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Special Section:

Magnetism in the Geosciences -Advances and Perspectives

Key Points:

- · PuffinPlot is a popular application for paleomagnetic data analysis
- We document a number of significant features added since the initial release in 2012
- · Features include declination realignment, VGP and RPI calculation, and data bundle export

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New Developments in the PuffinPlot Paleomagnetic **Data Analysis Program**

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Abstract PuffinPlot is a program for paleomagnetic data analysis and plotting, first released in 2012 and under continuous development since then. It is free, cross-platform software and provides both a graphical desktop interface for interactive use and an application-programmer interface for scripting. We present a major new release of the program, describe significant new features added since the first release, and demonstrate their application to real-world data. New features include automatic magnetic declination realignment, relative paleointensity calculation, virtual geomagnetic pole determination, calculation of inclination-only statistics, support for reproducible research via the export of self-contained data bundles, and support for reading a number of popular paleomagnetic file formats. We also discuss the application of unit tests in ensuring PuffinPlot's long-term reliability and outline directions for future development of the software.

Plain Language Summary By analyzing the remanent magnetization of ancient rocks and sediments, we can work out the strength and direction of the Earth's magnetic field when they were formed. We do this with laboratory measurements of the magnetic properties of rock samples or sediment cores, combined with treatments to remove any unwanted magnetic signals from them. PuffinPlot is a program which analyses these laboratory measurements to estimate the original magnetic field. In this paper we present a new release of PuffinPlot and describe and demonstrate some of its new features. These include a way to calculate magnetic field directions even when a sediment core has been rotated or when it has no azimuthal orientation, combining multiple measurements to estimate the strength of the original magnetic field, and generating a self-contained software and data package to let other researchers verify and redo the analysis automatically. We also discuss automated tests which make the software more reliable and features that we plan to include in future releases.

1. Introduction

The paleomagnetic data analysis and plotting program PuffinPlot was introduced in a 2012 paper (Lurcock & Wilson, 2012). As is the case for much scientific software, initial development was focused on the immediate needs of a research group, in this case the paleomagnetism group at the University of Otago, New Zealand. In the intervening years, PuffinPlot has gained many users worldwide and has been used in the preparation of dozens of peer-reviewed publications. In response both to the needs of the program's author and coworkers and to requests from external users, features have been added more or less continuously since the initial release. As a result, the size of the codebase has more than doubled, and PuffinPlot has gained a large number of capabilities not documented in the 2012 paper. This paper describes a new release of Puffin-Plot (version 1.4.1) and provides an overview of the more significant and scientifically interesting features added to PuffinPlot since the first public version.

1.1. Brief Introduction to Puffinplot

PuffinPlot implements most of the common, standard paleomagnetic plots and analysis techniques, such as demagnetization-intensity biplots, Zijderveld (1967) orthogonal component plots, Lambert (1772) equal-area plots, principal component analysis (PCA; Kirschvink, 1980), Fisher (1953) statistics, and great-circle intersection analysis (without sector constraints; McFadden & McElhinny, 1988).

Two interfaces are provided: a user-friendly, interactive, graphical user interface (GUI; shown in Figure 1) and a well-documented application-programmer interface (API), allowing PuffinPlot to be controlled by scripts or used as a library in other applications. The API is also accessible via PuffinPlot's built-in Python

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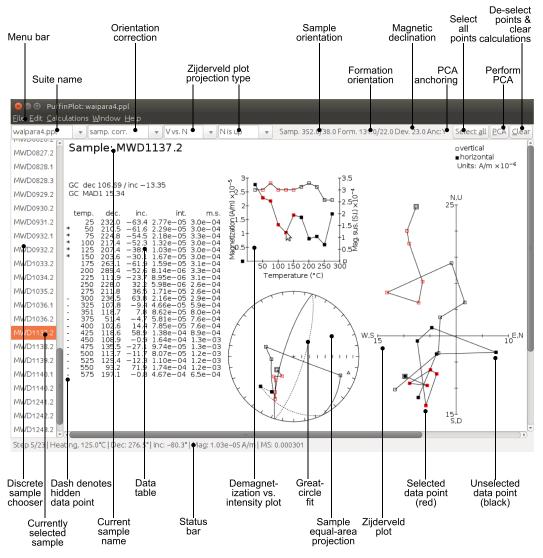


Figure 1. Annotated screenshot of PuffinPlot's desktop graphical user interface. This screenshot shows the default layout, containing only a few commonly used plot types. Many other plots and tables are available. The size and positioning of the plots within the window is also fully customizable.

and JavaScript scripting support. In this way, we attempt to combine the virtues of both interactive, graphical programs like Paleomag (Jones, 2002) and Paleomac (Cogné, 2003) and flexible, scripting-centric software like PmagPy (Tauxe et al., 2016) and ZPLOTIT (Acton, 2011). The GUI is well suited to exploratory data analysis and the API to automated analysis of large volumes of uniform data and integration into larger data processing workflows. Figure 2 gives a high-level overview of the program's architecture.

PuffinPlot is written in Java and runs on any operating system for which a Java runtime is available, including Windows, Linux, and Mac OS X. The entire program is free software released under the GNU General Public License; the source code, as well as the compiled program itself, is thus freely available to read, download, modify, and redistribute. The program and all associated resources are distributed via the official website (at https://www.talvi.net/puffinplot/).

1.2. Overview of New Developments

In section 2, we describe and demonstrate the major new features, including automatic realignment of the declinations of core sections, calculation of relative paleomagnetic intensity (RPI), determination of virtual geomagnetic poles (VGPs), analysis by means of inclination-only statistics, Fisherian analysis of demagnetization steps, and improved scripting support; the more significant features are demonstrated by applying them to real-world data.

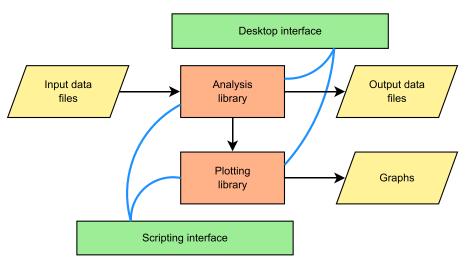


Figure 2. High-level schematic overview of the program structure of PuffinPlot.

In section 3, we list and describe the additional file formats which the new version of PuffinPlot can import, as well as improvements made to existing file importers.

Section 4 describes *data bundles*, which make it easier to share and reproduce analyses performed using PuffinPlot.

Section 5 briefly outlines the numerous smaller features which have been added since the initial release.

In section 6, we discuss some changes focused on improving and maintaining the quality of PuffinPlot's source code, in particular the implementation of unit tests to ensure the present and future reliability of analysis results.

In section 7, we describe the challenges involved in the continuing improvement of PuffinPlot and outline directions for future development.

2. New Analysis Features

2.1. Automatic Declination Realignment

In some paleomagnetic long-core studies of paleosecular variation (PSV), the core sections lack azimuthal orientations: Each section thus contains a "floating" relative record of paleomagnetic declination, with an unknown rotation relative both to the declination records of its neighboring core sections and to the original, absolute orientation. PuffinPlot now has a feature which can be used to realign the declinations of core sections in order to reconstruct a continuous declination record. The procedure is as follows:

- 1. A paleomagnetic direction is calculated for every core depth for which this is possible.
- 2. For each core section, a "top declination" and "bottom declination" is calculated. The top declination is the Fisherian mean declination of the top few samples in the section (the number of samples is user configurable); similarly, the bottom declination is the mean declination of the bottom few samples.
- 3. The user specifies an absolute declination for the top of the entire core; in the case of a high-resolution core where the deposition has continued up to the present day, it may be appropriate to take the absolute declination from the modern field direction. If the whole-core declination record is intended to be rotated empirically to match a reference curve, any absolute declination can be used.
- 4. The horizontal components of the magnetic moments of the entire top core section are rotated as a whole; the rotation is such that it aligns the top declination with the absolute declination.
- 5. In the same way, the second core section (i.e., the one below the top section) is rotated so as to align its top declination with the top section's already realigned bottom declination.
- 6. The process continues section by section down the core, with each section being rotated to align its top declination with the bottom declination of the section above it.

Provided that paleomagnetic declinations have already been calculated, the entire procedure is automated: The user only needs to specify the number of samples to average for a top or bottom declination and the absolute declination for alignment of the uppermost core top.

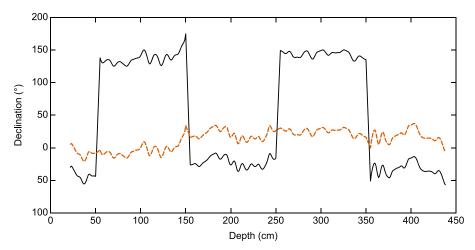


Figure 3. Automatic declination realignment applied to declinations from Core C5 of NEXTDATA cruise AMICA2013 (Margaritelli et al., 2016). Before plotting and processing, the top two and bottom two samples from each core section were removed to exclude artifacts at the extreme ends of the cores. Black solid line: original declinations as calculated by principal component analysis. Orange dashed line: automatically realigned declinations using an absolute declination of 0 and a mean direction from six samples at each core section end.

The algorithm implemented by PuffinPlot is essentially a formalization of a technique already in use (e.g., by Sagnotti et al., 2011); its inclusion in PuffinPlot allows the technique to be applied very quickly and conveniently—and, more importantly, in a well-defined and fully reproducible way. Figure 3 gives an example of the application of the algorithm to measured core data.

There are of course caveats to bear in mind when applying this technique: The alignment is dependent on the reliability of the calculated paleomagnetic declinations at the core ends and on the assumption that there will be minimal rotation across the short interval used for alignment. Increasing the number of samples averaged at the core ends reduces the first of these problems, at the cost of increasing the second. Nevertheless, the realignment algorithm is a powerful and useful tool for compiling a continuous declination record in cases where more accurate techniques are not available.

2.2. Inclination-Only Statistics

Particularly in long-core studies which lack azimuthal orientation, it is often useful to calculate statistics on paleomagnetic inclinations only, ignoring the declination: provided that the site paleolatitude is sufficiently high, polarity can be determined from inclination alone. Neither Fisher statistics nor a simple arithmetic mean give a reliable average inclination, and several algorithms have been devised to produce more accurate estimates of the mean inclination and confidence interval from inclination-only data (see Arason & Levi, 2010, Table 2, and references therein). PuffinPlot now incorporates what we believe to be the first Java implementation of the Arason and Levi (2010) maximum-likelihood algorithm for inclination-only statistics, based on the published JavaScript version and tested against the original Fortran implementation. Currently, Arason-Levi statistics are provided only via the API; a GUI for them will be added in the next release.

2.3. RPI Calculation

PuffinPlot can now calculate RPI estimates from a pair of data sets, each loaded as a PuffinPlot suite. One suite contains the natural remanent magnetization (NRM) demagnetization data, and the other the data to be used as a normalizing parameter. Normalization can be done to magnetic susceptibility (MS), stepwise acquisition of anhysteretic remanent magnetization (ARM), or stepwise alternating-field (AF) demagnetization of an ARM or isothermal remanent magnetization (IRM). For MS normalization, the initial NRM is simply normalized to the corresponding MS value. For estimates based on stepwise demagnetization of an ARM or IRM, the procedure is as follows:

- 1. The NRM is stepwise demagnetized with a series of AF treatments at increasing field strengths. The magnetic moment is remeasured after each step.
- 2. An ARM or IRM is applied to the core.

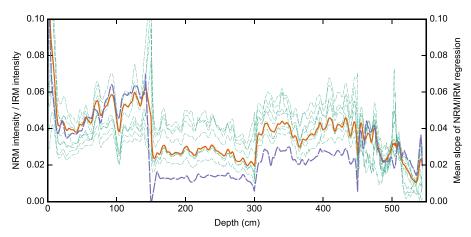


Figure 4. Results from PuffinPlot's RPI estimation tool, using data from the 6m1a core of the Lake Ohau Climate History project (Levy et al., 2018). The NRM was stepwise demagnetized at fields of 5, 10, 20, 30, 40, 50, 70, 80, 90, and 100 mT, then a 900-mT IRM was applied and the core demagnetized again at the same alternating field strengths. The thin, green, dashed lines show the downcore NRM/IRM ratios at individual treatment steps; the thick orange line is an RPI estimate obtained by taking the arithmetic mean of the ratios for all treatment steps at each depth; the thick dashed purple line is an RPI estimate obtained as the slope of a least squares linear regression on NRM and IRM values for all steps at each depth. RPI = relative paleomagnetic intensity; NRM = natural remanent magnetization; IRM = isothermal remanent magnetization.

3. The ARM or IRM is stepwise demagnetized in the same way as the NRM, with the same series of AF field strengths.

Like the UPmag program of Xuan and Channell (2009), PuffinPlot uses two different techniques to produce two RPI estimates from the resulting data. With the first technique, the estimate is calculated by computing a series of subestimates: For each AF field strength, the remaining NRM moment measured after that treatment step is normalized to the moment remaining after the corresponding ARM or IRM demagnetization step; an overall estimate is then produced by taking the arithmetic mean of these subestimates. The second technique calculates the RPI as the slope of a least squares linear regression on a collection of points. Each point corresponds to a single AF treatment step; its y coordinate is the NRM moment after that step, and its x coordinate is the ARM or IRM moment after the corresponding step. The R^2 value for this fit additionally gives an indication as to the reliability of the estimate. This technique can also be applied in the same way with a normalizer data set created by imparting an ARM in a stepwise manner with a series of increasing AF steps; in this case, the inverse slope gives the RPI estimate. Figure 4 gives an example of RPI calculation with an IRM normalizer.

2.4. VGP Calculation

PuffinPlot can now calculate VGPs from paleomagnetic site directions using the equations of spherical geometry (e.g., section 3.6, Irving, 1964). It can also calculate and display Fisherian statistics on VGPs. Since site locations are required for this calculation and are not included in most paleomagnetic file formats, the site locations can be specified in a dedicated file and imported separately. In the GUI, VGPs and their associated statistics are shown in a newly implemented VGP parameter table, and the VGP locations can be plotted on a world map; VGP data are also exported along with other site statistics. Figure 5 shows an example of VGP calculation in PuffinPlot.

2.5. Fisher Analysis of Demagnetization Steps

While paleomagnetic directions for a sample are most usually determined by PCA, there are some cases in which it may be useful to calculate Fisherian statistics on the directions of magnetic moments at individual treatment steps to obtain a mean direction for a sample. PuffinPlot now provides this functionality.

2.6. Improvements to Scripting Support

PuffinPlot now supports scripting in JavaScript as well as Python, and the user-defined great circle validity check now uses JavaScript rather than Python. Since only a minority of users make use of the Python scripting features, the Jython package (which provides Python support) is no longer bundled as part of PuffinPlot, dramatically reducing the download size. Jython is now downloaded and installed automatically if and when

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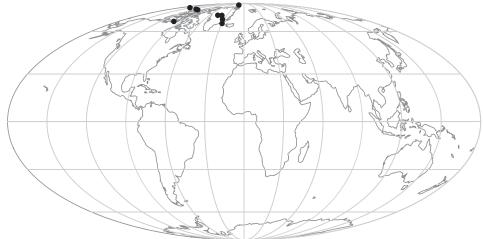


Figure 5. An example of VGP calculation on synthetic data in PuffinPlot. Data were generated for nine sites at different geographic locations, with 10 samples at each site. Sample directions were generated by adding random noise to the direction calculated by the IGRF-12 geomagnetic model for the year 1900. (top) Suite parameter table, giving Fisherian statistics on site and sample directions and VGPs. (middle left) Site parameter table, showing paleomagnetic direction at each site. (middle right) VGP parameter table, showing locations of sites and site VGPs. VGP = virtual geomagnetic poles.

it is required; additionally, separating Jython into an optional download has made it practical to use a more complete version of the package, including a larger range of Python libraries than was available with the previous, integrated Jython installation.

3. New File Formats

The most common feature request for PuffinPlot is support for reading an additional file format. Initially, PuffinPlot could import DAT files from 2G cryomagnetometers and TXT files from the "Zplot" program written by Steve Hurst at the Woods Hole Oceanographic Institution, and provided a custom importer which could be configured by the user to read many simple tabular file formats. There was also limited support for reading and plotting anisotropy of magnetic susceptibility (AMS) data from Advanced Geoscience Instruments Company (AGICO) ASC files. In the latest version, support has been added for reading the following file formats:

- 1. The text-based paleomagnetic data (PMD) format developed by R. Enkin and supported by several paleomagnetic programs including PMGSC, Paleomac (Cogné, 2003), and Remasoft (Chadima & Hrouda, 2007). The importer handles several variants of the format, including those exported from Remasoft 3.
- 2. The JR6 format developed by AGICO and supported by programs including REMA6W (AGICO, 2017), Remasoft, and Paleomac. The JR6 format allows an unusual degree of flexibility in specifying sample orientations: Four orientation parameters are given, together representing one of 64 possible conventions for the representation of the orientation of the fiducial mark, the sample dip and azimuth, and the formation dip direction. On importing, PuffinPlot standardizes all these representations to its own convention, rotating the input data as required.



- 3. The California Institute of Technology (CIT) or Caltech format used by the Paleomag (Jones, 2002) software. This format stores the data for each sample in a separate file and lists the sample files in an index file with a SAM extension. The PuffinPlot importer takes the SAM file and uses it to read data from the listed sample files.
- 4. The Interactive Analysis of Paleomagnetic Data (IAPD) format native to the IAPD and Super-IAPD series of programs by Trond Torsvik and others. This is a fairly straightfoward tabular format, but incompatible with PuffinPlot's general-purpose tabular file importer, so a specialized importer has been implemented for it
- 5. PuffinPlot can now import sample directions directly as declinations and inclinations stored in a CSV file, without requiring data at the demagnetization step level. This allows PuffinPlot's facilities to be used for general-purpose analysis and plotting of both paleomagnetic data sets lacking demangetization data and nonpaleomagnetic directional data.
- 6. Site location data can now be imported from a comma-separated value (CSV) file; this is particularly useful if VGP directions need to be calculated (see section 2.4).

Additionally, a number of improvements have been made to existing file importers:

- 1. We have made several significant improvements to AMS data import from AGICO ASC files. There are several variants of the ASC file format produced by different versions of AGICO's two programs for AMS measurement, SUSAR (AGICO, 2003) and SAFYR (AGICO, 2009). PuffinPlot now supports files from version 4.0 of SUSAR and versions 1.5 and 2.6 of SAFYR. Like the JR6 format, the ASC format supports multiple orientation conventions. Previously, ASC files had to conform to PuffinPlot's own orientation convention but now, as with JR6 files, all conventions are supported and are converted automatically on import. Finally, PuffinPlot can now read sample and formation orientations from the ASC file and optionally use them to update any existing values in the current suite.
- 2. The custom file importer has gained features: Measurement units can be selected by the user, and the sample volume field (previously ignored) is handled correctly. The importer also sets default values for the sample and formation corrections if these are not specified in the file.
- 3. In general, file reading and import is more robust to corrupted data and unexpected formats. Error messages and warnings during file import are clearer; measurement types are checked for consistency when opening a file; the measurement type in 2G files is guessed more reliably when not explicitly specified; and some situations which may previously have resulted in an unhandled error (e.g., an incorrectly specified 2G protocol) are now caught and dealt with more thoroughly, usually by showing a dialog box which explains the problem to the user.

4. Data Bundles and Reproducible Research

In recent years there has been increasing recognition of the importance of reproducibility in scientific research, in geoscience as in other disciplines, in particular with regard to data dissemination and processing (e.g., Gil et al., 2016; Thompson & Burnett, 2012). PuffinPlot now incorporates features to make it easier for users to publish data in a way which makes it easy for others to reproduce their results. This is done by creating a "data bundle," a self-contained archive comprising a PuffinPlot file of input data, CSV files containing the results of data analysis, and an automated processing script which uses PuffinPlot in non-GUI mode to automatically reproduce the analysis results from the original data. Optionally, a copy of the Puffin-Plot program itself may be included in the archive, meaning that only a Java runtime is required to reproduce the analysis. The data bundle is envisaged as a simple, straightforward way to package supporting data for inclusion with an article submission or upload to a data repository and can be used in several ways:

- 1. The pregenerated results in the CSV files can be used directly.
- 2. The results can be regenerated and verified by rerunning the analysis using the supplied script.
- 3. The PuffinPlot file can be opened and browsed in PuffinPlot's GUI to examine the data and the choices made in analyzing it. The analysis can be modified and rerun to explore the impact of different settings.
- 4. The PuffinPlot input file has a simple, text-based, tabular format and is fully documented in the manual; it can therefore be used as a convenient input format for further analysis of the original data by other software.



5. Other New Features

The following are other new features:

- 1. Various functions have been added to edit the data in a suite. Samples can now be removed by depth or treatment type, sample moments can be inverted, PCA and GC fits can be cleared individually, treatment type can be set manually, site definitions can be cleared, and sample volume can be edited. Data from a file can be added to an already opened suite as well as being loaded into a new one, and a discrete suite can be converted into a continuous one by supplying a file listing the depths of the samples.
- 2. A large number of minor improvements have been made to the desktop interface. For instance, treatment steps can be deselected by dragging a box, the suite name is shown in the title bar, and a status bar (showing the details of the demagnetization step under the mouse pointer) has been added to the main window. These changes are too numerous to list in full, but in combination they make the desktop GUI significantly more user-friendly and powerful.
- 3. A new data display has been added—a parameter table showing mean directions and VGPs—and features have been added to existing plot types. Data points can be annotated with their treatment step or sample name; current site and sample are highlighted in the relevant data tables and plots; Zijderveld plots support west-upward projections; site direction confidence intervals can be shown in the suite equal-area plot; and site equal-area plots more clearly distinguish different types of data.
- 4. More data fields are included in exported data files: custom flags and notes, great circle strikes and dips, and (in the sample parameter file) the n and α_{95} values. The precision of exported numerical parameters has also been increased. For Fisherian statistics, the R value (total vector path length) is now included in both the on-screen display and exported data.
- 5. Many minor bug fixes, mostly relating to display glitches. No bugs leading to data loss or incorrect analysis results have been reported or found.

6. Behind the Scenes: API Changes, Unit Tests, and Build Processes

Several of the recent improvements are largely invisible to the typical desktop GUI user but are of interest to anyone writing scripts that use PuffinPlot and also help to ensure the long-term health of the project.

The API has been improved most noticeably in the renaming of many classes and methods to make their purposes clearer and more self-explanatory. For instance, the originally somewhat cryptic method <code>Datum.getMeasType()</code> has now become <code>TreatmentStep.getMeasurementType()</code>. This makes scripting easier as well as making the codebase itself more maintainable.

One major expansion of PuffinPlot's codebase is invisible to the user: the addition of several hundred unit tests covering virtually all of the data processing and file reading code. Unit testing (e.g., Barbey & Strohmeier, 1994) helps to ensure the correctness of a software implementation by testing the operation of its component units (classes, functions, and methods) in isolation with predefined inputs and checking the outputs against precalculated values. As well as verifying the software's current behavior, unit testing helps to guard against the accidental introduction of bugs in future versions. It is of particular value in scientific and analytical software, where a bug may produce incorrect results without resulting in any obvious error visible to the user. A unit test often makes use of a so-called "test oracle" (e.g., section 9.1.2, Jalote, 1997): an independently calculated result known to be correct, against which the program unit's output is checked. Wherever possible, PuffinPlot's unit tests check results against worked examples in textbooks or papers (e.g., Robert, 1992, for VGP calculation and McFadden & McElhinny, 1988, for great-circle direction estimates), reference implementations of algorithms (e.g., Arason's own Fortran implementation for the Arason & Levi, 2010, algorithm), or independent implementations in other published paleomagnetic software (e.g., Remasoft Chadima & Hrouda, 2007, for JR6 file import and PmagPy; Tauxe et al., 2016, for Fisher statistics). It is, of course, possible that there may be an error in a test oracle, but the probability of a PuffinPlot unit and an independent source both producing the same wrong answer is vanishingly small, so matching results can be taken as strong evidence of correctness.

Ongoing development of PuffinPlot now uses the test-driven development methodology (Beck, 2003), whereby unit tests are written before the implementing code itself. While no methodology can ever guarantee entirely bug-free software, this technique gives good confidence that new features will also be correctly implemented.



We have made efforts to make it easier to work on the PuffinPlot codebase: Building the software from source has been simplified by the use of an automated dependency manager (Apache Ivy), and development has been moved to the popular Git version control system and GitHub source hosting site. As well as making the source code easier to find, download, and compile, these changes lower the barrier to entry for new contributors to the project.

7. Future Work

Despite PuffinPlot's steadily increasing capabilities, development is far outpaced by the rate of feature requests: The wish list of new features currently stands at around 180 items, ranging from the relatively trivial to those that would require significant rearchitecting of the program and data structures. As a single-developer, part-time project, PuffinPlot develops slowly, and feature requests have to be prioritized carefully with regard to demand and feasibility. New feature implementation also has to be balanced against refactoring and maintenance of existing code, which becomes a larger burden as the size of the project increases over time. For the next major release, we are aiming to implement the following features:

- 1. More sophisticated algorithms for determination of paleomagnetic directions, including the use of sector constraints in great-circle analysis and the estimation of direction uncertainty by the technique of Heslop and Roberts (2016).
- 2. Interoperability with the online Magnetics Information Consortium (MagIC) database (Jarboe et al., 2018), including import and export of the recently updated MagIC file format.
- 3. A more flexible system for organizing plots, allowing for multiple plot windows, multiple plots of the same type, and more flexible configuration of plotting options.
- 4. Improvements to the file import system, making it simpler to implement new file importers and allowing the use of plug-in file import scripts which do not need to be compiled into the main PuffinPlot distribution.
- 5. Multiple directional fits for a single sample. This feature has been frequently requested but has so far remained unimplemented because of the large changes it will require to the internal data model.

PuffinPlot has now been in use for somewhat over 10 years, including its initial internal deployment at the University of Otago. Like several paleomagnetic programs before it, it seems destined for a long life and is entering its second decade with undiminished vigor.

Acknowledgments

PuffinPlot version 1.4.1 may be downloaded via the official website at https://www.talvi.net/puffinplot/, which provides links to installable packages, documentation, and the full source code. The release and the entire current source code repository have also been permanently archived in the Zenodo research data repository (Lurcock, 2019). The development of PuffinPlot has been financially supported by the Project of Strategic Interest NextData PNR 2011-2013. We thank the many users who have reported bugs and requested features over the years. Both this paper and the program itself have benefited from thorough and constructive reviews by Gillian Turner and an anonymous

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