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An R package for statistical provenance analysis

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December 20, 2015

Abstract

This paper introduces `provenance`, a software package within the statistical programming environment `R`, which aims to facilitate the visualisation and interpretation of large amounts of sedimentary provenance data, including mineralogical, petrographic, chemical and isotopic provenance proxies, or any combination of these. `provenance` comprises functions to: (a) calculate the sample size required to achieve a given detection limit; (b) plot distributional data such as detrital zircon U-Pb age spectra as Cumulative Age Distributions (CADs) or adaptive Kernel Density Estimates (KDEs); (c) plot compositional data as pie charts or ternary diagrams; (d) correct the effects of hydraulic sorting on sandstone petrography and heavy mineral composition; (e) assess the settling equivalence of detrital minerals and grain-size dependence of sediment composition; (f) quantify the dissimilarity between distributional data using the Kolmogorov-Smirnov and Sircombe-Hazelton distances, or between compositional data using the Aitchison and Bray-Curtis distances; (e) interpret multi-sample datasets by means of (classical and nonmetric) Multidimensional Scaling (MDS) and Principal Component Analysis (PCA); and (f) simplify the interpretation of multi-method datasets by means of Generalised Procrustes Analysis (GPA) and 3-way MDS. All these tools can be accessed through an intuitive query-based user interface, which does not require knowledge of the `R` programming language. `provenance` is free software released under the GPL-2 license and will be expanded based on user feedback.

keywords: provenance – statistics – U-Pb – zircon – heavy minerals – petrography – geochemistry

1 Introduction

Sedimentary provenance analysis, in which chemical, mineralogical and isotopic properties of siliciclastic sediments are used to trace the flow of sand (or silt) through a sediment routing system, has entered an era of 'Big Data' (Vermeesch and Garzanti, 2015). Thanks to technological improvements, it is now common practice to analyse thousands of grains in dozens of samples. These large datasets can be prohibitively difficult to interpret without statistical aids. Over the past few years, sedimentary geologists and geochronologists have developed a plethora of methods to address this issue, which are scattered in many different places and implemented in a variety of different software environments (e.g., Ludwig, 2003; Marshall, 1996; Sircombe and Hazelton, 2004; Sircombe, 2004; Resentini et al., 2013; Templ et al., 2011; van den Boogaart and Tolosana-Delgado, 2008; Vermeesch, 2004, 2012, 2013; Vermeesch and Garzanti, 2015). This paper aims to group some of the most useful tools under a common umbrella, the `provenance` package. The various sections of this article are arranged in order of increasing complexity and dimensionality, using a published dataset from Namibia for examples (Section 2).

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Section 3 covers some functions that deal with a single provenance proxy applied to a single sample of sediment. This includes sample size calculations (Section 3.1) and functions to plot detrital age distributions as Kernel Density Estimates and Cumulative Age Distributions (Section 3.2). Sections 3.3 and 3.4 show how the effects of selective entrainment of dense minerals can be undone and how mineralogical and petrographic provenance proxies are affected by hydraulic sorting. Section 4 introduces Principal Component Analysis and Multidimensional Scaling as dimension reducing techniques which facilitate the interpretation of multi-sample datasets analysed by a single method. This Section also presents a brief overview of different approaches to quantify the 'dissimilarity' between distributional and compositional data. Finally, section 5 covers functionality to combine large datasets comparing multiple samples analysed with multiple methods, using Procrustes analysis and 3-way Multidimensional Scaling. The various functions in this paper are illustrated with many code snippets. Further examples are provided at `http://provenance.london-geochron.com` and in the built-in documentation. To run these examples and use the `provenance` package, one should first install `R`. This is an increasingly popular programming environment similar in scope and purpose to `Matlab`, which is available free of charge on any operating system at `http://r-project.org`. The actual package can then be installed by typing

```
install.packages('provenance')
```

at the command prompt. Once installed, the package can be loaded by typing

```
library(provenance)
```

The easiest way to use `provenance` is by typing:

```
provenance()
```

which brings up a query-based user interface, removing the need to master the syntax of the `R` programming language (Figure 1). The `provenance()` user interface is self explanatory and won't be discussed further in this paper. Instead, the different tools within the `provenance` package will be illustrated with short code snippets which more advanced users may incorporate in their own `R` scripts for enhanced flexibility and automation. Internal documentation of these functions can be accessed through the `?` command. For example, to display the documentation for the `procrustes` function (Section 5):

```
?procrustes
```

2 Data handling

Over the years, geologists have tried and tested literally dozens of provenance proxies (e.g., Basu and Molinaroli, 1989; Matter and Ramseyer, 1985; Morton, 1985; Owen, 1987; Renne et al., 1990; Hurford and Carter, 1991; McLennan et al., 1993; Vermeesch and Garzanti, 2015). Most of these can be diviced into two broad classes:

1. `distributional` data cover single-mineral proxies such as detrital zircon U-Pb or mica ^{40}Ar/^{39}Ar ages, in which samples can be summarised as lists of ordinal values.
2. `compositional` data cover multi-mineral proxies such as petrography, heavy mineral analysis and bulk geochemistry, in which samples can be summarised as one-way tables in which each row can be (re)normalised to unity.

`provenance` reads raw data as `.csv` files and casts these into two classes by separate functions. For example:

```
DZ <- read.distributional(DZ.fname.csv,DZ.err.fname.csv)
HM <- read.compositional(HM.fname.csv)
```

Here DZ.fname.csv and DZ.err.fname.csv stand for the file names of some U-Pb age data and their analytical uncertainties (where the latter argument is optional). Different columns of these files correspond to different samples, with the rows containing the numerical values of the single grain analyses. HM.fname.csv stands for the file name of a heavy mineral dataset, stored as a table with samples arranged by row and each column corresponding to a different type of mineral. The data objects produced by the two read functions are treated differently by all subsequent functions.

2.1 Built-in datasets

To illustrate provenance's functionality, the package is bundled with a published dataset from Namibia (Vermeesch and Garzanti, 2015). Entering

```
data(Namib)
```

loads a variable called Namib into memory, which is comprised of one distributional and five compositional datasets: (1) Namib$DZ contains the zircon U-Pb ages and their analytical uncertainties; (2) Namib$PT the bulk petrography; (3) Namib$HM the heavy mineral compositions less the opaque minerals; (4) Namib$PTHM the combined petrography and heavy minerals, including micas and opaque minerals, normalised to unity; (5) Namib$Major the major element composition of the bulk sediment; and (6) Namib$Trace the trace element composition of the bulk sediment. To avoid having to repeatedly type the preamble Namib$, we can attach the dataset to the search path:

```
attach(Namib)
```

After which we can access its data members as DZ, PT etc. Additionally, provenance also includes a table of mineral and rock densities (densities) as well as the petrographic/mineralogical end-member compositions (endmembers) of various tectonic settings which will be used to evaluate the settling equivalence of detrital components (Section 3.4). Also these two datasets can be loaded with the data function:

```
data(densities,endmembers)
```

The built-in datasets are based on the following ten files: DZ.csv, DZ.err.csv, PT.csv, HM.csv, PTHM.csv, Major.csv, Trace.csv, densities.csv and endmembers.csv. The system paths of these files can be retrieved as follows:

```
HM.fname.csv <- system.file("HM.csv",package="provenance")
```

Further details about these datasets can be obtained from the built-in help functions ?Namib, ?densities and ?endmembers.

2.2 Basic data manipulation

provenance includes a number of basic operations to query and manipulate the large datasets contained within distributional and compositional data objects. For example, to extract the coastal samples of the Namibian geochronology and heavy mineral datasets:

```
coast.samples <- c('N1','N2','T8','T13','N12','N13')
coast.DZ <- subset(DZ,select=coast.samples)
coast.HM <- subset(HM,select=coast.samples)
```

For compositional data, the subset function also allows the user to extract subcompositions. For example, to extract the zircon, tourmaline and rutile content of all samples in the heavy mineral dataset:

```
ZTR <- subset(HM,components=c('zr','tm','rt'))
```

Of course, both options can also be combined:

```
coast.ZTR <- subset(HM,select=coast.samples,components=c(’zr’,’tm’,’rt’))
```

which returns the zircon, tourmaline and rutile contents of the coastal samples alone. For compositional data, it is often useful to add several components together, an operation which is referred to as ‘amalgamation’ (Aitchison, 1986). This is useful for removing missing components (‘zero counts’) prior to logratio analysis (Section 4.2). For example, to extract the QFL (Quartz – Feldspar – Lithics) composition from the petrographic dataset by amalgamation:

```
QFL <- amalgamate(PT,Q=’Q’,F=c(’KF’,’P’),L=c(’Lm’,’Lv’,’Ls’))
```

where `KF` and `P` stand for K-feldspar and plagioclase, and `Lm`, `Lv` and `Ls` refer to the lithic fragments of metamorphic, volcanic and sedimentary origin respectively. In the special case of a three component system, amalgamation can also be achieved by a different function:

```
QFL.tern <- ternary(PT,’Q’,c(’KF’,’P’),c(’Lm’,’Lv’,’Ls’))
```

This produces an object of class `ternary` which is handled by a special, overloaded version of the `plot` function (Section 3.2). The statistical field of compositional data analysis is very rich, and `provenance` does not attempt to cover all but its most basic operations. The user is referred to other `R` packages such as `compositions` (van den Boogaart and Tolosana-Delgado, 2008) and `robCompositions` (Templ et al., 2011) for a more comprehensive toolset. Three functions are provided to facilitate the interaction between `provenance` and these other packages. `as.acomp` and `as.data.frame` convert `compositional` datasets to objects of class `acomp` and `data.frame`, for use in `robCompositions` and `compositions`, repectively. For example:

```
PT.acomp <- as.acomp(PT)           # can be used in ’compositions’
PT.data.frame <- as.data.frame(PT) # can be used in ’robCompositions’
```

Conversely, the `as.compositional` function translates `acomp` or `data.frame` objects to `compositional` data for use in `provenance`. For example, using the `Kongite` and `skyeLavas` datasets which are built into `compositions` and `robCompositions`:

```
library(compositions)
data(Kongite)
Kongite.comp <- as.compositional(Kongite)
library(robCompositions)
data(skyeLavas)
skyeLavas.comp <- as.compositional(skyeLavas)
```

where `Kongite.comp` and `skyeLavas.comp` can be further analysed by the functions described later in this paper.

3 Functions applying to a single sample

3.1 Sample size calculations

On the most basic level, provenance analysis requires the geologist to identify certain properties in a representative number of grains from each sample. The question then arises how many grains constitute a ‘representative’ number of grains. The answer to this question depends on the geological problem of interest. If the main purpose of the study is merely to characterise the general shape of the distribution (e.g., ‘young’ vs. ‘old’ or ‘narrow’ vs. ‘wide’), then a few dozen grains may be enough (Avdeev et al., 2011). If instead one is looking for a particular component comprising, say, a fraction f=1/N of the total population (where N is an integer denoting the number of fractions), then the likelihood of missing this fraction is given by $(1-f)^n$, where n is the number of grains (Dodson et al., 1988). Finally, if, we are interested in collecting all fractions of a sample (Vermeesch, 2004), then the likelihood of missing any of them is given by

$$p = \sum_{i=1}^{N} (-1)^{i-1} \binom{N}{i} (1-if)^n \tag{1}$$

where $\binom{N}{i}$ is the Binomial coefficient. To calculate the probability that at least one 10% fraction is missing from a 60-grain sample in `provenance`:

```
p <- get.p(n=60,f=0.1)
```

Conversely, to estimate the largest fraction (f) which one can be 95% confident not to have missed in the same 60-grain sample:

```
f <- get.f(n=60,p=0.05)
```

Finally, to compute the number of grains needed to be 95% certain that no fraction greater than 5% of the total population is missed:

```
n <- get.n(p=0.05,f=0.05)
```

which is 117 (Vermeesch, 2004).

3.2 Plotting individual samples

The geologically meaningful information carried by distributional data does not so much lie in their values as, like their name suggests, in their distribution. A first step towards interpreting such data in `provenance` is to plot them as either cumulative or density plots. To illustrate this, consider an infinite population characterised by a uniform distribution between 100 and 110 Ma. Plotting an infinite number of values collected from this population on a histogram with infinitessimal binwidth yields a simple step function (red line in Figure 2.a). This is the probability density function of the population. The corresponding cumulative distribution (red line in Figure 2.b) is a straight line rising from 0 at 100 Ma (0% of the population falls below 100 Ma) to 1 at 110 Ma (100% of the population falls below 110 Ma). Of course, in real life geologists never have the luxury of exhaustively collecting an entire population. Instead, they must work with a representative subset of that population, the sample. Suppose that we have collected a random sample of 100 values from our uniform population (black ticks on Figure 2.a). Further suppose that these values are analysed with infinite analytical precision. From this sample of random values, we cannot reconstruct the step function. Instead, the density must be *estimated* using histograms or kernel density estimates (KDEs). For a sample of limited size, these estimates never exactly agree with the true age distribution, but are smooth approximation thereof (black line in Figure 2.a). In contrast, the Empirical Cumulative Distribution Function (ECDF, a.k.a. 'Cumulative Age Distribution' or CAD in a geochronological context, Vermeesch, 2007) is a method to visualise distributional datasets without the need for any smoothing. Let $x = \{x_1, x_2, ..., x_n\}$ be a sample of distributional data, then the cumulative distribution F_x is defined as follows:

$$F_x(t) = \frac{1}{n}(\#x_i \leq t) \tag{2}$$

where '$\#x \leq t$' stands for "the number of items in x that are smaller than or equal to t". In contrast with density estimates, CADs do not suffer from oversmoothing (Figure 2.b). Despite this significant advantage of CADs over KDEs, the latter are still preferred by many practitioners of detrital geochronology because they are more intuitive to interpret.

In real life, analytical precision is never infinite, but measured ages are offset from their true values by some experimental error. Suppose that this error is characterised by a Normal distribution with standard deviation $\sigma = 2$ Ma. Convolution of the error distribution with the uniform distribution of the true ages yields a smooth probability density function which spreads into values beyond the 100-110 Ma interval (red line in Figure 2.c). The corresponding cumulative distribution rises gently from 0 at ~95 Ma (0% of the distribution falls below 95 Ma) to 1 at ~115 Ma (100% of the distribution falls below 115 Ma), with a linear section in between (red line in Figure 2.d). Like before, the KDE of the measurements (black line in Figure 2.c) oversmooths the theoretical probability density function (red line). And like before, the correponding CAD (black line in Figure 2.d) does not suffer from this problem. Note that Probability Density Plots (PDPs), which are a popular way to account for the variable precision of detrital data by using the analytical uncertainty as a bandwidth estimator (Ludwig, 2003; Sircombe, 2004) unfortunately suffer from significant levels of undersmoothing for small datasets and oversmoothing for large datasets (Vermeesch, 2012). For this reason, PDPs are not implemented in `provenance`.

Figure 2 here.

In `provenance`, CADs are obtained using an overloaded `plot` function. For example, for detrital zircon U-Pb sample `N1` (Figure 3a):

```
plot(DZ,snames='N1',CAD=TRUE)
```

Both histograms and KDEs are implemented in standard `R` as the `hist` and `density` functions, respectively. These built-in functions work very well for relatively simple, unimodal distributions (Silverman, 1986). However, the distributions occurring in detrital geochronology tend to be more complex than that, causing the `density` function to overestimate the kernel bandwidth and oversmooth the resulting distribution. For this reason, the `provenance` package includes a separate function for kernel density estimation using a hybrid adaptive kernel density algorithm, adopted from `DensityPlotter` (version 3.0 and above, Vermeesch, 2012). This algorithm consists of two steps. First, the fixed bandwidth algorithm by Botev et al. (2010) is used to calculate a 'pilot' density. Then, the bandwidth is adjusted at each sample point to scale with the square root of the local density, normalised by the geometric mean of the entire distribution (Abramson, 1982). Thus, the fixed bandwidth estimate is converted into an adaptive density estimate, which assigns a narrower bandwidth to densely sampled segments of the age distribution and a wider bandwidth to those segments which are sparsely sampled. This increases the resolution of the density estimates where sufficient data are available, whilst smoothing out those parts with insufficient data. As an example, the following code plots the U-Pb age distribution of sample `N1` from the Namibian dataset with the default settings (Figure 3b):

```
N1 <- DZ$x$N1       # extract the ages of sample N1
dens <- KDE(N1)     # create the density estimate
plot(dens)          # plot the density estimate
```

The appearance of the plot can be changed by modifying the optional arguments. The following example plots the data on a logarithmic scale from 10 to 3,000 Ma with a fixed bandwidth of 50 Ma and turns off the sample point indicators on the x-axis (Figure 3c):

```
dens <- KDE(N1,bw=50,from=100,to=4000,adaptive=FALSE,log=TRUE)
plot(dens,pch=NA ) # pch = the symbol used for the sample points
```

`provenance` also includes some basic functionality to plot compositional data on ternary diagrams. For example, to plot the petrography of the Namib dataset on Dickinson et al. (1983)'s QFL diagram (Figure 3d):

```
plot(QFL.tern,type='QFL.dickinson')
```

where `QFL.tern` was produced by the `ternary()` function (Section 2.2). The graphical output can be saved as a vector-editable PDF for further processing in software such as Adobe Illustrator©, CorelDraw©or Inkscape:

```
dev.copy2pdf(file="QFL.tern.pdf")
```

Figure 3 here.

3.3 The SRD correction: a simple way to correct for environmental bias

To facilitate the comparison of detrital modes for provenance analysis or stratigraphic correlation, we need to first remove the often significant compositional differences among sediment samples that are caused by hydrodynamic processes in the depositional environment. Intersample modal variability can be corrected for by a simple principle. In the absence of provenance changes and environmental bias, the weighted average Source Rock Density (SRD) of terrigenous grains should be equal, for each sample and each grain-size class of each sample, to the weighted average density of source rocks. By correcting relative abundances of detrital minerals in proportion to their densities, we can restore the appropriate SRD index for any provenance and subprovenance type in each sample or grain-size class (Garzanti et al., 2009). Modal variability is effectively reduced by this procedure, which can be applied confidently to modern sediments deposited by tractive currents in any environment. Good results are obtained even for placer sands and finest grain-size fractions where heavy-mineral concentration is strongest. Such 'SRD correction' also successfully compensates for biased narrow-window modes, thus providing a numerical solution of general validity to the problem of environmental bias in sedimentary petrology.

The SRD index, used to assess average density of source rocks in the absence of hydrodynamic effects or to detect hydraulic-controlled concentration of denser minerals, is defined as the weighted average density of terrigenous grains (spurious and intrabasinal particles such as bioclasts are neglected in the calculation; Garzanti and Andò, 2007):

$$SRD = \sum_{i=1}^{n} (\%m_i \; \rho_{m_i}) = 1/\sum_{i=1}^{n} (\%M_i/\rho_{m_i}) \tag{3}$$

where %m and %M are the volume and weight percentages of mineral m, and ρ_m its density. In order to compensate for selective-entrainment effects, we must recalculate detrital modes for each sample until the same SRD index is restored for each. The mathematical procedure is similar to that used to convert volume percentages to weight percentages, and vice-versa:

$$\%M = \%m \; \rho_m/SRD = \%m \; \rho_m/\sum_{i=1}^{n} (\%m_i \; \rho_{m_i}) \tag{4}$$

$$\%m = \%M \; SRD/\rho_m = \%M/\left[\rho_m \sum_{i=1}^{n} (\%M_i/\rho_{m_i})\right] \tag{5}$$

The 'SRD correction' assumes the form of Equation 4 for heavy-mineral-poor samples:

$$\%m^* = \%m \; \rho_m/\sum_{i=1}^{n} (\%m_i \; \rho_{m_i}) \tag{6}$$

and the form of Equation 5 for heavy-mineral-rich samples:

$$\%m^* = \%m/[\rho_m \sum_{i=1}^{n} (\%m_i/\rho_{m_i})] \tag{7}$$

To remove environmental bias by the SRD correction we need to assume an appropriate common SRD value for all samples. Such a value may be determined empirically, by averaging SRD indices of 'normal' samples with the same provenance. Or we may proceed in reverse, and find through successive approximations the SRD value which minimizes the residual variance in the data set. In any case, we need criteria to tell us which SRD value is appropriate and which should be considered anomalous. In the absence of hydrodynamic effects, the SRD index faithfully reflects the average density of source rocks (Garzanti et al., 2006). With the exception of less dense glass-rich volcanic and porous sedimentary rocks, and of denser mafic and ultramafic rocks, rocks densities typically lie in the 2.6-2.8 g/cm^3 range (Daly et al., 1966). Therefore, besides monogenic detritus supplied locally by specific rock types (e.g., ignimbrite, gypsum, gabbro, peridotite, granulite, eclogite), SRD indices of homogenized detritus derived long-distance from diverse crustal sources must lie in a narrow range (2.70 ± 0.05). Given the regional geology and geomorphology of southern Africa, we can confidently rule out exotic compositions and safely assume an SRD of $\sim$ 2.71. Restoring all samples from the Namib dataset to this reference value:

```
rescomp <- restore(PTHM,dens=densities,target=2.71)
HMcomp <- c("zr","tm","rt","sph","ap","ep","gt","st","amp","cpx","opx")
PHO <- amalgamate(rescomp,Plag="P",HM=HMcomp,Opq="opaques")
plot(ternary(PHO),showpath=TRUE)
```

where `HMcomp` is a list of heavy minerals and `amcomp` amalgamates the restored `PTHM` composition to the reference SRD density. Setting `showpath=TRUE` in the overloaded `plot` function displays the intermediate steps of the iterative SRD correction algorithm on the ternary diagram. In the above example, plagioclase, the amalgamated transparent heavy minerals and the opaque minerals are plotted together because they cover a wide range of densities (2.67, $\sim$3.5 and 5 g/cm^3, respectively). For the Namib dataset, the correction path clearly shows that samples N8 and N9 are most strongly affected by the SRD correction and, hence, hydraulic sorting effects. This is entirely consistent with the interpretations of Garzanti et al. (2012), Vermeesch and Garzanti (2015), and Section 5. Finally, to illustrate the combined use of `provenance` with the `compositions` package, the following code adds an ellipse from the mean and the variance to the SRD-corrected data, using the `compositions` package's `ellipses` function:

```
PHO.acomp <- as.acomp(PHO) # convert to class 'acomp'
ellipses(mean(PHO.acomp),var(PHO.acomp),r=2)
```

Figure 4 here.

3.4 Size-density sorting of detrital grains and intrasample variability

The settling velocity of a detrital particle represents the balance between gravitational forces and drag resistance due to both turbulence and viscosity. Settling of clay and silt particles in water is resisted by viscosity, whereas turbulence is the dominant drag component during settling of pebbles or in air. Different empirical formulas have been proposed to model settling of particles by tractive currents, accounting for the wide range of grain sizes displayed by sedimentary deposits and their diverse depositional facies (aeolian vs. fluvial vs. marine). The settling velocity of clay and silt particles can be calculated by Stokes' Law:

$$v = gR_xD_x^2/18\eta \tag{8}$$

where g is the gravitational constant, R_x is the submerged density (ρ_{grain}-ρ_{fluid}), D_x is the diameter of the particle, and η is the fluid viscosity. The settling velocity of sand-sized particles in water must be calculated by empirical formulas, such as the relatively simple one proposed by (Cheng, 1997):

$$v = (\eta/D_x)\left[\sqrt{25 + 1.2(gR_xD_x^3/\eta^2)^{2/3}} - 5\right]^{3/2} \tag{9}$$

The settling velocity of granules and pebbles can be described by Newton's Impact Law:

$$v = \sqrt{2gR_xD_x/(3\rho_f)} \tag{10}$$

where ρ_f is the fluid density. The same formula has been shown empirically to be sufficiently accurate also to calculate the settling of particles of any grain size in air (Garzanti et al., 2008). These three formulas allow us to calculate the difference in nominal diameter (the 'size shift', SS) between two settling-equivalent particles for any size, in any transporting medium, and usually referred to quartz. For clay and silt particles, size shifts between any mineral x and a reference mineral or the bulk sediment are calculated as:

$$SS_x = log_2(R_x/R_{ref})/2 \tag{11}$$

For sand sized particles:

$$SS_x = log_2(R_x/R_{ref}) - (3/2)log_2(\Xi_m/\Xi_{ref}) \tag{12}$$

where $\Xi = v/\eta + \sqrt{(v/\eta)^2 + 48(g\ R_x/\eta^2)^{2/3}}$. For granules and pebbles or any sediment settling in air, size shifts are twice those predicted by Stokes' Law:

$$SS_x = log_2(R_x/R_{ref}) \tag{13}$$

The average settling velocity for each given sediment sample can be calculated with formulas 8, 9 or 10 according to its mean grain size, grain density (SRD index of the bulk sediment, see Section 3.3) and depositional environment (air, freshwater or seawater). For each detrital mineral or rock fragment, the size shift referred to the bulk-sediment (SRD index) is calculated with formulas 11, 12 or 13. To account for shape effects (Komar et al., 1984), the density of micas is lowered by 0.5 g/cm^3 (Garzanti et al., 2008). Finally, a Gaussian size-frequency distribution is calculated for each detrital component by combining its size shift referred to the mean size of the bulk sediment and the sorting value of the latter.

In `provenance`, all these calculations are performed by the `minsorting` function, so named after the spreadsheet application of Resentini et al. (2013) on which it is based. To illustrate the use of the `minsorting` function, the following code snippet applies it to one of the end-member compositions included with the package, assuming a mean grain size of (Krumbein) Φ=2 and standard deviation Φ=1:

```
data(endmembers,densities)
distribution <- minsorting(endmembers,densities,sname='ophiolite',
                           phi=2,sigmaphi=1,medium="seawater",by=0.05)
plot(distribution,components=c('F','px','opaques'))
```

Which yields the grain size distribution of feldspar, pyroxene and opaque minerals (in 0.05 Φ intervals), so chosen because of the great contrast in density between them (Figure 5). When - as is commonly done in geochronological analysis - one specific mineral is targeted (e.g., apatite or zircon), we can use such information to choose the most suitable size window for laboratory treatment and analysis, and thus obtain a most faithful characterization of the sediment sample.

Figure 5 here.

4 Jointly considering multiple samples

`provenance` allows multiple samples to be plotted together. For example, to plot all 16 detrital age distributions from the Namibian dataset on a scale from 0 to 3,000 Ma in four columns:

```
UPb <- KDEs(DZ,from=0,to=3000,normalise=TRUE)
summaryplot(UPb,ncol=4)
```

where the `normalise` flag sets the area under each of the KDEs to the same value. The resulting plot contains 16 kernel density estimates, resulting in 16 × 15 / 2 = 120 pairwise comparisons (Figure 6). The first step towards simplifying this multi-sample comparison problem is to convert the raw data into a table of pairwise distances. This can be achieved using a number of different dissimilarity measures.

Figure 6 here.

4.1 Dissimilarity measures

A crucial first step towards simplifying the interpretation of multi-sample datasets is to replace the visual comparison of age distributions, histograms and pie charts with numerical values expressing the 'dissimilarity' between samples. For distributional data, the default method is the Kolmogorov-Smirnov (K-S) statistic (δ^{ks}_{AB}), which uses the maximum absolute difference between two cumulative distributions (Feller, 1948). Given two samples A and B, the K-S distance is defined as

$$\delta^{ks}_{AB} = \underset{t}{max}|F_A(t) - F_B(t)| \tag{14}$$

where F_A and F_B are defined by Equation 2 and $|\cdot|$ stands for the absolute value. One nice feature of the K-S distance is that it obeys the triangle inequality, which states that, for any three samples A, B and C, the distance between A and C is less than or equal to the distance between A and B plus the distance between B and C. The triangle inequality makes the K-S distance behave like the physical distances which we are familiar with in the real world. On the other hand, the K-S statistic also has limitations, such as its inability to take into account the effect of unequal analytical uncertainties. This makes it difficult to objectively compare samples acquired on different mass spectrometers characterised by differing analytical precision. This problem was addressed by Sircombe and Hazelton (2004) using the squared overlap between so-called Kernel Functional Estimates (KFEs):

$$\delta^{sh}_{AB} = \sqrt{\int \left(f_A(t) - f_B(t)\right)^2 dt} \tag{15}$$

where f_A and f_B are the KFEs of samples A and B. KFEs are a special type of KDEs, in which a variable degree of deliberate oversmoothing is applied to the different samples to account for the differing analytical uncertainties between them (Sircombe and Hazelton, 2004). Although KFEs are useful as a point of comparison between different samples, they have limited value as a data visualisation tool due to the oversmoothing. To use the S-H dissimilarity, the user needs to supply the analytical uncertainties in a separate `.csv` file. The following code demonstrates the calculation of K-S and S-H dissimilarities in `provenance`:

```
KS.diss <- diss(DZ,method='KS')
SH.diss <- diss(DZ,method='SH')
```

For compositional proxies such as petrographic, heavy mineral or chemical data, `provenance` provides a further two dissimilarity measures. If the dataset is free of zero values, Aitchison's central logratio distance is used by default:

$$\delta^{ait}_{AB} = \sqrt{\sum_{i=1}^{n} \left[ln\left(\frac{A_i}{g(A)}\right) - ln\left(\frac{B_i}{g(B)}\right)\right]^2} \tag{16}$$

where 'g(x) stands for 'the geometric mean of x (Aitchison, 1986; Vermeesch, 2013). Note that the same distance is obtained irrespective of whether the input data are expressed as fractions or percentages. The Aitchison distance breaks down for datasets comprising 'zero counts' ($A_i = 0$ or B_i=0 for any i). This problem can be solved by pooling several categories together (see Section 2.2), or by using a different dissimilarity measure such as the Bray-Curtis distance:

$$\delta_{AB}^{bc} = \sum_{i=1}^{n} |A_i - B_i| \Big/ \sum_{i=1}^{n} (A_i + B_i) \tag{17}$$

The following example yields the dissimilarity matrices of the heavy mineral and major element compositions using the Bray-Curtis and Aitchison measures, respectively:

```
HM.diss <- diss(HM,method='bray')
Major.diss <- diss(Major,method='aitchison')
```

4.2 Principal Component Analysis and Multidimensional Scaling

Although the dissimilarity matrices introduced in the previous section make the comparison of two samples more objective, it remains difficult to discern any meaningful patterns in large numbers of such pairwise comparisons. Multidimensional Scaling (MDS) is a dimension-reducing technique which can make the comparison of multiple samples more objective (Borg and Groenen, 2005). MDS is widely used in other scientific disciplines and can easily be adapted for provenance studies (Vermeesch, 2013). Given a table of pairwise distances between samples, MDS produces a configuration of points in which similar samples plot close together and dissimilar samples plot far apart. `provenance` implements both *classical* MDS, in which the physical distances between the different points in the MDS configuration are directly proportional to the dissimilarities between the corresponding samples; and *nonmetric* MDS, which merely aims to reproduce the relative ranks of the dissimilarities (Borg and Groenen, 2005). In the latter case, provenance allows the user to graphically assess the goodness of fit by plotting the dissimilarities against the fitted distances on a so-called 'Shepard Plot' (Kruskal and Wish, 1978). `provenance` uses nonmetric MDS by default because it produces better fits than classical MDS and accepts a wider range of dissimilarity measures (Kruskal and Wish, 1978; Borg and Groenen, 2005). The `MDS` function accepts as input either data of class `compositional` or `distributional`, or a dissimilary matrix (class `diss`). The following two lines of code are therefore equivalent to each other:

```
MDS.DZ.1 <- MDS(DZ)
MDS.DZ.2 <- MDS(diss(DZ))
```

In contrast with nonmetric MDS, classical MDS can only be used for dissimilarity measures are proper distances and therefore fulfil the triangle inequality (Borg and Groenen, 2005), which is the case for the Kolmogorov-Smirnov and Aitchison distances. For example, using the latter dissimilarity measure, the major element composition can be plotted as a classical MDS configuration:

```
Major.diss <- diss(Major,method='aitchison')
MDS.Major <- MDS(Major.diss,classical=TRUE)
plot(MDS.Major,xaxt='s',yaxt='s')
```

Where the `xaxt` and `yaxt` flags add tick marks and labels to the x and y axes (these are turned off by default). By definition, the Aitchison distance does not only fulfil the triangle inequality but is a Euclidean distance as well. In this case, MDS is equivalent to Principal Component Analysis (PCA, Aitchison, 1983; Cox and Cox, 2000). This equivalence can be demonstrated by the fact that:

```
PCA.Major <- PCA(Major)
plot(PCA.Major)
```

produces identical output as the previous code snippet (Figure 7). The main advantage of PCA over MDS is that it can be visualised as a 'biplot', in which the configuration is accompanied by a set of vector 'loadings' showing the relationship between the categorical input variables (Figure 7.b). Thus, the PCA biplot facilitates the interpretation of the configuration in terms of underlying processes (Aitchison and Greenacre, 2002). In this respect, compositional biplots are similar to a 3-way extension of the MDS method called INDSCAL, which is discussed in the next section. One limitation of compositional PCA is its inability to handle datasets containing zero values, which is due to its dependence on logratios (see Section 4.1). Various ways have been proposed to deal with this problem (e.g., Martín-Fernández et al., 2003), but none of these are implemented in `provenance` (yet). Instead, the user is presented with two options. The zero-value problem can either be circumvented by employing non-metric MDS using the Bray-Curtis dissimilarity; or by resorting to the PCA functionality implemented in the `compositions` and `robCompositions` packages.

Figure 7 here.

5 Combining multiple methods in multiple samples

The entire 5-proxy dataset can be visualised together with the `summaryplot` command, producing a diagram with 16 KDEs and 64 pie charts:

```
PT$colmap <- 'cm.colors'
Trace$colmap <- 'rainbow'
UPb <- KDEs(DZ,from=0,to=3000,normalise=TRUE)
summaryplot(UPb,HM,PT,Major,Trace,ncol=2)
```

Which assigns a different colour map to the pie charts of the petrographic and trace element data from the default `heat.colors`. The summary plot manages to squeeze 16,125 numerical values into a single diagram, which provides a good visual illustration of the term 'Big Data', but is next to impossible to interpret geologically. Using the methods introduced in Section 4, we can produce five MDS maps and thereby facilitate the multi-sample comparison for each dataset (Vermeesch and Garzanti, 2015). Unfortunately, the subtle differences between these maps present a second type of multiple comparison problem, which calls for second layer of statistical simplification. The `provenance` package provides two alternative solutions for this: Procrustes analysis and 3-way MDS.

Procrustes analysis is the process by which a combination of shape-preserving transformations is used to match the shape of one object with that of another. Generalised Procrustes Analysis (GPA) is a generalisation of this procedure to multiple objects. In a provenance context, GPA extracts a single 'consensus' view from a collection of MDS configurations, by rotating, reflecting and scaling them to minimise a least squares criterion (Gower, 1975; Vermeesch and Garzanti, 2015). The following code applies this method to the Namib dataset:

```
proc <- procrustes(DZ,HM,PT,Major,Trace)
plot(proc)
```

GPA is a two step process, in which the individual datasets are first subjected to an MDS analysis, and the resulting configurations are then transformed into a group configuration. Alternatively, the same type of graphical output can be generated in a single step, using the final technique discussed in this paper, 3-way MDS.

As the name suggests, 3-way MDS is a generalisation of the methods discussed in Section 4.2 from two- to three-dimensional dissimilarity matrices. For the Namib dataset, the combination of 16 samples and 5 methods results in a dissimilarity matrix of size 15 × 15 × 5. There exist many types of 3-way MDS algorithms, the oldest and most widely used of which is called INdividual Differences SCALing (INDSCAL, Carroll and Chang, 1970). In contrast with 2-way MDS and GPA, INDSCAL produces not one but two pieces of graphical output: the 'group configuration' and the 'source weights'. For the Namib dataset, the former reproduces the relative dissimilarities between the samples, whereas the latter displays the relationship between the provenance proxies (Vermeesch and Garzanti, 2015). This is similar in a way to the compositional biplots produced by PCA (Section 4.2), which simultaneously display the configuration of the samples and the relationship between the variables (e.g. minerals or chemical elements). In the case of INDSCAL, the ‘source weights’ quantify the relative importance attached by each of the data sources (i.e. provenance proxies) to the horizontal and vertical axis of the ‘group configuration’ (Carroll and Chang, 1970; De Leeuw and Mair, 2011; Vermeesch and Garzanti, 2015). In `provenance`:

```
IND <- indscal(DZ,HM,PT,Trace,Major)
plot(IND)
```

Note that the resulting group configuration (Figure 8.a) looks significantly different from that presented by Vermeesch and Garzanti (2015). This is due to an error in the original petrographic data table, which has been fixed in the present paper. The ‘source’ weights (Figure 8.b) show that the major and trace element compositions attach much greater weight to the horizontal axis of the group configuration than the other proxies. This is attributed to hydraulic sorting, which affects bulk compositions more than it does mineral separates (Vermeesch and Garzanti, 2015). This is entirely consistent with Figure 4, which showed that samples N8 and N9 are particularly affected by winnowing effects.

Figure 8 here.

Although, in principle, 3-way MDS yields more insightful output than GPA, in practice things do not always work out so well. The problem is that the output of INDSCAL is often very sensitive to subtle changes in the input data. For example, running INDSCAL on the same data as before, but using the S-H dissimilarity instead of the K-S distance for the DZ data and the Bray-Curtis distance instead of the Aitchison distance for the bulk chemistry results in a similar looking group configurations (Figure 8.c), but a significantly different subject weights (Figure 8.d).

```
DZ$method <- "SH"
Major$method <- "bray"
Trace$method <- "bray"
IND.SH <- indscal(DZ,HM,PT,Trace,Major)
plot(IND.SH)
```

It is therefore advisable not to overinterpret these weights, and thus in practice INDSCAL often does not outperform GPA as might be hoped.

6 Conclusions

It is increasingly being recognised that, in order to truly understand sediment routing systems, the combination of multiple proxies teaches more than the sum of its parts (Garzanti, 2015). This paper introduced an `R` package named `provenance` to facilitate the joint interpretation of large datasets comprising many samples and several provenance proxies. Technological advances such as fast scanning electron microscopes (e.g, QEMSCAN, Allen et al., 2012) and high-throughput LA-ICP-MS (e.g., Frei and Gerdes, 2009) promise to fully unlock the power of multi-method provenance analysis and further increase the need for the ‘Big Data’ analysis tools provided by `provenance`. Much work remains to be done to extend the methods presented in this paper. One example is the incorporation of dissimilarity measures to compare distributional data of higher dimensionality, such as paired U-Pb ages and Hf- or O-isotopic compositions (e.g., Owen, 1987). Another example is the introduction of weighted MDS (de Leeuw and Mair, 2009) to handle, say, datasets containing samples of widely different sizes.

We would like to conclude this paper with the advice not to rely exclusively on statistics for the interpretation of provenance data. It is our opinion that statistical provenance analysis should be used as a complement to rather than a substitute for expert geological knowledge. It is sometimes found that petrographic information, especially the composition of the lithic fragments, allows an experienced analyst to unequivocally constrain provenance with much greater confidence than any machine or computer algorithm

(Garzanti, 2015). Like any 'black box' technique, statistical methods such as MDS or INDSCAL can easily be abused. By exhaustively going through all the options provided by `provenance`, it may be possible to 'cherry pick' a configuration that supports a pre-conceived model. Paraphrasing Andrew Lang, we would like to urge the user to resist the temptation of using `provenance` in the same way that a drunk uses lamp-posts – for support rather than illumination. It is important to keep in mind that good scientific practice involves testing and rejecting rather than 'proving' hypotheses (Popper, 1959). We hope that `provenance` will be used according to this philosophy, along with all the other techniques at the disposal of sedimentary geologist today.

Acknowledgments

The author would like to thank István Dunkl, Luca Caracciolo, Hilmar von Eynatten and Guido Meinhold for organising the 2014 Working Group for Sediment Generation workshop in Göttingen and inviting him to present the work behind the `provenance` package. This research was funded by NERC standard grant #NE/1009248/1 and ERC starting grant 259505 ('KArSD'). Raimon Tolosana-Delgado and two anonymous reviewers are gratefully acknowledged for their critical but constructive comments which truly transformed the paper.

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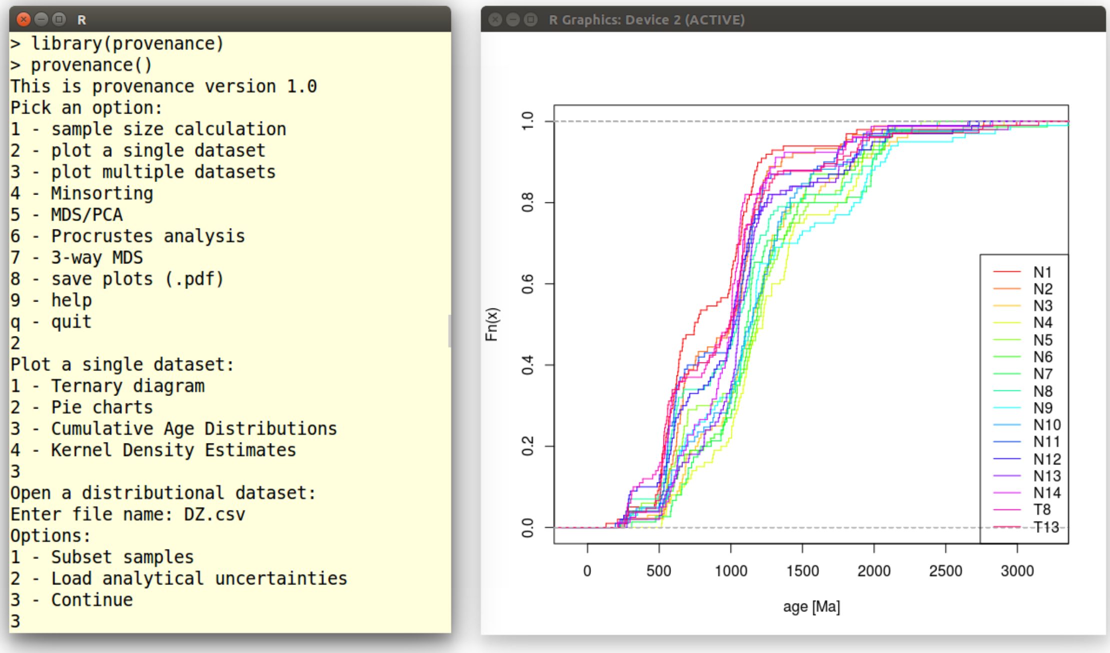

```
> library(provenance)
> provenance()
This is provenance version 1.0
Pick an option:
1 - sample size calculation
2 - plot a single dataset
3 - plot multiple datasets
4 - Minsorting
5 - MDS/PCA
6 - Procrustes analysis
7 - 3-way MDS
8 - save plots (.pdf)
9 - help
q - quit
2
Plot a single dataset:
1 - Ternary diagram
2 - Pie charts
3 - Cumulative Age Distributions
4 - Kernel Density Estimates
3
Open a distributional dataset:
Enter file name: DZ.csv
Options:
1 - Subset samples
2 - Load analytical uncertainties
3 - Continue
3
```

Figure 1: The query-based user interface.

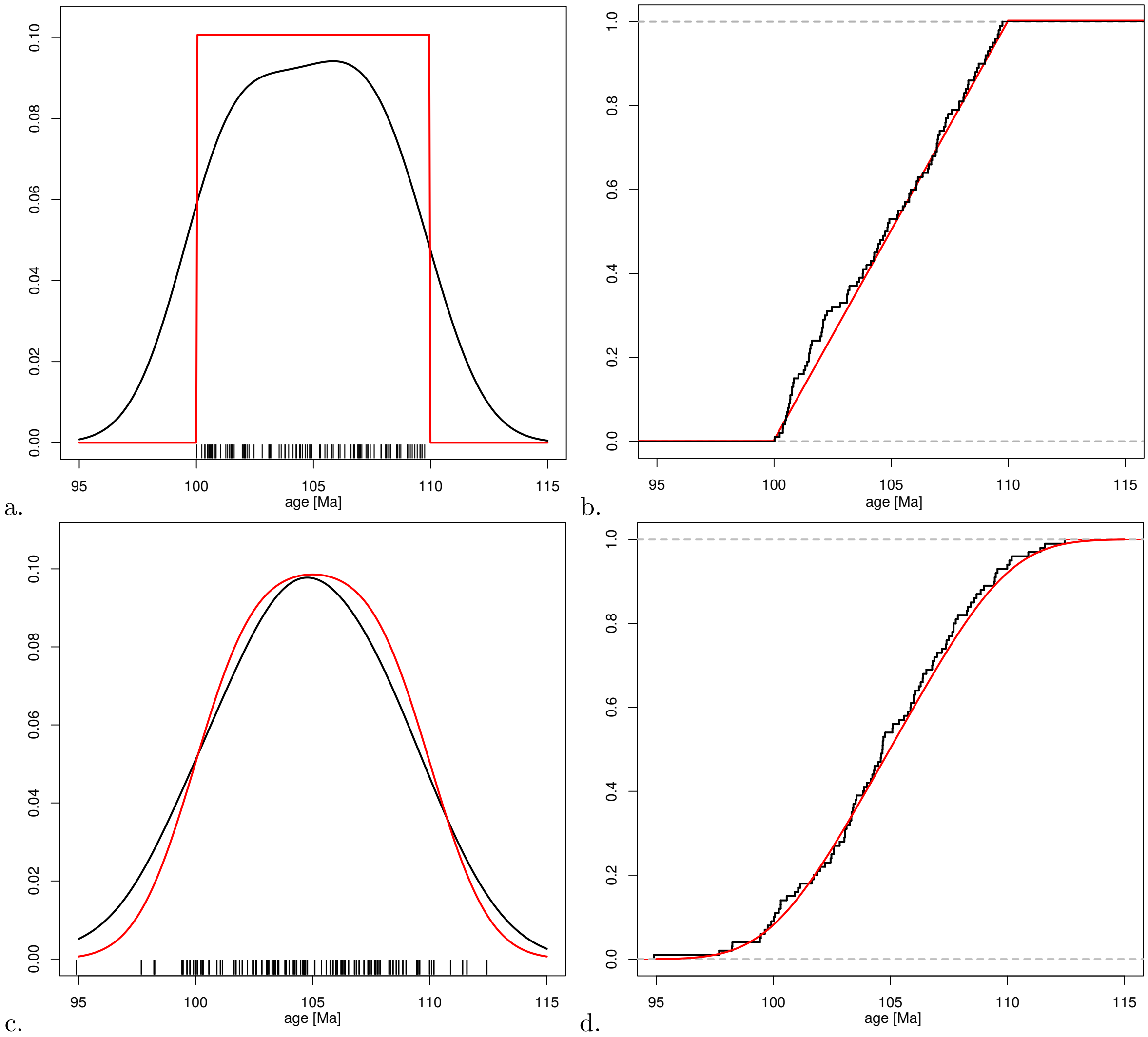

Figure 2: a. red – a uniform distribution between 100 and 110 Ma, black – a kernel density estimate (KDE) of 100 randomly selected values, which oversmooths the theoretical distribution; b. red – cumulative version of a., black – Cumulative Age Distribution (CAD) of the 100 random samples, which does not oversmooth the theoretical curve; c. red – theoretical sampling distribution in the presence of normally distributed analytical uncertainties (σ=1), black – the KDE of 100 random samples which again oversmooth the theoretical curve; d. red – the cumulative measurement distribution, black – the CAD of the 100 randomly selected measurements is an unbiased estimator of the theoretical distribution.

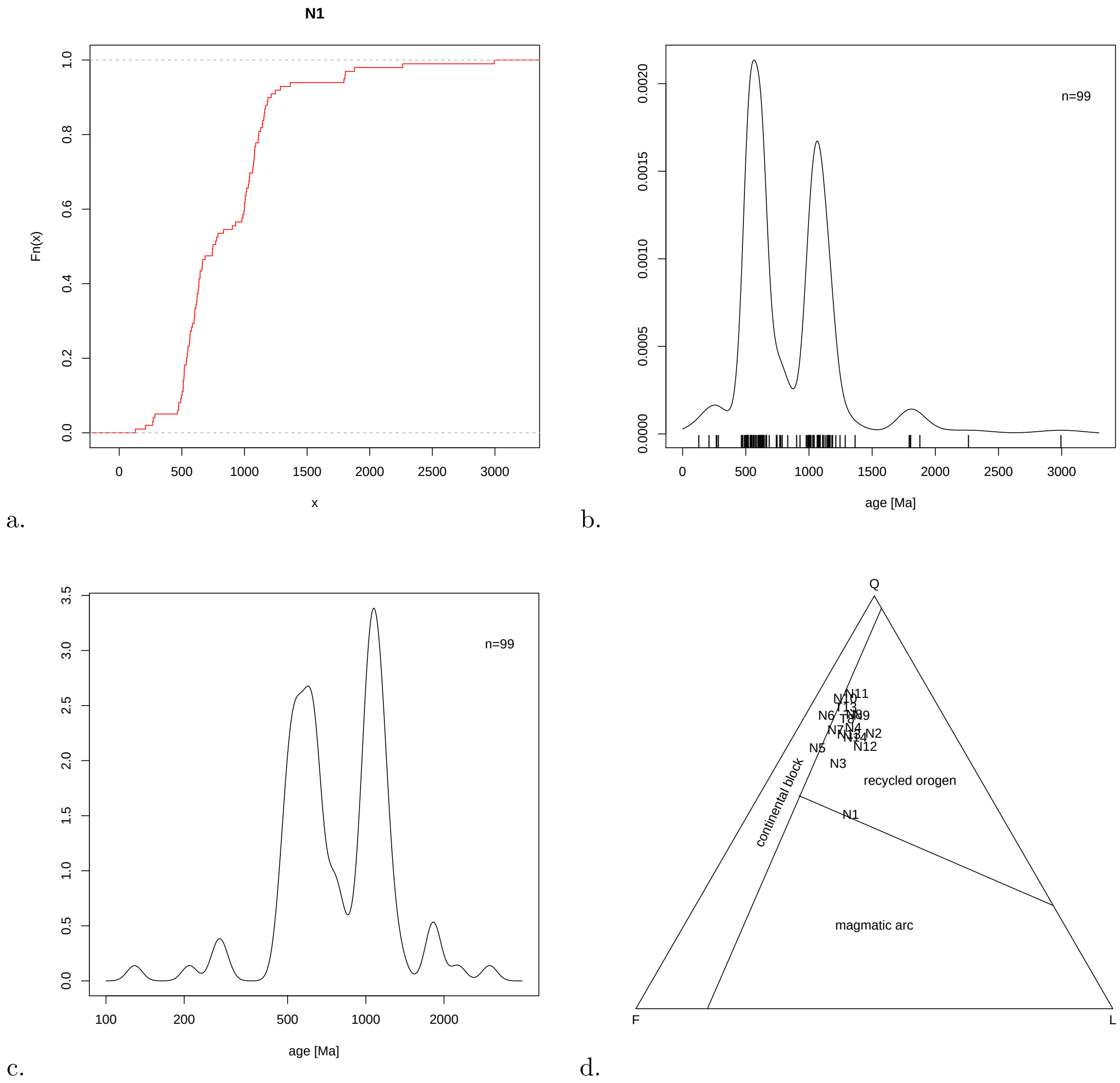

Figure 3: Graphical output generated by `provenance` for `distributional` and `compositional` data. a. the CAD of sample N1; b. the KDE of sample N1, using a the hybrid adaptive bandwidth algorithm outlined in Section 3.2, plotted on a linear scale; c. a KDE using a fixed bandwidth of 50 Ma and a log scale; d. the quartz - feldspar - lithic composition of the Namib samples on Dickinson et al. (1983)'s QFL diagram.

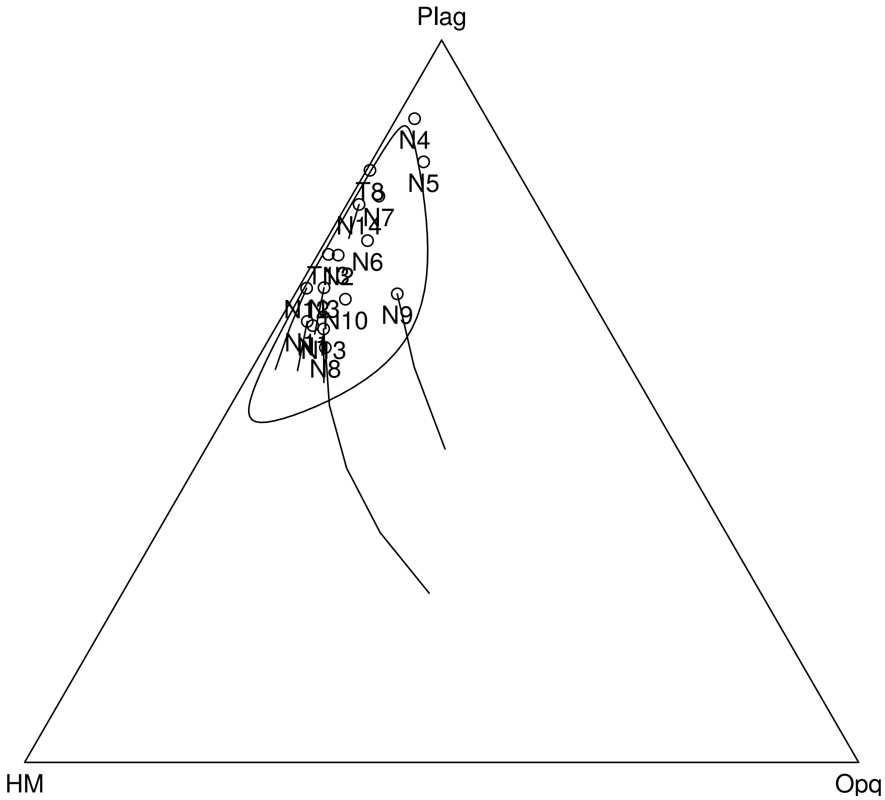

Figure 4: The effect of the Source Rock Density (SRD) correction on the Namib dataset, shown on a ternary diagram with P = plagioclase ($\rho = 2.67$ g/cm^3), HM = heavy minerals ($\rho = 3.5$ g/cm^3), and Opq = opaque minerals ($\rho = 5$ g/cm^3). Circles mark the restored compositions, lines connect the intermediate values of the SRD correction algorithm. It is evident that samples N8 and N9 are most strongly affected by hydraulic sorting and benefit from the SRD correction the most. The ellipse was drawn using the `compositions` package's `ellipses` function.

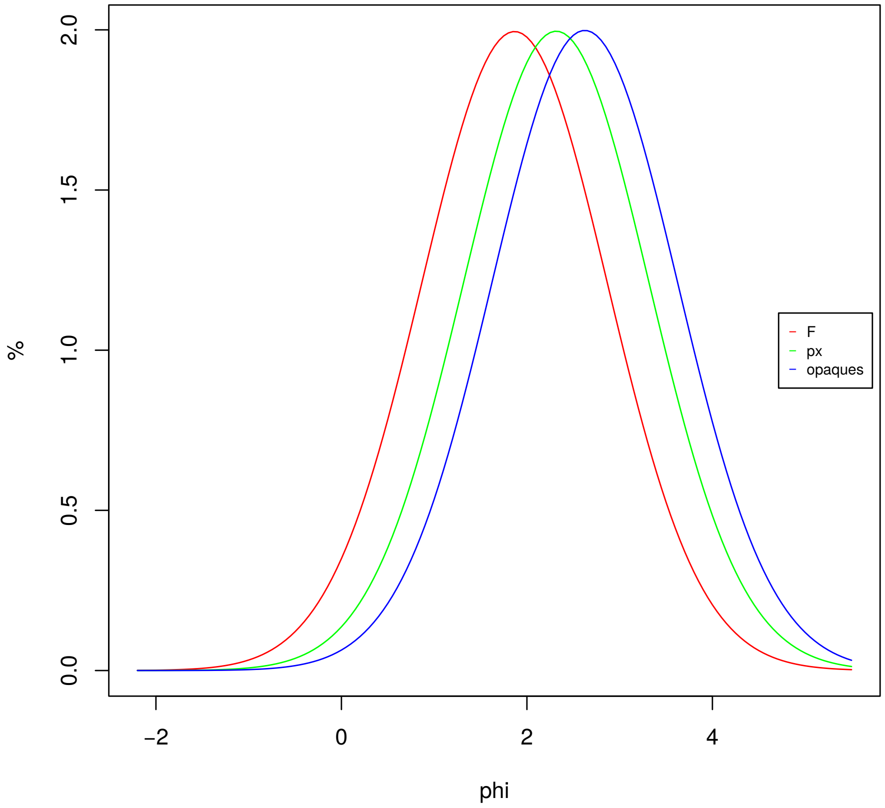

Figure 5: Graphical output of the `minsorting` routine applied to an ophiolitic end-member composition. Different colours show the inferred grain-size distribution of feldspars ('F', red), pyroxene ('px', blue) and opaque minerals (green) in Krumbein's Φ units, assuming a mean grain size for the bulk sediment of Φ=2 with standard deviation Φ=1. It can be seen that relatively coarse grains of the comparatively light minerals are hydraulically equivalent with finer grains of the dense minerals.

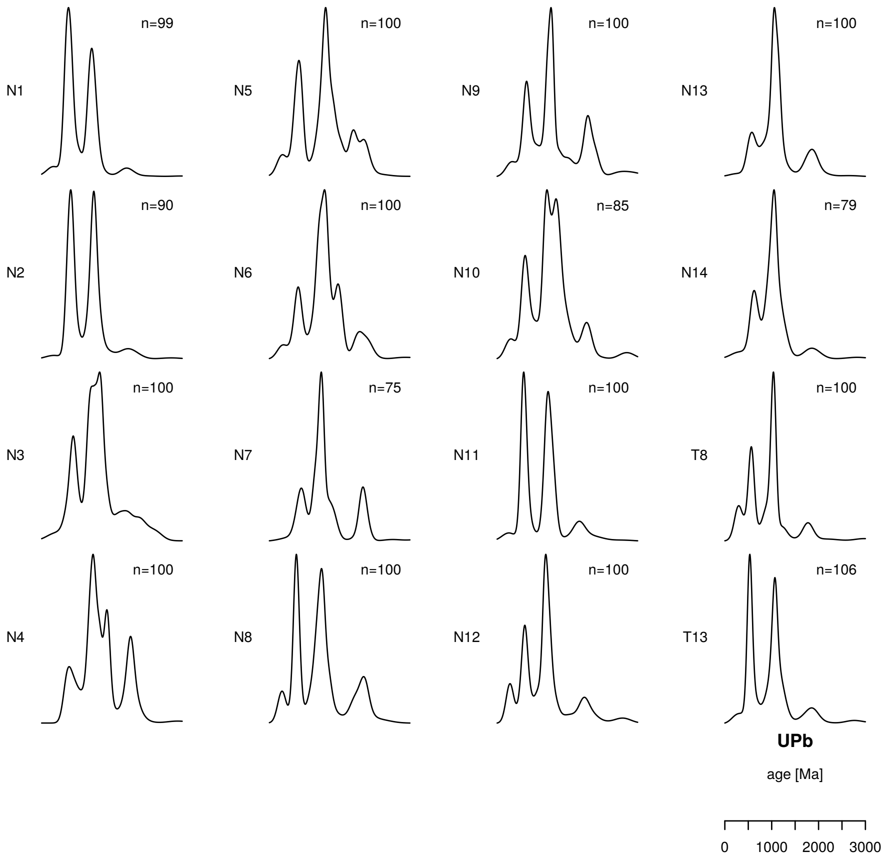

Figure 6: Graphical output of the `summaryplot` function, applied to the detrital zircon U-Pb age data. The areas under the KDEs have been normalised to the same value.

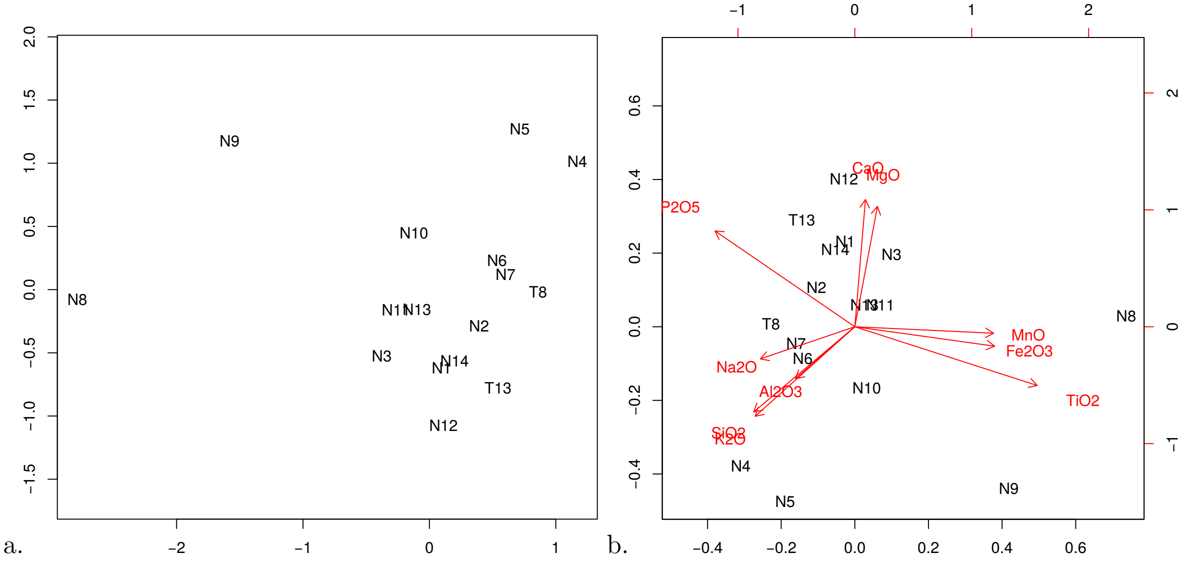

Figure 7: Illustration of the equivalence of Multidimensional Scaling (MDS, a) and Principal Component Analysis (PCA, b) for compositional data using the Aitchison dissimilarity, using the major element composition of the Namib samples as an example. The two configurations are identical apart from an arbitrary rotation.

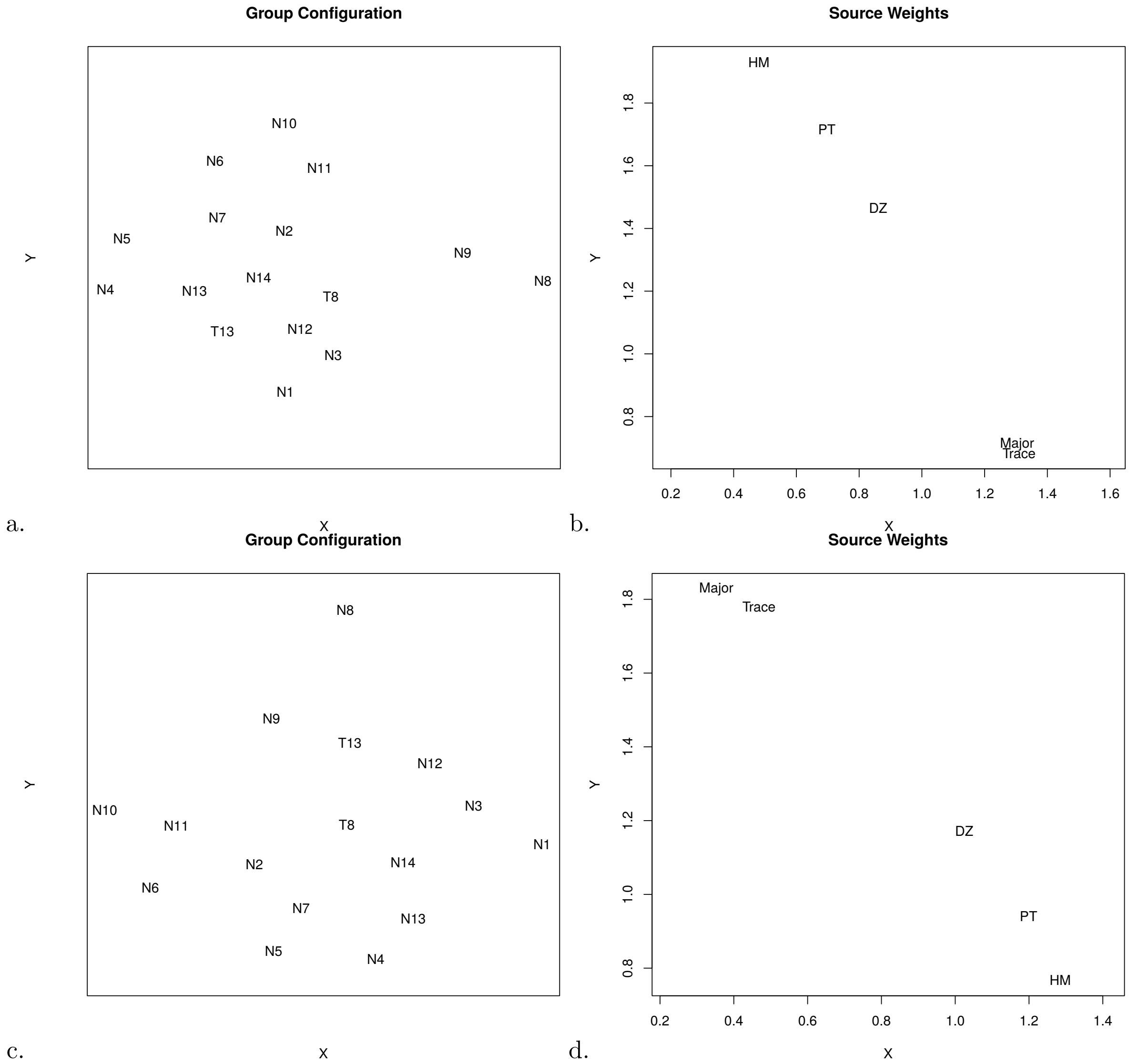

Figure 8: a. group configuration of an INDSCAL analysis of the Namib dataset using the Kolmogorov-Smirnov dissimilarity for the U-Pb data (DZ), the Bray-Curtis dissimilarity for the heavy mineral (HM) and bulk petrography (PT) data, and the Aitchison distance for the major and trace element compositions; b. the source weights, which show the relative importance which each of the five provenance proxies attach to the horizontal and vertical axis of the group configuration (Vermeesch and Garzanti, 2015); note that samples N8 and N9 plot on the far right of the group configuration, indicating that they have significantly different Major and Trace element compositions. This is consistent with these samples being affected by hydraulic sorting, as was previously shown in Figure 4. c. the group configuration of the same data, but using the Sircombe-Hazelton dissimilarity for the U-Pb data, and the Bray-Curtis dissimilarity for the major and trace compositions; d. the correponding source weights. Although the two configurations look very similar, the actual weights attached to each of the proxies are very different.