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UDECON: deconvolution optimization software for restoring high-resolution records from pass-through paleomagnetic measurements

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Abstract

The rapid accumulation of continuous paleomagnetic and rock magnetic records acquired from pass-through measurements on superconducting rock magnetometers (SRM) has greatly contributed to our understanding of the paleomagnetic field and paleo-environment. Pass-through measurements are inevitably smoothed and altered by the convolution effect of SRM sensor response, and deconvolution is needed to restore high-resolution paleomagnetic and environmental signals. Although various deconvolution algorithms have been developed, the lack of easy-to-use software has hindered the practical application of deconvolution. Here, we present standalone graphical software UDECON as a convenient tool to perform optimized deconvolution for pass-through paleomagnetic measurements using the algorithm recently developed by Oda and Xuan (Geochem Geophys Geosyst 15:3907–3924, 2014). With the preparation of a format file, UDECON can directly read pass-through paleomagnetic measurement files collected at different laboratories. After the SRM sensor response is determined and loaded to the software, optimized deconvolution can be conducted using two different approaches (i.e., "Grid search" and "Simplex method") with adjustable initial values or ranges for smoothness, corrections of sample length, and shifts in measurement position. UDECON provides a suite of tools to view conveniently and check various types of original measurement and deconvolution data. Multiple steps of measurement and/or deconvolution data can be compared simultaneously to check the consistency and to guide further deconvolution optimization. Deconvolved data together with the loaded original measurement and SRM sensor response data can be saved and reloaded for further treatment in UDECON. Users can also export the optimized deconvolution data to a text file for analysis in other software.

Keywords: U-channel sample; Superconducting rock magnetometer; Sensor response; Paleomagnetism; Deconvolution; Software

Introduction

The development of pass-through superconducting rock magnetometers (SRM) has allowed automated, fast, continuous, and high sensitivity measurement of remanent magnetizations in geological archives (Dodson et al. 1974; Goree and Fuller 1976; Weeks et al. 1993; Nagy and Valet 1993; Goree 2007), leading to rapid accumulation of high-resolution paleomagnetic and environmental magnetic datasets. Pass-through SRMs have been routinely used by Ocean Drilling Program (ODP), Integrated Ocean Drilling Program, and now International Ocean Discovery Program (IODP) expeditions onboard R/V *JOIDES Resolution* and *Chikyu* for paleomagnetic measurements of "archive" half-round core sections. A typical IODP expedition often involves pass-through SRM measurements for kilometers of core sections at every few centimeter intervals to produce timely magnetostratigraphic constraints for the drilled cores. Pass-through paleomagnetic and environmental magnetic measurements are also routinely conducted on continuous u-channel samples (Tauxe et al. 1983) using u-channel SRMs equipped with high-resolution pickup coils (Weeks et al. 1993; Nagy and Valet 1993) available at worldwide paleomagnetism laboratories. The continuous and rapidly growing records acquired on pass-through SRMs have revolutionized paleomagnetic

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research making it possible to reconstruct and exploit paleomagnetic field behavior at unprecedented resolution and scale. For instance, continuous sedimentary relative paleointensity records reconstructed mainly based on pass-through SRM measurements have greatly contributed to our understanding of the geodynamo and served as independent stratigraphic tool for correlating and dating worldwide sediment sequences at much higher-resolution than traditional magnetic polarity stratigraphy (e.g., Valet and Meynadier 1993; Guyodo and Valet 1999; Valet et al. 2005; Channell et al. 2009; Roberts et al. 2013).

Despite the exciting opportunities offered by pass-through SRMs, it is known that pass-through paleomagnetic measurements are inevitably smoothed and altered due to the convolution effects of the SRM sensor response. Cross terms among the SRM's three orthogonal pickup coils, and possible rotation of x–y pickup coils around the z-axis relative to the plane of measurement tray may even lead to directional and intensity artifacts in the resulting measurement (e.g., Parker and Gee 2002; Roberts 2006; Jackson et al. 2010; Oda and Xuan 2014). Deconvolution is necessary to overcome the convolution effect and obtain more accurate and significantly higher-resolution data comparable to that measured using back-to-back discrete samples (see Guyodo et al. 2002). Various algorithms have been presented for deconvolution of pass-through paleomagnetic data acquired on either whole-core or u-channel SRMs (e.g., Dodson et al. 1974; Constable and Parker 1991; Oda and Shibuya 1994; 1996; 1998; Jackson et al. 2010). Oda and Xuan (2014) recently developed an improved deconvolution algorithm based on the Akaike's Bayesian Information Criterion (ABIC) minimization method introduced by Oda and Shibuya (1994, 1996). The new deconvolution algorithm optimizes ABIC not only for smoothness of the signal but also for realistic error in sample length and shift in measurement position introduced during sampling and measurement in the laboratory. Reliability and accuracy of the algorithm have been demonstrated using synthetic pass-through data with realistic measurement noises (see Oda and Xuan 2014).

It is desirable to perform deconvolution as a routine for processing pass-through paleomagnetic measurement data to remove any artifacts (see Roberts 2006) and to restore higher-resolution paleomagnetic intensity and directional variabilities (e.g., excursions or reversals, see Guyodo et al. (2002)) as well as environmental changes that are crucial to our understanding of the Earth's past magnetic field and environment. The lack of easy-to-use software that can quickly implement the deconvolution schemes makes it difficult to deconvolve large amount of pass-through data on regular bases. In this paper, we present standalone graphical software UDECON designed to directly read pass-through measurement data file and allow fast and reliable deconvolution optimization using the algorithm developed by Oda and Xuan (2014). It should be noted that deconvolution optimization in UDECON is based on the following assumptions (see Shibuya and Michikawa 2000; Jackson et al. 2010; Oda and Xuan 2014): (1) sample magnetization varies only as a function of depth; (2) smoothness of the magnetization variations is similar throughout the sample; and (3) measurement errors follow Gaussian distribution. In the following sections, we first discuss necessary preparations for the pass-through measurement and SRM sensor response data prior to the use of UDECON and then provide detailed description of features available in the software as well as instructions to help accomplish successful deconvolution.

Preparation of measurement data for deconvolution

It is necessary to check and prepare the raw pass-through measurement data prior to deconvolution analyses. Corrections on raw measurement data are often needed, including corrections for drifts in the superconducting quantum interference device (SQUID) system and magnetization of the sample tray. Several factors can cause drifts in a SQUID magnetometer, for instance, thermoelectric effect in the SQUID electronics, or flux creep in the SQUID or flux transformer (Clark and Braginski 2004). External effects such as magnetic relaxation of mu-metal shield or decay of viscous remanent magnetization of the tray or the sample can also lead to drifts in the system. For typical pass-through paleomagnetic measurements, background magnetic moment is monitored at the beginning and the end of each measurement run and linearly interpolated through measurement time to correct for drifts. Magnetization of the sample tray is usually measured on regular bases and subtracted from the raw sample measurements. The tray and drift corrected magnetic moment data (usually in unit of emu) were then transformed to volume normalized intensity (in unit of emu/cc) using volumes estimated by the sample cross section area and effective lengths of the sensor responses. The manufacturer of SRM (2G Enterprises) usually provides the effective length of sensor response for all three orthogonal measurement axes at the time of installation. In addition, pass-through measurement on SRM should also include measurement of intervals immediately before and after passing the sample through the center of the sensor area. These measurement intervals are referred to as the "leader" and "trailer" and serve the dual functions of monitoring the background magnetic moment and allowing deconvolution analysis for measurements near the sample ends.

Pass-through paleomagnetic measurement sometimes includes flux jumps at random measurement positions on some measurement axes. Flux jumps are sudden changes in magnetic moment along particular measurement axis, after which the magnetic moment levels do not go back to that prior to the flux jump. Flux jumps in measurement could dramatically distort paleomagnetic direction and intensity estimation after drift correction (e.g., Oda and Shibuya 1996). In general, two types of flux jumps have been known to occur in SQUID magnetometers. The first type (type 1) of flux jumps present as a random integer value multiplication of one flux quantum and are caused by phase-slips along the periodic flux-to-voltage characteristic of the SQUID response curve (e.g., Clark and Braginski 2004). SRM manufacturer (2G Enterprises) usually provides the magnetic moment value of one flux quantum for each measurement axis based on factory calibration. Type 1 flux jumps appear to happen more often when measuring samples with strong magnetization at high track velocity. The second type (type 2) of flux jumps are characterized as low-frequency step noise with amplitudes smaller than one flux quantum. Type 2 flux jumps may originate from a trapped fluxon hopping between two positions within the SQUID or flux transformer's structure (see Clark and Braginski 2004). A type 2 flux jump was reported by Oda and Shibuya (1996) and referred to as "unknown jumps".

In addition to flux jumps, raw pass-through paleomagnetic measurement may also contain spike noises. Different to flux jumps after which magnetic moment level does not go back to a previous level, spike noise is a sudden change in magnetic moment at a measurement position, after which the magnetic moment level goes back to that prior to the spike noise. At measurement positions with spike noise, measurement values are apparently distinct from the average values of the surrounding measurement positions. Flux jumps and spike noises both significantly affect the resulting paleomagnetic measurement, and measurements containing flux-jumps or spike noises need to be repeated or corrected before any paleomagnetic interpretation or deconvolution can be made (e.g., Oda and Shibuya 1996). The UPmag software (Xuan and Channell 2009) provides convenient tools to check pass-through paleomagnetic measurement data and correct for flux jumps. We recommend using the UPmag software to check and correct pass-through paleomagnetic measurement data before deconvolution analysis.

Acquisition and preparation of magnetometer sensor response

To perform deconvolution for measurements made on an SRM, an accurate estimate of the SRM sensor response including cross terms among the three pickup coils is needed (e.g., Oda and Shibuya 1996; Parker and Gee 2002; Roberts 2006; Jackson et al. 2010), and a sensor response file should be prepared prior to deconvolution analysis (see Fig. 1). In order to acquire reliable sensor response suitable for deconvolution, high-resolution (e.g., every 1-mm interval) measurements of a magnetic point source over the possible sensor response interval (e.g., 40 cm) along the track are needed (Oda and Xuan 2014). The magnetic point source is repeatedly measured while it is placed at different grid positions on a cross section perpendicular to the direction of pass-through measurement along the track (e.g., 5×5 grid positions over an $\sim 2 \times 2$ cm^2 area), orienting parallel or antiparallel to each of the three orthogonal SRM measurement axes (see Figure 1 in Oda and Xuan (2014)). The measured sensor response curves for each grid position are then normalized by the magnetic moment of the point source used for the measurements. Subsequently, magnetometer sensor response over the cross area of the measured sample (typical u-channel has a cross area of $\sim 1.8 \times 1.8$ cm^2) needs to be calculated using the collected sensor response measurements. This can be done through spline interpolation of sensor response at the measured grid positions (i.e., 5×5 with 5 mm spacing) to higher resolution spacing (e.g., 1 mm), followed by integration of sensor response over the sample cross area. The integrated sensor response should be normalized by the cross area before it is used for deconvolution optimization in UDECON. As difference in the shape and area of the sample cross section will lead to different sensor response (e.g., Oda and Shibuya 1996; Roberts 2006; Lascu et al. 2012), different response data should be prepared and used for the deconvolution of samples with different geometry of cross section.

The final SRM sensor response data for deconvolution should be organized in a text file with standard format as shown in Table 1. The response file begins with six rows of header followed by sensor response data listed in ten columns. The first header row includes cross section area (in cm^2) of the sample, which is used for the integration and normalization of the response data. The second header row indicates the resolution (in cm) at which the sensor response measurements were conducted. The third header row in the response file provides information on number of measured data points on each side of the magnetometer sensor response excluding the center (number of data points should be the same on both sides). We recommend including sensor response data with values down to 1×10^{-3} of the peak value. The fourth header row in the response file is left blank and the fifth header row explains the orientations of the response data. For instance, the column marked as "*XZ*" should contain response data of the *Z*-axis sensor due to magnetic moment in the *X*-axis direction. The sixth header row lists the names of the ten columns of sensor response data in the response file. As the sixth

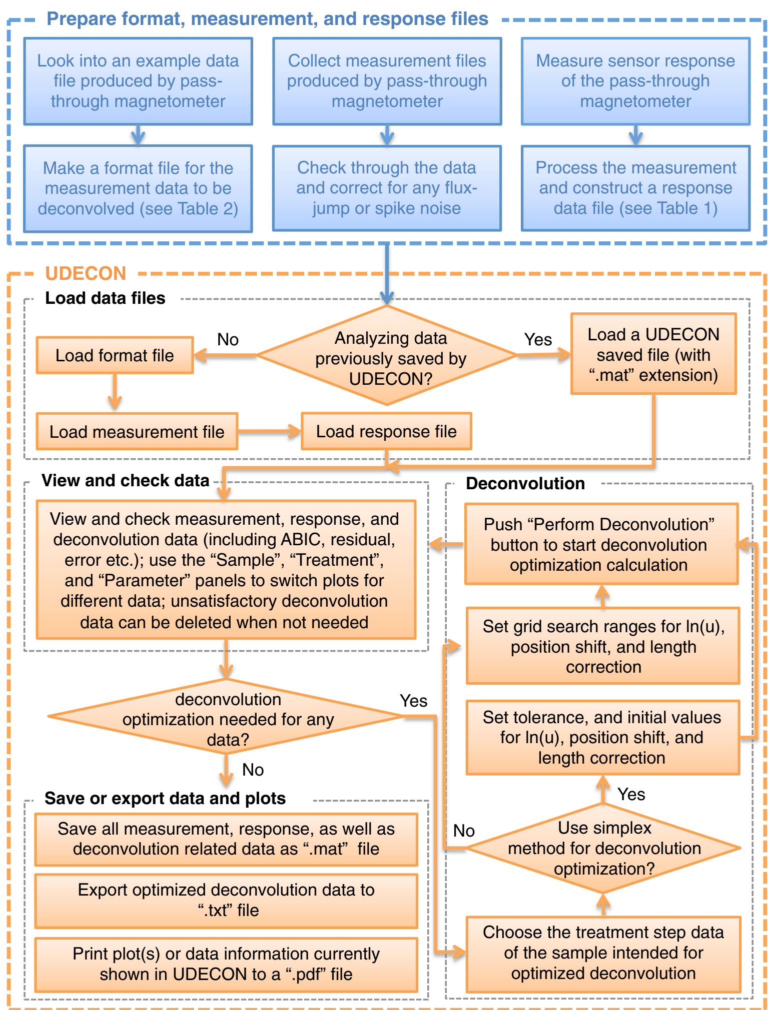

Fig. 1 A flowchart summarizing the major steps of using the UDECON software. The *blue section* on the *top* summarizes the preparation of format, measurement, and response files required by UDECON, and the *orange section* on the *bottom* shows operations to be conducted in UDECON

header row indicates, the main body of the response file contains the following ten columns of data: "Position" (in cm), "*XX*", "*XY*", "*XZ*", "*YX*", "*YY*", "*YZ*", "*ZX*", "*ZY*", and "*ZZ*". The different columns of response data are tab-delimited. Note that for the top three rows, the colons right before the numbers are required. While preparing the response file, we recommend that users copy the top six rows of text from the example response file, and only change the numbers in the top three rows as needed.

Optimized deconvolution using UDECON

To provide convenient and rapid realization of the optimized deconvolution algorithm developed by Oda and Xuan (2014) for pass-through paleomagnetic measurement data, we developed graphical software UDECON using the Graphical User Interface Design Environment (GUIDE) in MATLAB (version R2014a) on a Macintosh. Standalone versions of UDECON for both Macintosh and Windows PC are made available using the MATLAB Compiler. UDECON installation includes step-by-step guide to install MATLAB Compiler Runtime needed for the software to run without MATLAB. UDECON installation file, example SRM measurement, format, and response files are available at http://earthref.org/ERDA/2202/. A typical workflow for optimized deconvolution of pass-through paleomagnetic data using UDECON is summarized in Fig. 1.

User interface and loading of measurement and response files

The UDECON user interface comprises the following six groups of components (Fig. 2a). (1) A toolbar on the top of the interface with various function tools to load and save data, and to modify and export plots. (2) A "Sample" list box on the top right corner to show list of samples

Table 1 Example response file created for use in UDECON

Integrated area (square cm) on cross section: 4

Measurement interval thickness (cm): 0.1

Number of measured points on one side of the center (excluding the center): 190

IJ below is I-oriented magnetization response on J-axis, where I = X, Y, Z, and J = X, Y, Z.

Position	XX	XY	XZ	YX	YY	YZ	ZX	ZY	ZZ
−19	−8.78E-05	−1.77E-07	3.84E-08	2.73E-06	−3.67E-05	2.37E-06	−1.26E-05	5.53E-07	1.48E-06
−18.9	−9.36E-05	−2.94E-07	−3.18E-08	3.15E-06	−3.92E-05	2.38E-06	−1.37E-05	6.10E-07	1.45E-06
−18.8	−9.96E-05	−4.52E-07	−4.02E-08	3.47E-06	−4.20E-05	2.36E-06	−1.45E-05	4.95E-07	1.34E-06
−18.7	−1.06E-04	−6.00E-07	−1.19E-07	3.86E-06	−4.48E-05	2.38E-06	−1.52E-05	4.43E-07	1.25E-06
−18.6	−1.11E-04	−7.46E-07	−1.37E-07	4.16E-06	−4.76E-05	2.39E-06	−1.63E-05	5.57E-07	1.25E-06
−18.5	−1.18E-04	−9.30E-07	−1.82E-07	4.47E-06	−5.05E-05	2.37E-06	−1.71E-05	4.39E-07	1.14E-06
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
−0.5	9.95E-01	1.12E-01	6.50E-03	−1.04E-01	9.95E-01	2.59E-03	−2.27E-02	−4.63E-03	1.00E + 00
−0.4	9.97E-01	1.12E-01	6.40E-03	−1.05E-01	9.97E-01	2.35E-03	−2.29E-02	−4.33E-03	1.00E + 00
−0.3	9.98E-01	1.13E-01	6.34E-03	−1.05E-01	9.98E-01	2.25E-03	−2.34E-02	−4.04E-03	1.00E + 00
−0.2	9.98E-01	1.13E-01	6.18E-03	−1.05E-01	9.99E-01	2.15E-03	−2.37E-02	−3.69E-03	1.00E + 00
−0.1	9.99E-01	1.13E-01	6.04E-03	−1.05E-01	1.00E + 00	2.14E-03	−2.39E-02	−3.50E-03	1.00E + 00
0	9.99E-01	1.13E-01	5.88E-03	−1.05E-01	1.00E + 00	2.09E-03	−2.42E-02	−3.01E-03	1.00E + 00
0.1	9.99E-01	1.13E-01	5.76E-03	−1.06E-01	1.00E + 00	2.06E-03	−2.45E-02	−2.81E-03	1.00E + 00
0.2	9.99E-01	1.13E-01	5.63E-03	−1.06E-01	1.00E + 00	2.03E-03	−2.47E-02	−2.39E-03	1.00E + 00
0.3	9.98E-01	1.13E-01	5.54E-03	−1.06E-01	9.99E-01	1.96E-03	−2.49E-02	−2.05E-03	1.00E + 00
0.4	9.97E-01	1.12E-01	5.49E-03	−1.06E-01	9.98E-01	1.93E-03	−2.51E-02	−1.76E-03	1.00E + 00
0.5	9.96E-01	1.12E-01	5.56E-03	−1.06E-01	9.97E-01	1.86E-03	−2.52E-02	−1.30E-03	1.00E + 00
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
18.5	4.64E-05	−4.19E-06	9.96E-08	4.42E-06	−3.03E-05	−3.05E-06	1.10E-05	−2.27E-06	1.02E-06
18.6	4.36E-05	−3.98E-06	5.52E-08	4.22E-06	−2.44E-05	−3.01E-06	1.03E-05	−2.11E-06	9.81E-07
18.7	4.06E-05	−3.69E-06	4.76E-08	4.08E-06	−2.30E-05	−2.92E-06	9.62E-06	−2.07E-06	8.90E-07
18.8	3.74E-05	−3.39E-06	3.54E-08	3.87E-06	−2.20E-05	−2.84E-06	8.91E-06	−1.85E-06	8.29E-07
18.9	3.43E-05	−3.22E-06	−5.34E-09	3.75E-06	−2.09E-05	−2.77E-06	8.17E-06	−1.79E-06	7.87E-07
19	3.12E-05	−2.94E-06	4.79E-09	3.57E-06	−2.11E-05	−2.68E-06	7.61E-06	−1.80E-06	7.10E-07

contained in the measurement file. (3) A "Treatment" list box in the middle right to show a list of measured or deconvolved "Treatment" steps for currently selected sample. (4) A group of radio buttons to switch "Parameter" to be shown in the plot region. (5) A group of radio buttons and edit boxes and a push button to choose optimization method, adjust parameters, and perform optimized deconvolution. (6) A large area in the middle left to show plots or deconvolution-related information of data selected by the user.

UDECON can directly read a pass-through paleomagnetic measurement file created by the 2G Long Core software and allows the user to conveniently calculate, optimize, view, compare, and save deconvolved paleomagnetic data. As format of measurement files may vary from one laboratory to another depending on configuration in the 2G Long Core software, a format file needs to be created and loaded to UDECON before the loading of measurement file. The main body of the format file contains three columns of tab-delimited text listing the following information about the measurement file: column number (all columns in measurement file must be listed in order), type of data (i.e., numbers or strings represented by "%f" and "%s", respectively), and name string for each column (see Table 2). The top section of a format file (i.e., first 23 rows, enclosed by the symbol "#") contains instruction on the preparation of a format file. This instruction should be included in all format files prepared for use in UDECON. Note that some parameters are required by UDECON and they must present in the measurement file, i.e., sample ID, measurement position, and demagnetization level along *Z* measurement axis, run number for measurement steps,

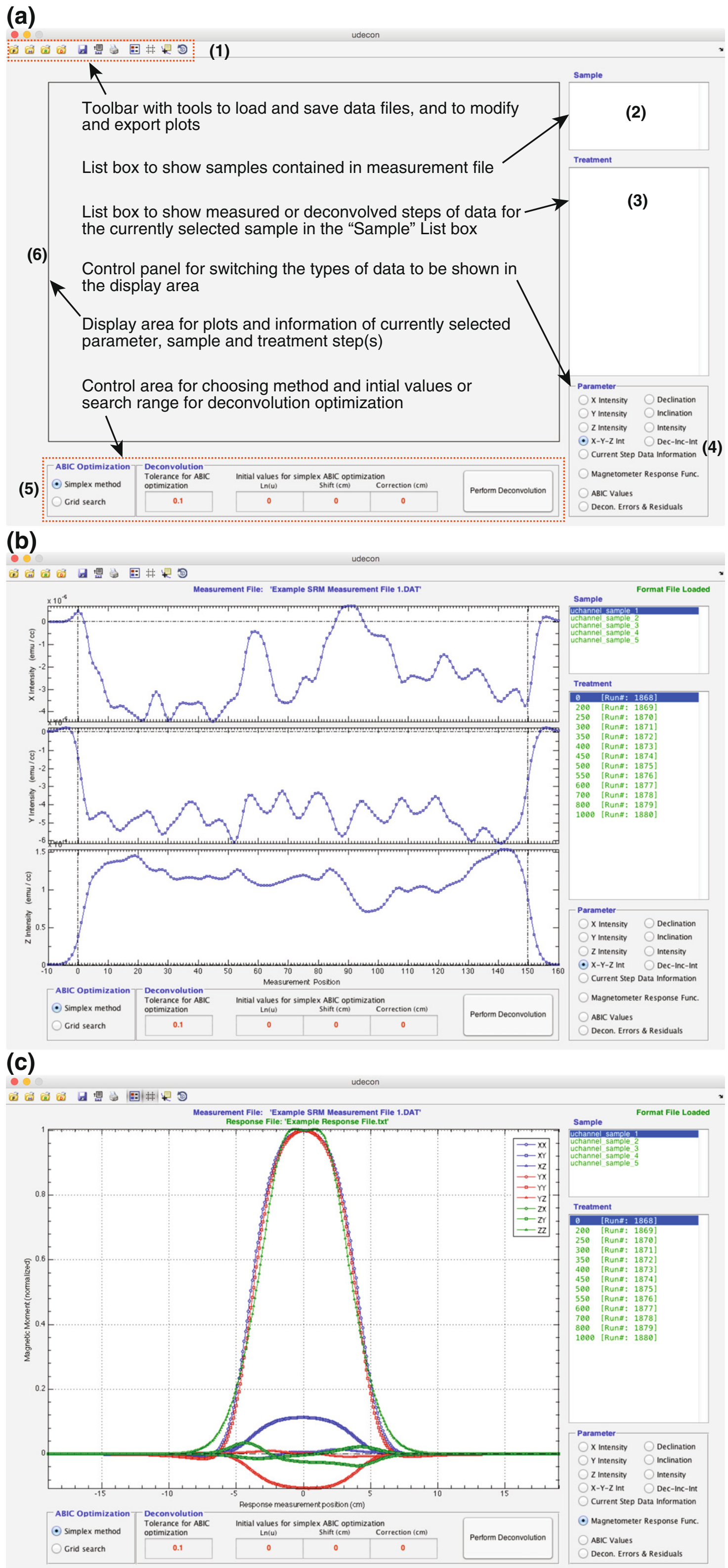

Fig. 2 (See legend on next page.)

(See figure on previous page.)
Fig. 2 UDECON user interface and the loading of required data files before deconvolution. (**a**) Initial UDECON user interface with description of the six main groups of components and examples of UDECON display after (**b**) loading a format file and an SRM measurement file and (**c**) loading an SRM response file. *Horizontal dashed lines* on the plots in (**b**) mark the zero levels of the intensity data, and *left* and *right vertical dot dashed lines* on the plots indicate the boundaries between leader and sample, and between sample and trailer measurements, respectively

lengths of leader and trailer measurements, magnetic moment and intensity along the three measurement axes after tray and drift correction, and declination, inclination, and total intensity. If any of the required data are missing in the measurement file, users need to calculate and add them to the measurement file and update the format file accordingly. Users may also consider modifying 2G Long Core software configuration (using "File Format Editor" in the Long Core software) to include all columns required by UDECON for future measurements.

After format file is created, it can be loaded to UDECON using the first icon in the toolbar. UDECON will automatically check if all required columns are listed in the format file. If any of the required columns is missing, UDECON will inform the user about the missing columns. If the format file is appropriate and successfully loaded, the name of the format file will be displayed on the top right corner of the UDECON interface (see Fig. 2b). The second icon in the toolbar can then be used to locate and load the measurement file. UDECON will check if data contained in the measurement file are consistent with what the format file indicates, and provide error message (and advices) if any inconsistency is detected. An example of UDECON interface after successful loading of the format and measurement files is shown in Fig. 2b. After loading the measurement file, list of samples and treatment steps will be displayed in the "Sample" and "Treatment" panels located on the right side of the software interface. The name of the measurement file will also occur in the top center of the UDECON interface above the plot area. By default, UDECON shows the *X*-, *Y*-, and *Z*-axis intensity data of the first treatment (demagnetization) step of the first sample on three individual plots (Fig. 2b).

After format and measurement files are loaded, users need to load the response file (see Table 1 and "Acquisition and preparation of magnetometer sensor response" section) by clicking on the third icon on the toolbar to locate and load the response file. If the response file is appropriately formatted and successfully loaded, UDECON will automatically plot the response file data and show the name of the response file just beneath the measurement file name (Fig. 2c). The procedures of loading format and measurement files followed by response file, are typical for deconvolution of a measurement file for the first time. If users have previously conducted deconvolution with these loaded files and saved a ".mat" file using UDECON (see "Saving deconvolution data and plots" section), deconvolution optimization analysis can be continued by directly loading the ".mat" file without loading any of the three files (see Fig. 1). The ".mat" file stores not only the deconvolution-related data but also the loaded measurement and response data. The ".mat" file can be loaded to UDECON using the fourth icon on the toolbar.

Viewing measurement and response data

UDECON provides a suite of convenient tools for users to view and check through measurement data for possible flux jumps, spike noises, and other unusual features. The plot area of UDECON is located in the left middle of the software interface and displays plots of measurement data (and/or deconvolution data when calculated) for selected sample and treatment steps, or sensor response function. The plot content will automatically update according to: changes of selection in "Sample" or "Treatment" list boxes, and changes of selection in the "Parameter" panel. The last four icons in the UDECON toolbar are designed for users to modify the appearance of plots. With these tools, users can add or remove legends (the eighth icon) and grid lines (the ninth icon), as well as show value of a selected data point (the tenth icon) and rotate a three-dimensional ABIC plot (the rightmost icon).

If the loaded measurement file contains data for multiple samples, a list of samples will be shown in the "Sample" list box, and users can click on a sample or use the up and down arrow keys to navigate from one sample to another to view data of that sample. UDECON supports measurement file that contains measurement data for multiple samples, but only one sample can be selected at a time. The "Treatment" list box displays the list of treatment and measurement steps for the currently selected sample. Data from multiple treatment steps can be selected for viewing and checking simultaneously. Note that list of treatment steps of a sample includes not only measurement step data but also steps of deconvolution data added by UDECON (see "Checking deconvolved data" section). Treatment step data can be switched either by left clicking or by using the up and down arrow keys. Users can choose any combination of treatment step data by left clicking the treatment steps while holding the Shift or the Command key (or the Control key in Windows OS).

Table 2 Example format file created for an SRM measurement file

```
################################################################################
# Follow the instruction below to prepare a format file for 2G Long Core software
# produced measurement data file.
#
# (1) Make sure different columns in the measurement file are tab-delimited.
# (2) In the first column below, write down column numbers for ALL columns present
#       in the measurement file without skipping any columns.
# (3) In the second column below, for each column in measurement file indicate if
#       that column contains number (%f) or string (%s).
# (4.1) In the third column below, give each column a name. Names can only contain
#        letters or numbers and should not start with a number.
# (4.2) Make sure there are no spaces before and after the column names.
# (4.3) The following 12 columns are required and must present in the measurement file:
#         "sampleID", "position" "runNumber", "afz", "leaderLength", "trailerLength",
#         "declination", "inclination", "intensity", "xcorr", "ycorr", "zcorr".
#         Column Names and Format Strings for the required columns must be exactly
#         the same (case-sensitive) as shown in this format file. If any of the required
#         columns are missing in the measurement file, users need to calculate and add
#         them to the measurement file. Users may consider modifying 2G Long Core software
#         configuration to include all columns required by UDECON for future measurements.
#
# Column                Format String               Column Name
######################## Do not edit contents above this line ########################
```

1	%s	sampleID
2	%f	position
3	%f	depth
4	%f	afx
5	%f	afy
6	%f	afz
7	%f	declination
8	%f	inclination
9	%f	intensity
10	%f	xintensity
11	%f	xmean
12	%f	xcorr
13	%f	yintensity
14	%f	ymean
15	%f	ycorr
16	%f	zintensity
17	%f	zmean
18	%f	zcorr
19	%s	armBias
20	%s	armAxis
21	%s	orientation
22	%f	leaderLength

Table 2 Example format file created for an SRM measurement file *(Continued)*

23	%f	trailerLength
24	%s	driftCorr
25	%s	trayCorr
26	%s	sampleTimeStamp
27	%s	trayTimeStamp
28	%f	runNumber

Selection in the "Parameter" panel located on the bottom right of the UDECON interface determines the types of data or information to be shown in the plot area. Users can choose to simultaneously show *X*-, *Y*-, and *Z*-axis intensity (Fig. 3a), or declination, inclination, and total intensity (Fig. 3b) for the selected "Sample" and "Treatment" steps on three individual plots. Alternatively, *X*-, *Y*-, and *Z*-axis intensity, declination, inclination, or total intensity can be shown on a single large plot to view multiple step data in more detail (Fig. 3c). The "Current Step Data information" provides a brief summary of information related to a treatment step of measurement or deconvolution data. The "Magnetometer Response Func." radio button allows the user to click and show the loaded SRM sensor response function at any time. The "ABIC Values" and "Decon. Errors & Residuals" options can only be chosen when a single step of deconvolved data (see "Checking deconvolved data" section) is selected in the "Treatment" list box.

Perform optimized deconvolution

After viewing and checking through the loaded measurement and response data, users should choose a treatment step data intended for optimized deconvolution. Note that only a single treatment step of original measurement data can be selected for deconvolution at a time. Optimized deconvolution in UDECON is controlled by options and parameters set in the "ABIC Optimization" and "Deconvolution" panels located on the bottom left of the software interface. The "ABIC Optimization" panel provides two options to implement the optimized deconvolution algorithm developed by Oda and Xuan (2014): (1) the "Simplex method" and (2) the "Grid search" method.

The "Simplex method" option in the "ABIC Optimization" panel uses an unconstrained nonlinear optimization based on Nelder–Mead simplex direct search algorithm (Lagarias et al. 1998). The algorithm searches for the optimum solution efficiently in the three-dimensional parameter space (i.e., smoothness, position shift, and length correction) using "Reflection", "Expansion", "Contraction", and "Reduction" of tetrahedrons depending on the values on the nodes without information of gradient at each node. MATLAB function "fminsearch" is used to implement the simplex-based deconvolution optimization in UDECON. Edit boxes in the "Deconvolution" panel are used to set the "Tolerance for ABIC optimization", as well as the initial values for ln(u) (i.e., smoothness), position shift, and length correction. After setting the tolerance and initial values, users can start searching for optimized deconvolution by left clicking on the push button "Perform Deconvolution" in the "Deconvolution" panel. UDECON will display and update ABIC value plot at each iteration step during the deconvolution optimization (see Fig. 4a). Upon completion of the optimization, the deconvolved *X*-, *Y*-, and *Z*-intensity data will be shown in the plot area.

The "Grid search" option in the "ABIC Optimization" panel uses a brute-force method to find the minimum ABIC out of all the "grid" nodes of ln(u), position shift, and length correction set in the edit boxes in the "Deconvolution" panel. Note that edit boxes shown in the "Deconvolution" panel will automatically update depending on the selection of optimization method in the "ABIC Optimization" panel. The grid of ln(u), position shift, and length correction values are defined by three edit boxes for each parameter, where the first and the third boxes define the minimum and maximum values for the parameter, respectively, and the middle box defines the increment of the parameter value within the range (note that step values must be non-zero). Realistic ranges for ln(u) should be between −10 and 10. It is usually a good practice to start with a large range and big increment (e.g., 1 or 2) to perform an initial optimized deconvolution, to guide the selection of a more constrained ln(u) range with finer increment. Position shift values should be within few centimeters (±2 cm) or much less (±few mm) if the measurement start line of the system is well calibrated and void space at the beginning of the continuous sample is negligible. Length correction should be between −0.5 and +0.5 cm, which correspond to an empty or full last sample slice respectively, assuming the paleomagnetic measurements are collected at every 1-cm interval resolution (see Oda and Xuan 2014). After ranges for all parameters are set, users can click on the push button "Perform Deconvolution" in the "Deconvolution" panel to start the deconvolution optimization. A progress bar will be shown on the screen during "Grid search" deconvolution. Upon completion of the calculation, the deconvolved *X*-, *Y*-, and *Z*-intensity data will be

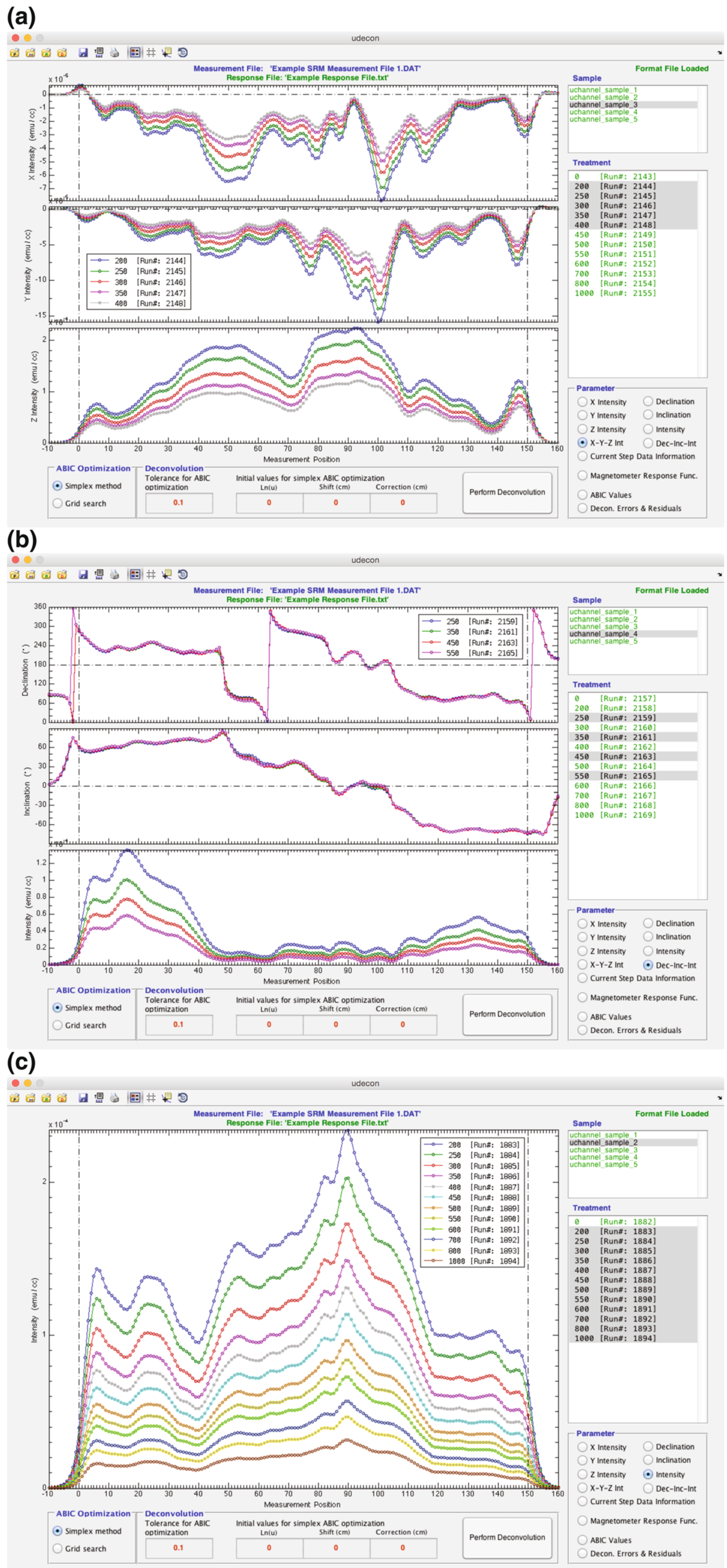

Fig. 3 Examples of viewing and checking measurement data in UDECON for (**a**) *X*-, *Y*-, and *Z*-axis intensity on multiple plots; (**b**) declination, inclination, and total intensity on multiple plots; and (**c**) total intensity on a single plot. Note that users can conveniently select any combination of treatment step data of a sample for viewing and checking

shown in the plot area. The "Grid search" method allows users to search optimized deconvolution with fixed length correction and position shift (see Fig. 4b), or just fixed length correction (Fig. 4c), or within three-dimensional space defined by ranges of all three parameters (Fig. 4d).

Although the "Simplex method" in UDECON generally provides a fast way for optimized deconvolution, it is an unconstrained optimization method and can result in optimized length corrections that are beyond the −0.5 to 0.5-cm range, and the optimization may also fall in a local minimum. We recommend that users utilize the "Grid search" method (default option in UDECON) with large ranges and big increment values to perform an initial optimization. The resulting optimum ln(u), position shift, and length correction values can then be used as initial values for further optimization using the "Simplex method". Alternatively, users can further optimize the deconvolution using the "Grid search" method with smaller range and small increment values for the optimization parameters. Optimized position shift and length correction values acquired from low demagnetization step data of a sample (usually with high signal-to-noise ratio compared with high demagnetization step data) can be used for optimized deconvolution for higher demagnetization step data of the same sample. For the "Grid search" method, this can be done by setting the "min." and "max." values of length correction or position shift both to the optimum value acquired from low demagnetization step data. This process will significantly increase the speed of deconvolution optimization in UDECON by reducing the amount of iteration needed to search for the minimum ABIC value. In addition, we recommend that users check the actual length of the sample if applicable. If the difference between the actual sample length and the length used in 2G Long Core software is beyond the −0.5 to 0.5-cm range, users may need to correct part of the trailer measurements as sample data or part of the sample data as trailer measurements.

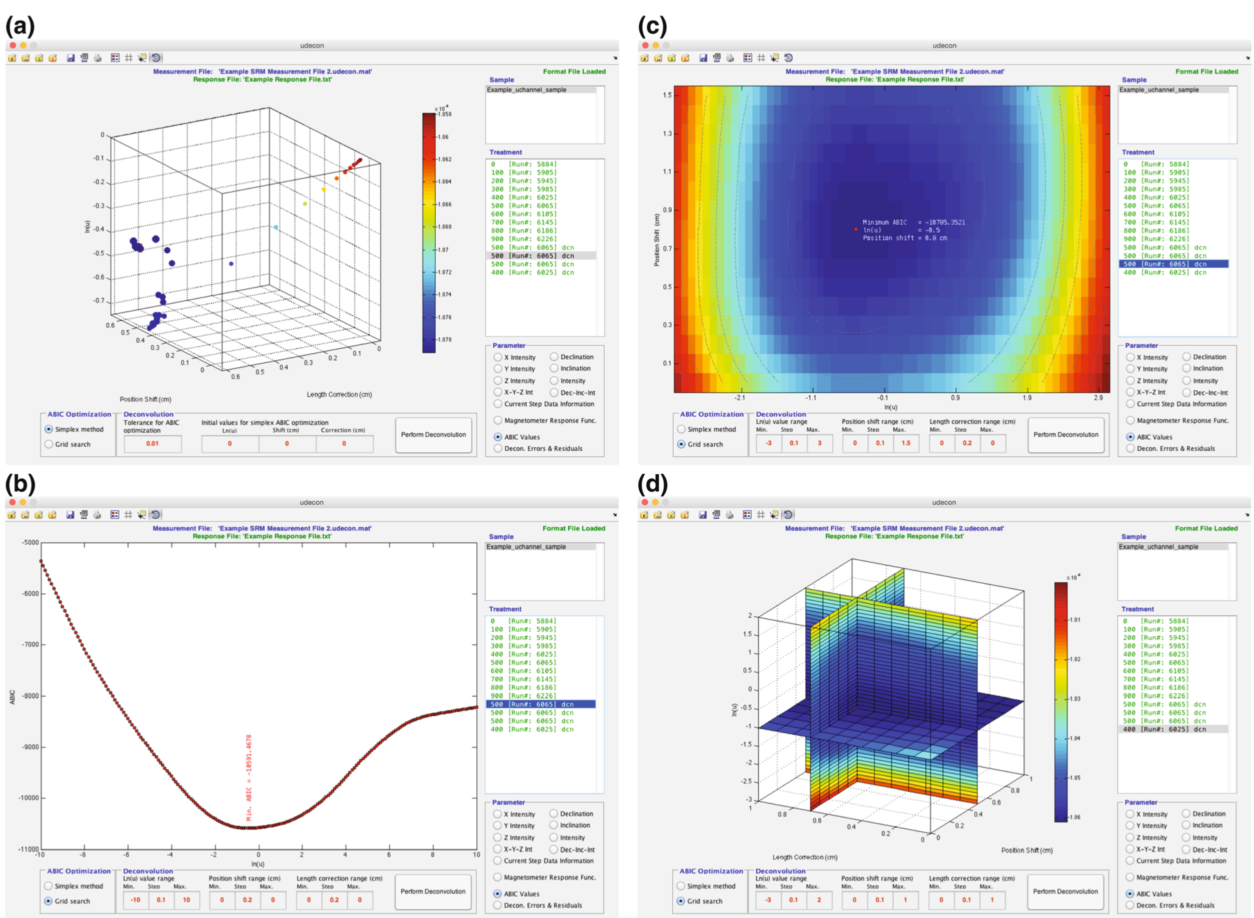

Fig. 4 Examples of ABIC plots associated with deconvolution optimization in UDECON for (**a**) optimized deconvolution using the "Simplex method"; and deconvolution optimization using the "Grid search" method with (**b**) fixed position shift and length correction values, (**c**) fixed length correction values, and (**d**) defined ranges for ln(u), position shift, and length correction. Note that for the "Simplex method", ABIC value plots are *color-coded*, and *larger symbols* indicate greater iteration number of the simplex optimization process

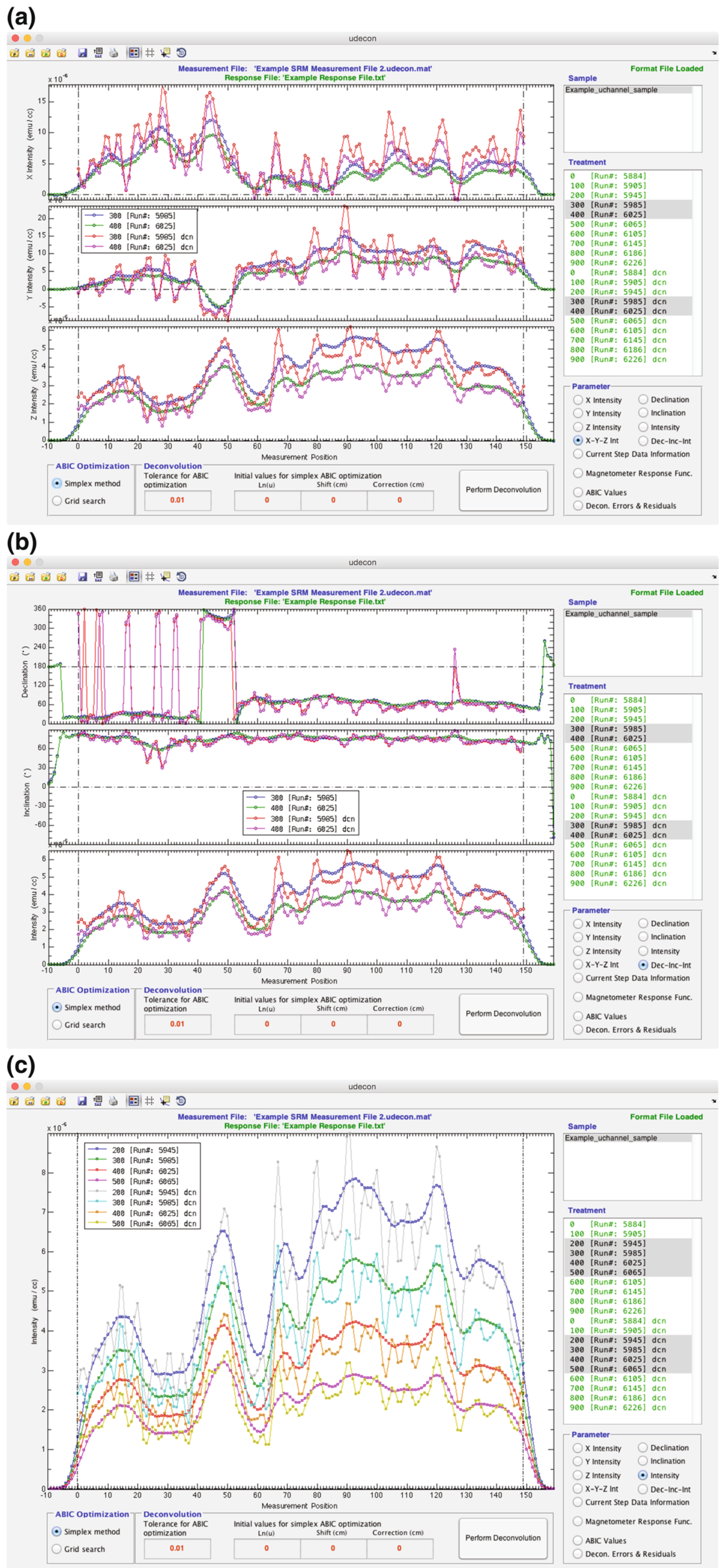

Fig. 5 Examples of comparison of multiple treatment step data of a sample before and after optimized deconvolution in UDECON for (**a**) *X*-, *Y*-, and *Z*-axis intensity on multiple plots; (**b**) declination, inclination, and total intensity on multiple plots; and (**c**) total intensity on a single plot

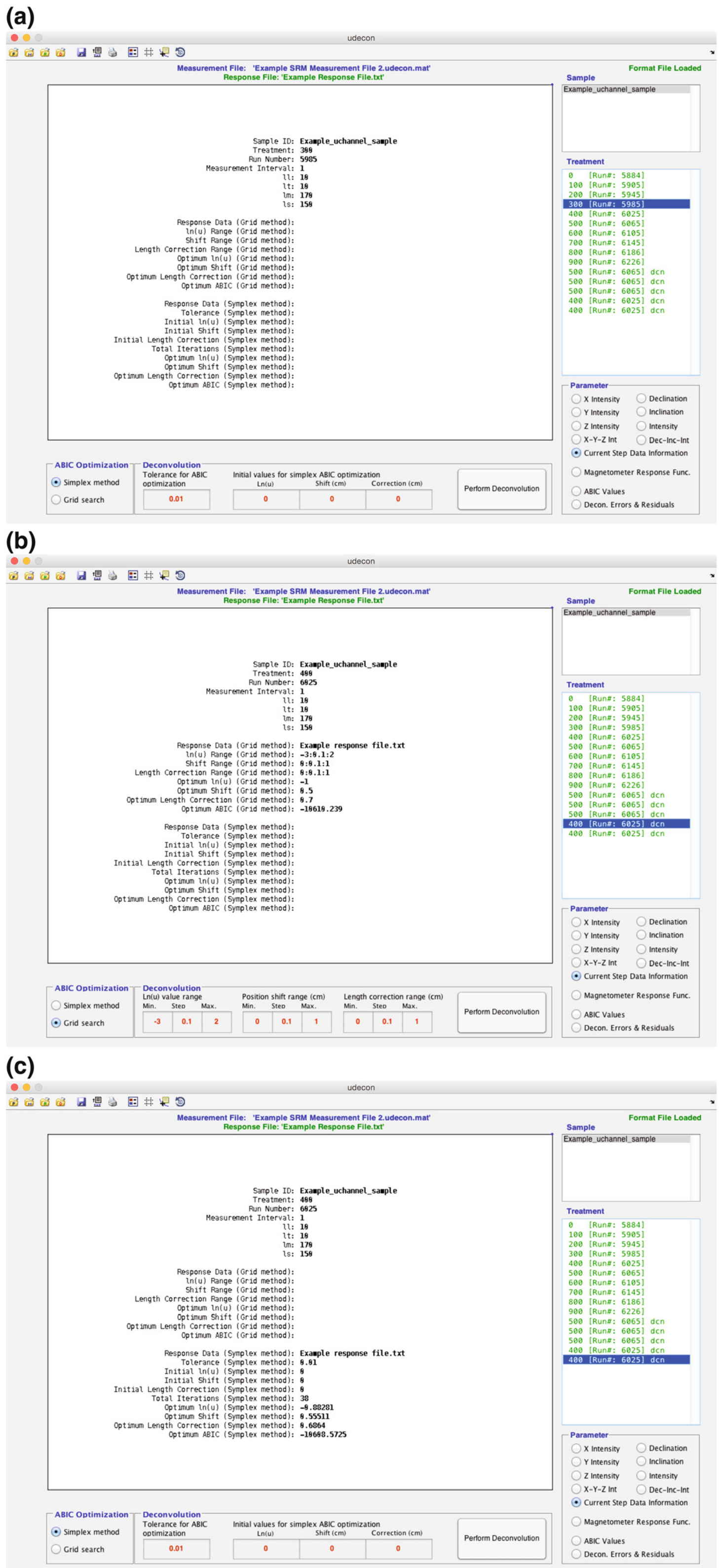

Fig. 6 Examples of display in UDECON on essential information and parameters related to deconvolution in (**a**) original measurement data, (**b**) deconvolved data using the "Grid search" optimization method, and (**c**) deconvolved data using the "Simplex method". Note that only one treatment step data of a sample can be selected a time to display the deconvolution-related information

Checking deconvolved data

When optimized deconvolution calculation is completed, deconvolved data will be added to the currently selected sample as a treatment step with the string "dcn" at the end of the treatment step labels (see Fig. 5a). Similar to treatment steps containing measurement data, the deconvolved data include *X*-, *Y*-, and *Z*-axis intensity, declination, inclination, and total intensity. Following the instructions in the "Viewing measurement and response data" section, the deconvolved data (treated as treatment step data) can be easily viewed and compared with the measurement data. Various parameters for multiple steps of data can be viewed simultaneously to check the consistence of optimized deconvolution through different treatment (demagnetization) steps. Examples of comparisons between two measurement step data before and after optimized deconvolution for *X*-, *Y*-, and *Z*-axis intensity, as well as for declination, inclination, and total intensity, are shown in Fig. 5a, b, respectively. Note that the intensities of measurement data before deconvolution are based on normalization using cross area of the sample and the effective lengths of sensor responses provided by 2G Enterprises. Inappropriate values of effective lengths and cross area of the sample may contribute to discrepancies between measurement data and deconvolved data. Figure 5c compares the total intensity of four demagnetization step data on a single large plot before and after optimized deconvolution. Repeatability of high-resolution variability (not observed in the original measurement data) in the deconvolved data at multiple treatment (demagnetization) steps provides strong evidence for the reliability of the optimized deconvolution.

For each optimized deconvolution operation using either the "Simplex method" or the "Grid search" method, UDECON stores the ABIC values calculated during the optimization process. These ABIC values can be plotted at any time using the radio button "ABIC Values" in the "Parameter" panel located on the bottom right of the software interface (see Fig. 4). In addition, a brief summary of deconvolution-related information for each treatment step data (measured or deconvolved) can be viewed by clicking on the radio button "Current Step Data Information" in the "Parameter" panel. Figure 6 shows examples of "Current Step Data Information" for treatment step

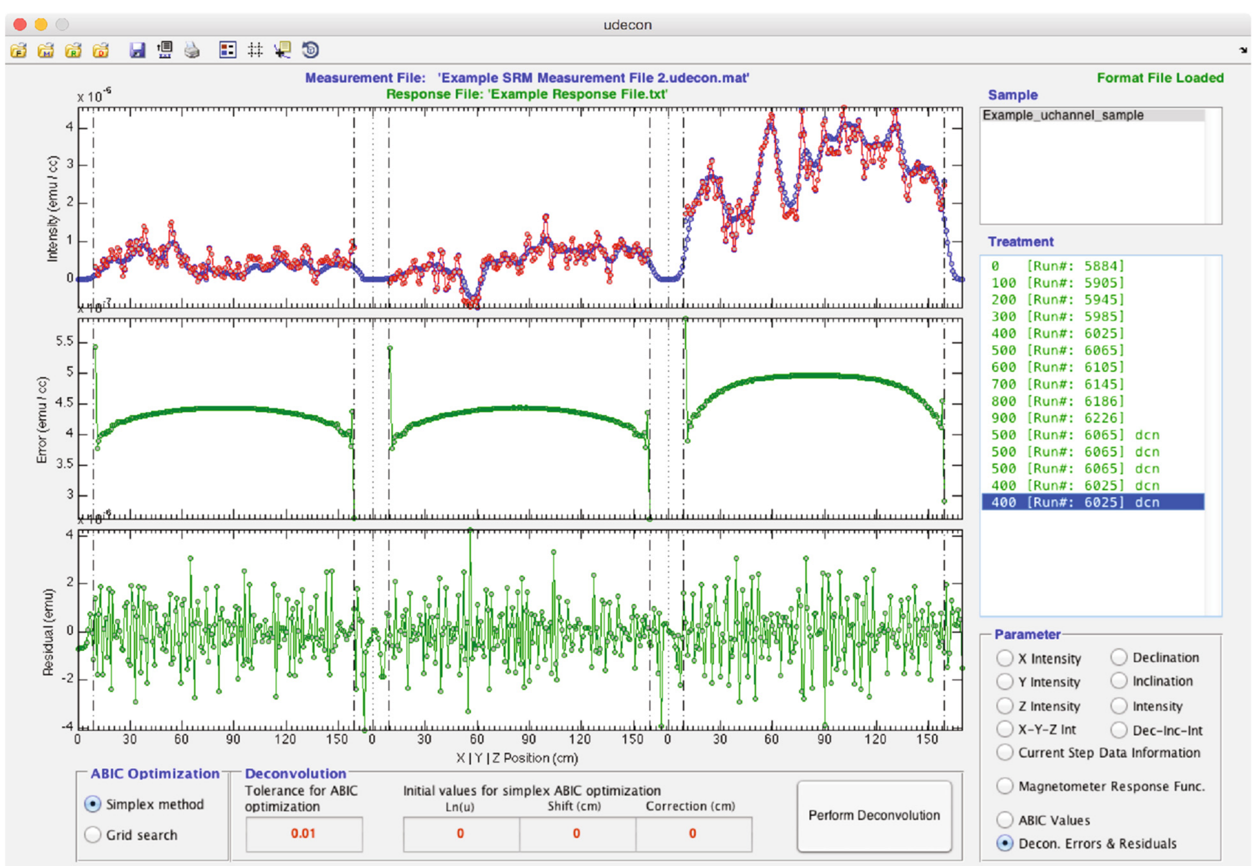

Fig. 7 Example of an integrated plot for comparison of intensity data on all axes before and after optimized deconvolution (*top plot*), as well as error (*middle plot*) and residual (*bottom plot*) data associated with the optimized deconvolution using UDECON

with original measurement data (Fig. 6a) and with optimized deconvolution data using "Grid search" method (Fig. 6b) or "Simplex method" (Fig. 6c). Treatment step with measurement data (Fig. 6a) contains information to be used by deconvolution calculation such as lengths of leader (ll), sample (ls), trailer (lt), total measurements (lm), and measurement increment, as well as Sample ID, treatment (demagnetization) level, and run number. For deconvolved treatment step (Fig. 6b, c), UDECON records tolerance and initial values (for "Simplex method") or parameter ranges (for "Grid search") used for the deconvolution optimization, together with the name of the response file. The deconvolved treatment step data also contain information of total number of iteration (if using "Simplex method"), the minimum (optimum) ABIC and parameter (ln(u), position shift, and length correction) values that yield the optimized result. This brief summary of information for each measurement and deconvolution step data can be conveniently displayed and compared to guide for any further optimization of deconvolution.

UDECON also provides estimates of errors and residuals associated with the optimized deconvolution. Residual is the difference between the measured magnetic moment and the convolution of response function with the optimized deconvolution data. In UDECON, error is also calculated according to the formulae provided by Oda and Xuan (2014). Error and residual data for optimized deconvolution data can be viewed by clicking on the radio button "Decon. Errors & Residuals" in the "Parameter" panel. Figure 7 shows an example of UDECON interface showing the error and residuals data together with the measurement and optimized deconvolution data for *X*-, *Y*-, and *Z*-axis intensity.

Table 3 Content of the UDECON exported file

Column number	Column header	Explanation
1	Sample ID	Name of samples (from measurement file)
2	Position	Measurement position in sample (from measurement file)
3	Run Number	Number ID assigned to a run step (from measurement file)
4	AF Z	Demagnetization level along *Z*-axis (from measurement file)
5	X Intensity	*X*-axis intensity based on optimized deconvolution
6	Y Intensity	*Y*-axis intensity based on optimized deconvolution
7	Z Intensity	*Z*-axis intensity based on optimized deconvolution
8	X Error	Estimated error in *X*-axis intensity for optimized deconvolution
9	Y Error	Estimated error in *Y*-axis intensity for optimized deconvolution
10	Z Error	Estimated error in *Z*-axis intensity for optimized deconvolution
11	Declination	Declination based on optimized deconvolution
12	Inclination	Inclination based on optimized deconvolution
13	Intensity	Total intensity based on optimized deconvolution
14	Dec. Error	Estimated error in declination for optimized deconvolution
15	Inc. Error	Estimated error in inclination for optimized deconvolution
16	Int. Error	Estimated error in total intensity for optimized deconvolution
17	Opt. ABIC	Minimum ABIC value for optimized deconvolution
18	Decon. Method	Optimization method used (Simplex or Grid Search)
19	Opt. ln(u)	Ln(u) value that yields the optimized deconvolution
20	Opt. Position Shift	Position shift value that yields the optimized deconvolution
21	Opt. Length Correction	Length correction value that yields the optimized deconvolution

Saving deconvolution data and plots

For each treatment step of measurement data, deconvolution optimization can be performed using different methods with different combinations of initial values or ranges for the three optimization parameters (i.e., ln(u), position shift, and length correction). Viewing and comparing deconvolution results acquired using different settings will allow users to further refine the optimization. Unsatisfactory and intermediate deconvolution results can be removed in UDECON by selecting the data from the "Treatment" panel and then press the "Delete" key. Any plots or data information displayed in the plot area in the center left of UDECON interface can be "Printed" to a pdf file using the seventh icon (with a printer shape) on the toolbar.

UDECON provides two options to save the deconvolution data: (1) save measurement and deconvolution data to a ".mat" file and (2) export deconvolution data to a ".txt" file. The first data saving option is realized by pressing the fifth icon (with a floppy disk shape) on the UDECON toolbar. The saved ".mat" file contains not only the deconvolved data but also the loaded measurement data as well as response data. All data associated with the deconvolution for each treatment step including ABIC values (along with optimization parameter values and optimum results), errors, and residuals are also saved. As mentioned in the "User interface and loading of measurement and response files" section, the saved ".mat" file can be reloaded to UDECON using the fourth icon on the toolbar. This option is particularly useful for storing deconvolution results that require further refinement later. The second option of exporting the deconvolution data to a ".txt" file is done by pressing the sixth icon on the UDECON toolbar. The exported ".txt" file can be read by other software for user customized plotting and comparison. Note that the exported file only contains the optimized deconvolution data including *X*-, *Y*-, *Z*-axis intensity, declination, inclination, total intensity, the errors associated with these data, and the optimized ABIC values as well as the optimized ln(u), position shift, and length correction that yield the minimum ABIC. Content of the exported ".txt" file is listed and explained in Table 3.

Conclusions

We present user-friendly graphical software UDECON to provide convenient and rapid realization of the optimized deconvolution algorithm recently developed by Oda and Xuan (2014) for restoring high-resolution records from pass-through paleomagnetic measurements. The improved deconvolution algorithm implemented in UDECON optimizes not only for smoothness of the magnetization data but also for realistic corrections in sample length and measurement position. UDECON is a compiled MATLAB Graphical User Interface (GUI) and is made available as standalone applications for both Macintosh and Windows PC. The software provides a simple and organized environment for users to quickly conduct optimized deconvolution.

With the preparation of a format file, UDECON directly reads pass-through paleomagnetic measurement files produced at different laboratories. Sensor response of an SRM needed for deconvolution can be accurately estimated through repeated measurements of a magnetic point source and prepared as a response file readable by UDECON (see "Acquisition and preparation of magnetometer sensor response" section). Once measured, the same sensor response data of an SRM can be edited and used to deconvolve any pass-through measurement made on that SRM. With a simple click in UDECON, optimized deconvolution can be searched using two different methods (i.e., "Simplex method" or "Grid search") with adjustable choices of initial values or ranges for smoothness, position shift, and length correction. A suite of tools can be used to easily view and compare various types of data before and after optimized deconvolution for single or multiple treatment steps. Deconvolution-related ABIC values, error and residual, as well as the parameters used for the calculation, can be conveniently compared to refine the deconvolution optimization. Unsatisfactory or preliminary deconvolution data can be easily removed when not needed. Any plots shown in UDECON can be saved as pdf files, and users can save all measurement, response, and deconvolved data for further analysis later in UDECON, or export just the deconvolved data to text file for editing or plotting in other software.

Abbreviations

ABIC: Akaike's Bayesian Information Criterion; GUI: Graphical User Interface; GUIDE: Graphical User Interface Design Environment; IODP: International Ocean Discovery Program; ODP: Ocean Drilling Program; SQUID: superconducting quantum interference device; SRM: superconducting rock magnetometer.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

CX designed the software interface and programmed majority of the UDECON functions, and wrote and edited the manuscript. HO contributed to the design of the software as well as the writing of the manuscript. In particular, HO contributed to the programming and checking of the deconvolution optimization algorithm and the visualization of deconvolution optimization process for the "simplex" method. Both authors read and approved the final manuscript.

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