approach to saturation correction (Fabian, 2006; Jackson and Solheid, 2010).

612 The linear correction assumes that the high-field portion of the ferromagnetic component is
613 saturated and fits a linear model to the high-field data to correct the slope by removing the
614 antiferro-, para- and diamagnetic contributions (i.e., non-saturated components). The approach to

615 saturation correction assumes that the high-field portion of the ferromagnetic component is not yet
616 fully saturated, but is in the reversible regime approaching saturation. This method fits the high-
617 field data with a model of the form:

618 $$M(B) = \chi_{HF} B + M_s + \alpha B^{\beta}, \quad (5)$$

619 where χ_{HF} is the high-field susceptibility, M_s is the saturation moment, and α and β are approach to
620 saturation coefficients (Fabian, 2006; Jackson and Solheid, 2010). The approach to saturation
621 model is fitted similarly to the method outlined by Jackson and Solheid (2010), whereby 100 β
622 values evenly distributed on the interval [-2, -1] are specified and equation 5 is solved to determine
623 the remaining coefficients and the model that best fits the data.

624 *HystLab* includes an automated slope correction routine that tests if a high-field slope correction
625 should be applied and then tests the appropriateness of a linear correction versus an approach to
626 saturation correction at 70%, 80%, and 90% of the peak field. A schematic outline of the decision
627 process is shown in Figure 9.

628 The first step is to perform a lack-of-fit F-test for whole loop linearity using the data before slope
629 correction (Jackson and Solheid, 2010). This test assesses if the lack-of-fit between the data and a
630 linear model fit to the whole loop is significant. If the p-value of this test is < 0.05 (5% significance
631 level) then we can reject the null hypothesis that the misfit between the data and a linear loop is
632 due to random noise, hence conclude that it is primarily due to a lack-of-fit (i.e., the loop is not
633 linear). If the null hypothesis cannot be rejected (i.e., the whole loop appears linear) then no high-
634 field slope correction is applied.

635 If a linear loop is rejected, *HystLab* assesses whether the loop is closed at high-fields. Loops that
636 are distinctly open at high-fields indicate that a specimen is not saturated and not in the approach
637 to saturation regime (e.g., Figure 10a). In such cases, no form of high-field slope correction can
638 currently be applied.

639 Here we introduce two new statistics to assess loop closure at high-fields. First, at a given field
640 above which closure is to be tested, the signal-to-noise ratio (SNR) of the high-field M_{rh} curve to
641 high-field noise is assessed – An open loop will have a non-zero M_{rh} curve over the defined high-

642 field range, which should be distinctive above the noise (i.e., have a high SNR). To assess the M_{rh}
643 signal, the negative field M_{rh} curve is inverted around the origin and averaged with the positive field
644 half and all negative moments are set to zero (they are a result of noise and setting them to zero
645 removes them from the estimation of signal power). The M_{rh} signal power is taken as the RMS of
646 this average M_{rh} curve. The power of the noise is take as the RMS of the high-field noise and the
647 SNR is calculated in decibels as $20 \times \log_{10}\left(signal/noise\right)$. High values of SNR indicate the non-zero
648 nature of the M_{rh} curve is distinct above the noise and indicate that the loop may be open.

649 The second statistic assesses the relative contribution of the high-field M_{rh} signal to the entire M_{rh}
650 signal. A perfectly closed loop will have zero area under the high-field portion of the M_{rh} curve, but
651 for most real data measurements the high-field M_{rh} is non-zero and a level tolerance is needed to
652 assess loop closure. To assess this, we define the high-field area ratio (HAR), which is the ratio of
653 the area under the high-field M_{rh} curve to the area under the entire M_{rh} curve. The areas are
654 calculated using the averaged M_{rh} curve described above and, following the SNR calculation, HAR
655 is calculated in dB. High values of HAR indicate that the high-field portion of the M_{rh} curve forms a
656 notable part of the total curve and indicate that the loop may be open; extremely low values
657 indicate that the high-field contribution is small and the loop may reasonably be assumed to be
658 closed.

659 The automatic correction determines that a loop is closed if the SNR is less than 8 dB or the HAR
660 is less than -48 dB. An 8 dB SNR corresponds to an average M_{rh} signal ~2.5 times stronger than
661 the noise, while an HAR of -48 dB corresponds to a high-field area ~1/250th of the total M_{rh} area.
662 These thresholds tend to prefer loop closure, for which high-field slope correction methods are
663 viable. For loops where closure is rejected, no correction is applied and the user should manually
664 consider the appropriateness of high-field slope corrections.

665 Figure 10a is an example of an open loop for which no correction can be rigorously applied. At
666 90% of the peak field, SNR = 15.8 dB and HAR = -47.8 dB. It is possible to test for closure at
667 higher peak fields, but it should be kept in mind that even minor loops that are far from saturation
668 will close at their peak field. Therefore, any loop will appear closed near the peak field.

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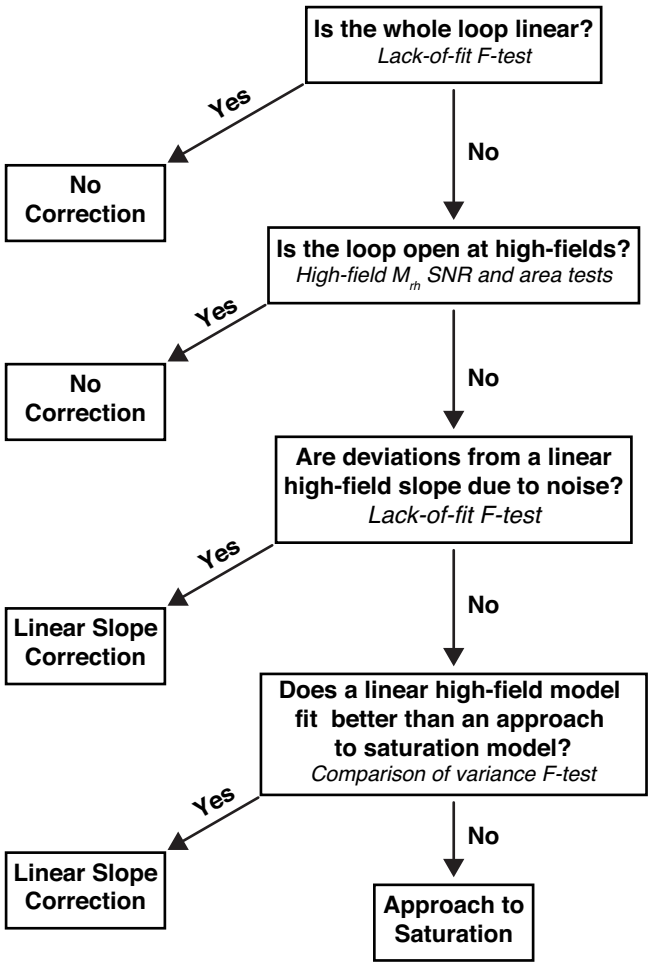
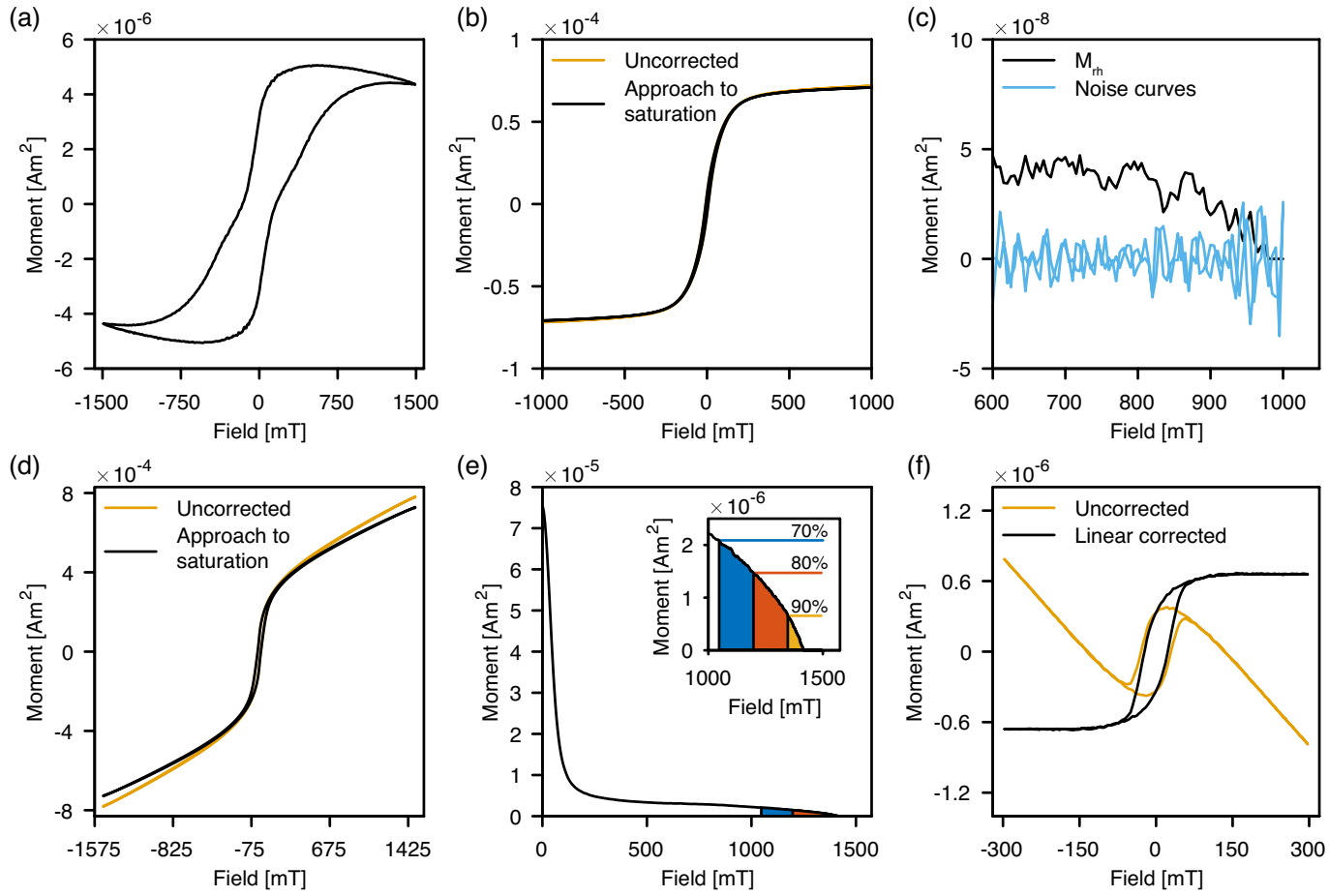


670

671 **Figure 9. Schematic of the decision process when applying an automated high-field slope**

672 **correction.**

673



674

675 **Figure 10. Examples of high-field slope corrections.** (a) An oxidized granite specimen with
676 mixed high and low coercivity components yields a hysteresis loop that remains open at high-
677 fields. Currently, no high-field slope correction is strictly valid for such a loop. (b) A hysteresis loop
678 of volcanic chip before and after automatic correction, which applies an approach to saturation
679 correction. (c) The high-field averaged M_{rh} curve and high-field portions of the noise curve
680 (negative field half inverted to positive fields) for the loop in part (b). At 70%, 80% and 90% of the
681 peak field (700, 800 and 900 mT, respectively), M_{rh} signal-to-ratios are 10.6, 7.8, and 1.9 dB,
682 respectively. (d) A hysteresis loop of a thermally stabilized basalt before and after automatic
683 correction, which applies an approach to saturation correction. (e) The averaged M_{rh} curve for the
684 loop in part (d), where the high-field portions used to calculate high-field to total M_{rh} signal ratios
685 are shaded in color. The inset enlarges the high-field region. The HAR values at 70%, 80% and 90
686 of the peak field are -24.7, -32.4, and -50.1 dB, respectively. Above 90% of the peak field, the loop
687 can be considered closed. (f) An MTB specimen with a strong diamagnetic component. The
688 automatic correction favors loop closure and a linear high-field slope correction.

689 In Figure 10b we show a hysteresis loop that visually appears to close at high-fields. The
690 corresponding high-field M_{rh} and noise curves are shown in Figure 10c. At 70%, 80% and 90% of
691 the peak field (700, 800 and 900 mT, respectively), M_{rh} SNR values are 10.6, 7.8, and 1.9 dB,
692 respectively. Above 80% of the peak field, the SNR falls just below our threshold of 8 dB and,
693 because M_{rh} becomes comparable to the level of noise, the loop can be considered closed. HAR at
694 the three field levels are -32.5, -38.0, and -49.4 dB.

695 In Figure 10d we show another loop that visually appears to be closed. In this case, the SNR
696 values at 70%, 80% and 90% of the peak field are all > 19.3 dB. The averaged M_{rh} curve is shown
697 in Figure 10e and the high-field areas are highlighted. The high-field regions have HAR values -
698 24.7, -32.4, -50.1 dB for 70%, 80%, and 90% of the peak field, respectively. These correspond to
699 total M_{rh} areas 17, 42, and 320 times larger than the respective high-field regions. The high SNR
700 values indicate the high-field M_{rh} segments are not unduly affected by noise, but the extremely low
701 HAR value at 90% peak field indicate the high-field M_{rh} signal is small and it is reasonable to
702 assume loop closure.

703 If an open loop is rejected, *HystLab* further tests the linearity of the high-field portion of the
704 hysteresis loop to evaluate whether a loop is saturated or approaching saturation (cf. Jackson and
705 Solheid, 2010). For a given field above which the specimen is assumed to be saturated or
706 approaching saturation, two styles of F-test are performed to assess which mode of slope
707 correction should be applied. Firstly, a linear model is fitted to the high-field data. Using the
708 negative high-field data as replicates of the positive high-field data, we perform a lack-of-fit F-test
709 to test the null hypothesis that the misfit between the data and the model can be explained by the
710 noise of the data. If the p-value of this test is < 0.05 (5% significance level), then we reject the null
711 hypothesis. That is, the poor fit of a linear model to the high-field data cannot be explained by
712 noise and may be better explained by an alternative model (i.e., approach to saturation).

713 The second test is an F-test comparison between the variance accounted for by a linear model
714 (with 2 free parameters) and the variance accounted for by an approach to saturation model (with
715 4 free parameters). If the p-value of this test is < 0.05 (5% significance level), then we reject the

716 null hypothesis that the simpler linear model fits the data adequately and conclude that the more
717 complex approach to saturation model is justified.

718 If one or both of these F-tests come out in favor of a linear high-field slope, a linear high-field
719 correction is applied. Only if both tests reject linearity is an approach to saturation correction
720 applied. This automated approach tends to favor applying a linear high-field slope correction
721 because of the ill-conditioned nature of the approach to saturation correction (see Jackson and
722 Solheid (2010) for a full discussion of the challenges of applying an approach to saturation
723 correction). We note that the F-tests are for general guidance and can be influenced by the
724 smoothing introduced by loop interpolation and drift corrections. For specimens where the
725 automated correction suggests approach to saturation, we recommend consideration of the
726 physical validity of the correction and a careful inspection and manual checking of fields around the
727 field above which the correction is applied. Furthermore, if possible, measuring hysteresis to higher
728 peak fields can help better resolve the saturation regime of many specimens.

729 The loops shown in Figure 10b and d are examples where a linear high-field slope is rejected and
730 an approach to saturation correction is applied. In Figure 10f we show a hysteresis loop from an
731 MTB specimen with a strong diamagnetic signal (the offset corrected loop shown in Figure 7a).
732 Both F-tests cannot reject a linear high-field slope, hence a linear correction is applied.

733 ### *4.6 Loop fitting*

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

739 Firstly, the remanent (M_{rh}) and induced (M_{ih}) hysteretic curves are calculated (von Dobeneck,
740 1996). The negative field halves are inverted and averaged with the positive field halves to reduce
741 noise – *HystLab* fits to these averaged half curves. Like Jackson and Solheid (2010), *HystLab* fits
742 a combination of hyperbolic and sigmoid logistic basis functions to the M_{rh} and M_{ih} curves. In

743 *HystLab*, however, the basis functions are not a pre-defined set, but are defined for each specimen
744 such that the median fields of the basis functions correspond to equally spaced moments on the
745 M_{rh} and M_{ih} curves.

746 For each curve, a maximum of 22 basis functions are fitted, for a total maximum of 44 per
747 hysteresis loop. The M_{rh} curve is fitted with 10 hyperbolic secant functions, 10 sigmoid logistic
748 functions, and 2 linear functions with positive and negative slopes. The M_{ih} curve is fitted with 10
749 hyperbolic tangent functions, 10 sigmoid logistic functions, and 2 linear functions (to account for
750 any paramagnetic and diamagnetic components of uncorrected loops). The mathematical form of
751 the basis functions is given in the *HystLab* instruction manual (see also von Dobeneck, 1996;
752 Jackson and Solheid, 2010). Where insufficient data are available to perform the lack-of-fit F-test,
753 *HystLab* reduces the number of hyperbolic and sigmoid functions to less than 10 each.

754 The relative contribution of the basis functions is estimated using the sparse unmixing by variable
755 splitting and augmented Lagrangian (SUnSAL) algorithm of (Bioucas-Dias, 2009). In addition to the
756 sparsity enforced by SUnSAL, basis functions with a relative contribution of < 0.01% are omitted
757 from the final fit to minimize the total number of used functions.

758 The quality of the fit is assessed using the F-test for lack-of-fit (Jackson and Solheid, 2010). This
759 lack-of-fit test, which is performed on the whole hysteresis loop, tests the null hypothesis that the
760 misfit between the model and the data can be attributed to i.i.d. Gaussian noise. If the p-value of
761 this test is < 0.05 (5% significance level), then we can reject the null hypothesis. That is, the poor
762 fit of the basis functions to the loop cannot be explained by noise. In these cases, the quality of the
763 data should be sufficient to estimate the various hysteresis statistics from the data directly. Users
764 should consider each specimen carefully and note the F-test results are for guidance and can be
765 influenced by the smoothing introduced by loop interpolation and drift corrections.

766 In **Figure 11**a, we show an example of a visibly noisy loop and its fit (the loop is one of the 30
767 repeated loops measured in continuous mode with 100 ms averaging described in Section 3.1). In
768 **Figure 11**b we also show a higher quality, lower noise loop from the same specimen alongside the
769 fit to the loop in **Figure 11**a (the lower noise loop is the average of the 30 loops measured in
770 discrete field sweep mode with a pause time of 300 ms and 200 ms averaging time). The RMS

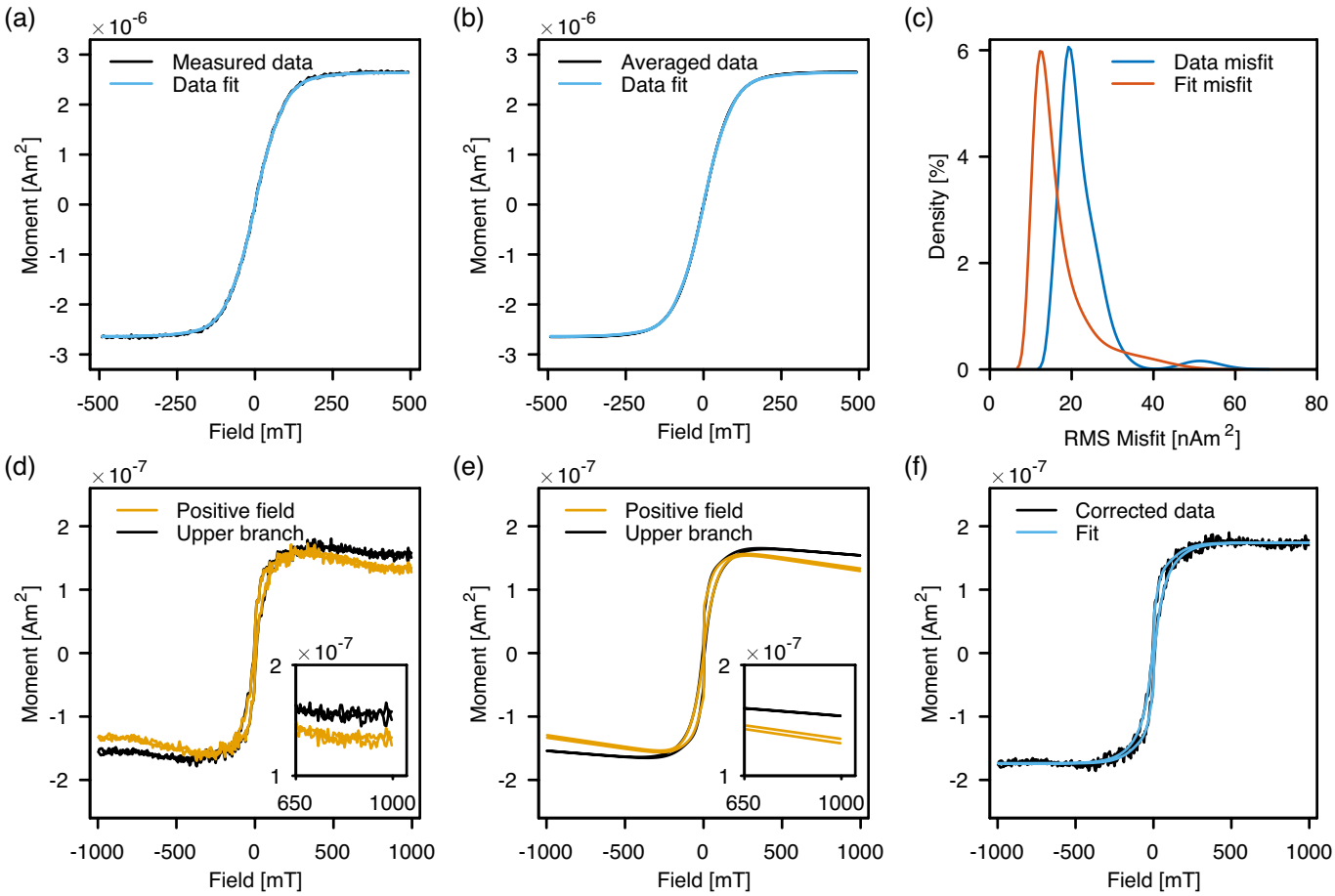
misfit between the measured loop and the averaged loop is 2.03×10^{-8} Am^2 and the RMS misfit between the loop fit and the averaged loop is 1.40×10^{-8} Am^2, indicating that the fit to the lower quality data is a better estimate of the higher quality loop. In **Figure 11**c we plot the density distributions of the RMS misfits between higher quality averaged loop and (1) the 30 noisier loops and (2) the model fits to the 30 noisier loops. For 24 of the 30 loops the model fit more accurately represents the lower noise loop than the measured data, which illustrates how fitting hysteresis loops can help to filter noisy data.

Fitting loops can also be a useful diagnostic tool for determining appropriate processing for noisy or otherwise problematic loops. The hysteresis loops for a weak carbonate specimen (Jackson and Swanson-Hysell, 2012) after positive field drift correction and after upper branch correction are shown in **Figure 11**d (a linear high-field slope correction has been applied to both loops); the loop closure errors are 7.03×10^{-9} Am^2 and 7.60×10^{-9} Am^2, respectively. Note the upward and downward curvature in strong positive and negative fields, respectively. In the absence of a metamagnetic transition, such curvature can be assumed to be the result of an unknown experimental artifact. A comparison between the fits to these two loops is shown in **Figure 11**e. The fit to the positive field drift corrected loop does not close (parallel and non-intersecting high-field upper and lower branches; inset **Figure 11**e), but the fit to the upper branch corrected loop yields a more closed loop, indicating it is a more appropriate drift correction to apply for this specimen.

In both cases, however, the high-field slope correction underestimates the high-field diamagnetic susceptibility. As a consequence, after linear high-field slope corrections, both loops and their fits have negative high-field slopes – the correction is inadequate. This incomplete correction is due to unusual high-field drift, present in all four high-field segments, that results in slight anomalous curvature of the high-field segments (**Figure 11**d). *HystLab* provides the option to apply slope correction and estimate loop parameters for the fitted loop in addition to the measured data. The resultant loop after upper branch drift correction using the fitted loop to correct the high-field slope with a linear correction is shown in **Figure 11**f. Applying the slope correction to the fitted loop yields more satisfactory high-field behavior that fully corrects for the diamagnetic component.

798 Fitting a noisy hysteresis loop can have a number of advantages, including removing high
799 frequency noise as well a means of assessing the appropriateness of processing and correcting
800 high-field slope behavior. We emphasize, however, that although fitting can help to analyze noisy
801 data, it is no substitute for remeasuring extremely noisy hysteresis loops.

802



803

804 **Figure 11. Examples of hysteresis loop fitting.** (a) Fitting of a loop measured with a 100 ms
805 averaging time in continuous sweep mode. (b) The average of 30 loops for the same specimen in
806 part (b), but measured with a 200 ms averaging time in discrete sweep mode with 200 ms settling
807 time. The fitted loop is the same as shown in part (a). (c) The distribution of misfits between 30
808 replicates of the loop shown in part (a) and the averaged loop in part (b) (blue curve) and the
809 distribution of misfits between the model fits to the 30 repeat loops and the averaged loop in part
810 (b) (orange curve). Twenty-four of the 30 replicates have model fits that more accurate represent
811 the higher quality loop than the original measurements. (d) A weak carbonate specimen after
812 positive field and upper branch drift corrections, both of which yield apparently similarly closed
813 loops. The high-field region is expanded in the inset. (e) Fitting results of the loops shown in (d)
814 reveal a distinct lack of loop closure after positive field drift correction. The high-field region is
815 expanded in the inset. (f) Using the high-field segment of the fitted loop yields a better linear slope
816 correction than using the data directly.

817

5 *HystLab* features

5.1 Supported data

Within the rock and paleomagnetic community, a range of magnetometers can be used to measure hysteresis loop data. These include vibrating sample magnetometers (VSMs), alternating gradient magnetometers (AGMs), variable field translation balances (VFTBs), as well as superconducting quantum interference device (SQUID) magnetometers coupled with high-field magnets. This variety, combined with a range of manufacturers, means that numerous data formats are available, which can complicate consistent analysis.

HystLab supports the most widely used data formats including, multiple format versions for the Princeton Measurements Corporation MicroMag 3900 VSM and 2900 AGM, Lake Shore 7400 and 8600 VSMs, Quantum Designs Magnetic Properties Measurement System (MPMS), Magnetic Measurements VFTBs, and MicroSense VSMs. *HystLab* allows users to append data to the current session, which allows multiple data formats to be loaded and analyzed together. Once data are loaded into *HystLab* users can save their *HystLab* session, allowing them to complete their analyses at a later date or to share their results with collaborators. If any users encounter an unsupported data format, they should contact the authors with an example file and it will be added to *HystLab*.

5.2 Interface

The main *HystLab* window is shown in Figure 12. Data can be loaded via the menu bar (Figure 12a) and will be plotted in the three main plots (Figure 12b). Here, the original, raw data can be plotted alongside the processed data as well as the fitted data. In addition to the hysteresis loop, the remanent (M_{rh}) and induced (M_{ih}) hysteretic curves, as well as the noise curve are also shown (Figure 12b). Multiple specimens can be loaded at once and the user can browse through each (Figure 12c). On loading data, loops are processed to correct for offset and apply the automatic drift and high-field slope corrections. Additional processing can then be performed on a specimen-by-specimen basis using the control panel shown in Figure 12d. The plot control panel (Figure 12e) allows for different moment/magnetization normalizations as well as controlling which data

are displayed. Panel f contains the analysis results and statistics – a comprehensive list and description of each statistic can be found the *HystLab* documentation (accessible through the "Help" menu, Figure 12a).

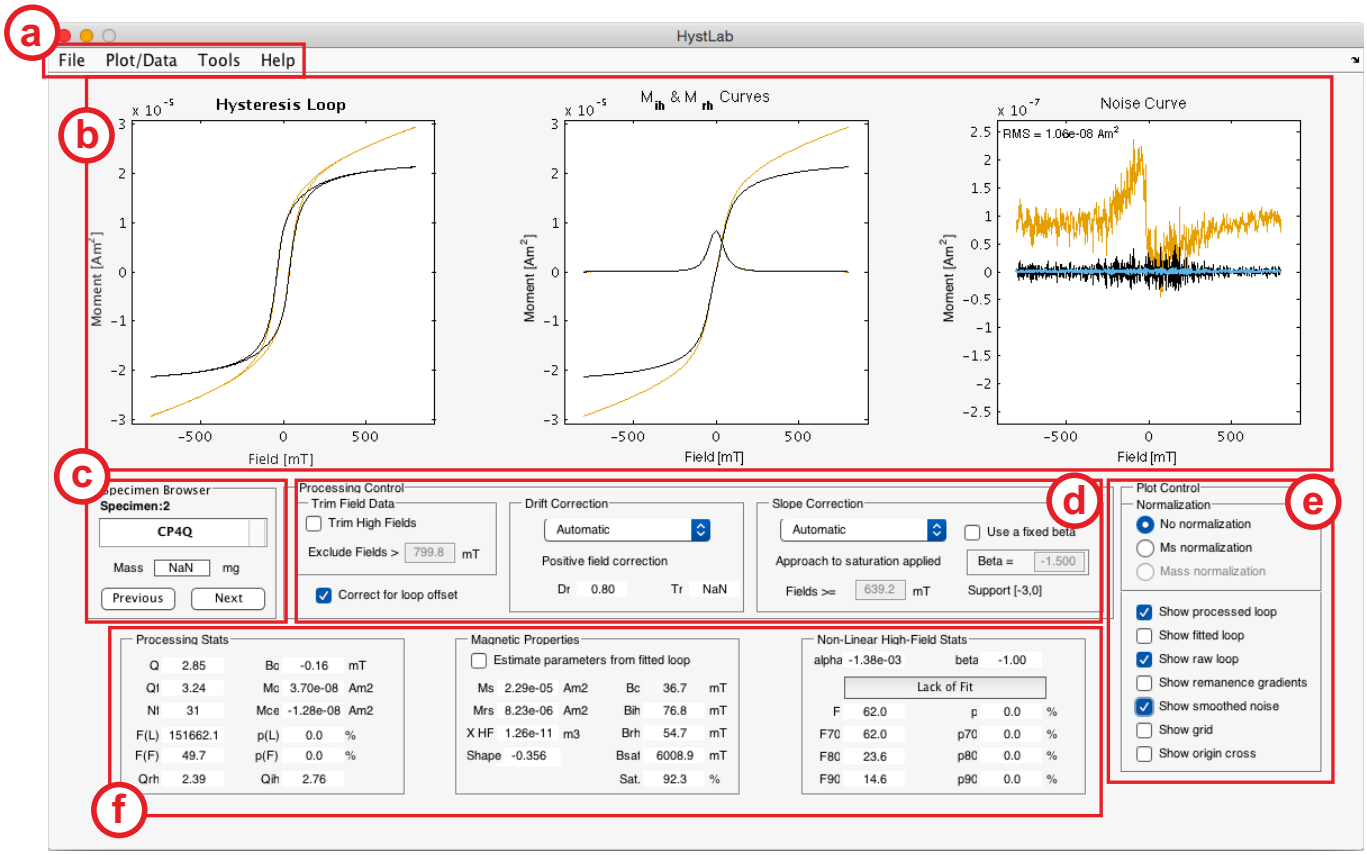


Figure 12. The main *HystLab* interface. (a) The menu bar for loading data and exporting results and plots. (b) The main data plots. (c) Specimen browser. (d) The processing control panel. (e) The plot control panel. (f) The analysis results and statistics.

5.3 Data and plots

Statistics and analysis parameters in *HystLab* can be exported to tab delimited text files. The default plot color schemes are chosen to enhance contrast for colorblind users (Wong, 2011), but are fully customizable and can be saved to a user preference file for future use. In addition, by clicking on each plot, a new MATLAB figure window will open, which allows further customization.

All plots presented in *HystLab* can be exported to encapsulated postscript files that are publication ready with little or no adjustment.

6 Summary

Magnetic hysteresis loops are one of the most ubiquitous rock magnetic measurements in the Earth magnetism community. These rapid to measure data provide a diverse variety of descriptive statistics that have a broad range of applications. However, despite their apparent ease and simplicity, in-depth and quantitative descriptions of measuring and processing hysteresis loops to avoid or correct for widely occurring detrimental factors (e.g., drift and loop offset) are rarely performed.

Here we have outlined a range of approaches that can be used to improve the measurement quality of hysteresis loops. Although these are largely developed from extensive experience using VSM systems, many are applicable to a wide range of instruments used to measure magnetic hysteresis. These strategies are also valid for other types of data measurable on the same equipment (e.g., isothermal remanent magnetization acquisition, back-field demagnetization, first-order reversal curves, among others).

Building on established processing recommendations, we have developed *HystLab*, which is a new software package for the advanced processing and analysis of hysteresis loop data. Supporting a wide range of data formats, with the ability to export data and generate publication ready figures, *HystLab* has a range of tools to correct for commonly occurring negative artifacts in hysteresis data. We hope that *HystLab* can enhance both productivity and accuracy when processing and analyzing large data sets, and we encourage users with suggestions or bug reports to contact us and help to improve the software.

Appendix: Glossary of Hysteresis Statistics and Parameters

Below is brief glossary of the major terms used in this paper. Further details and definitions are given in the documentation that accompanies *HystLab*.

885	α	The alpha parameter for the applied approach to saturation high-field slope correction (Fabian, 2006; Jackson and Solheid, 2010).
887	β	The beta parameter for the applied approach to saturation high-field slope correction (Fabian, 2006; Jackson and Solheid, 2010).
889	B_0	Hysteresis loop offset along the field (horizontal) axis.
890	B_c	Hysteresis loop coercivity.
891	B_{ih}	The median value of the induced hysteretic curve (von Dobeneck, 1996).
892	B_{rh}	The median value of the remanent hysteretic curve (von Dobeneck, 1996).
893	*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.
895	M_0	Hysteresis loop offset along the moment/magnetization (vertical) axis.
896	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.
899	M_f	Ferromagnetic moment/magnetization at a specific field.
900	M_{ih}	The induced hysteric moment/magnetization curve (Rivas et al., 1981; von Dobeneck, 1996). Calculated as half the sum of the upper and lower hysteresis branches.
903	M_p	Paramagnetic moment/magnetization at a specific field.
904	M_{rh}	The remanent hysteric moment/magnetization curve (Rivas et al., 1981; von Dobeneck, 1996). Calculated as half the difference of the upper and lower hysteresis branches.
907	M_{rs}	Saturation remanent moment/magnetization.
908	M_s	Saturation moment/magnetization.

909	Q	A measure of the quality of the raw hysteresis loop determined by taking the linear
910		correlation between the upper and inverted lower branches.
911	Q_f	A measure of the quality of the slope-corrected (ferromagnetic) hysteresis loop
912		determined by taking the linear correlation between the upper and inverted lower
913		branches.
914	Q_{ih}	A measure of the quality of the processed M_{ih} curve determined by taking the linear
915		correlation between the positive field half and the inverted negative field half.
916	Q_{rh}	A measure of the quality of the processed M_{rh} curve determined by taking the linear
917		correlation between the positive field half and the reflected negative field half.
918	*Shape*	Hysteresis loop shape factor, σ (Fabian, 2003).
919	*SNR*	The signal-to-noise ratio (SNR; in dB) of the high-field M_{rh} to the high-field noise.
920	T_0	The initial temperature of a specimen at the beginning of a measurement.
921	T_A	The ambient temperature between the pole pieces of the measurement equipment.
922	T_r	The ratio of the specimen initial temperature (T_0) to the ambient temperature
923		between the pole pieces (T_A). Estimated for the paramagnetic drift correction.
924	X_{HF}	High-field susceptibility (determined from the high-field slope correction).

925

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936

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