





Multidimensional Scaling of Varietal Data in Sedimentary Provenance Analysis

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Special Section:

Controls and Biasing Factors in Sediment Generation, Routing, and Provenance: Models, Methods, and Case Studies

Key Points:

- Varietal data are defined as lists of compositional tables
- Given an appropriate dissimilarity measure, varietal data can be subjected to multidimensional scaling
- This paper introduces three ways to quantify the pairwise dissimilarity of varietal data

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Abstract Varietal studies of sedimentary provenance use the properties of individual minerals or mineral groups. These are recorded as lists of numerical tables that can be difficult to interpret. Multidimensional Scaling (MDS) is a popular multivariate ordination technique for analyzing other types of provenance data based on, for example, detrital geochronology or petrography. Applying MDS to varietal data would allow them to be treated on an equal footing with those other provenance proxies. MDS requires a method to quantify the dissimilarity between two samples. This paper introduces three ways to do so. The first method (“treatment-by-row”) turns lists of (compositional) data tables into lists of vectors, using principal component analysis. These lists of vectors can then be treated as “distributional” data and subjected to MDS analysis using dissimilarity measures such as the Kolmogorov-Smirnov statistic. The second method (“treatment-by-column”) turns lists of compositional data tables into multiple lists of vectors, each representing a single component of the varietal data. These multiple distributional data sets are subsequently subjected to Procrustes analysis or 3-way MDS. The third method uses the Wasserstein-2 distance to jointly compare the rows and columns of varietal data. This arguably makes the best use of the data but acts more like a “black box” than the other two methods. Applying the three methods to a detrital titanite data set from Colombia yields similar results. After converting varietal data to dissimilarity matrices, they can be combined with other types of provenance data, again using Procrustes analysis or 3-way MDS.

Plain Language Summary The source of modern or ancient sediment can be determined by examining either the overall characteristics of the sediment or the chemical composition of individual sediment particles. With the help of recent analytical advancements, geologists can now analyze the complete chemical makeup of single grains of sand or silt. These types of data sets, known as “varietal” data sets, have the ability to uncover differences between sediments that are not visible through traditional methods. However, varietal data are incompatible with the statistical methods that geologists typically use to determine the origin of sediment. This paper addresses this issue by presenting three methods for quantifying the differences between varietal data sets, which is a crucial step in any further statistical analysis. Testing these methods on a varietal data set from Colombia shows similar outcomes. By using the techniques described in this paper, varietal data can now be combined with other conventional methods for determining sediment origin.

1. Introduction

Multidimensional Scaling (MDS; Kruskal & Wish, 1978; Shepard, 1980; Vermeesch, 2013) is a multivariate ordination technique that has gained considerable popularity in recent years as a method to interpret large data sets in sedimentary provenance analysis (Vermeesch, 2013). Given a table of pairwise “dissimilarities” between samples, MDS produces a lower (typically two-) dimensional “map” in which similar samples plot close together and dissimilar samples plot far apart. MDS can be applied to a wide variety of different provenance proxies by choosing an appropriate dissimilarity measure. Vermeesch (2019) distinguishes between three different types of provenance data, each of which is associated with a specific database format (Figure 1):

1. *Distributional data* such as detrital zircon U-Pb ages can be stored in *lists of decimal numbers*, where each list represents a sample and typically contains a different number of values (i.e., single grain ages). Two samples can be compared using the Kolmogorov-Smirnov distance or related nonparametric statistics (Vermeesch, 2018a). The resulting dissimilarity matrix fulfills the metric requirements and is therefore suitable for both classical and nonmetric MDS (Vermeesch, 2013).

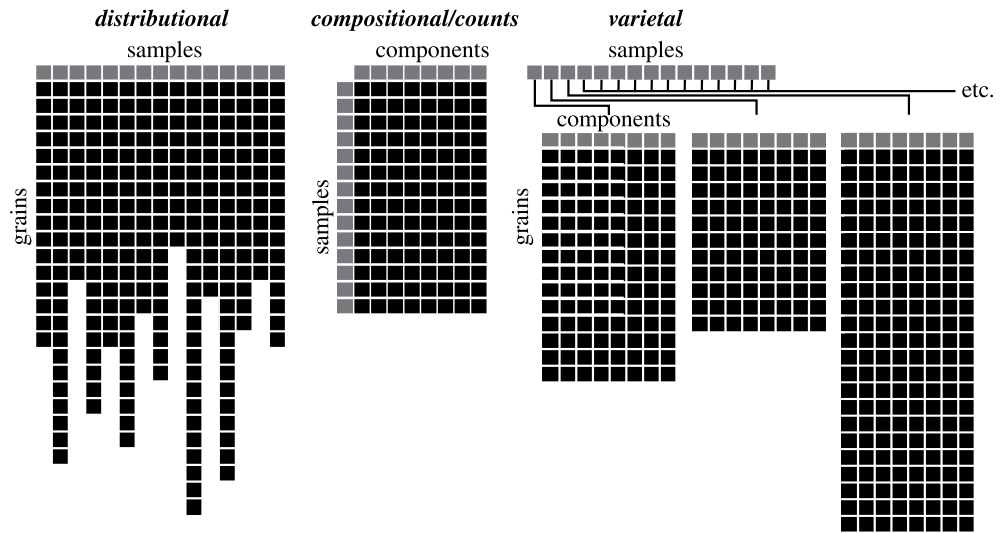


Figure 1. Schematic representation of the four classes of provenance data. Gray boxes represent labels and black boxes numbers. Distributional data can be stored as lists of vectors, compositional data as tables of positive decimal numbers, count data as tables of nonnegative integers, and varietal data as lists of tables with positive decimal numbers.

2. *Compositional data* such as the major and trace element compositions of bulk samples are stored in *tables of decimal numbers*, in which the rows represent samples and the columns represent components such as elements or isotopes. Pairwise comparison of the samples (rows) is best done using the Aitchison distance, which corresponds to a Euclidean distance of centered log ratios (Aitchison, 1986). It can be shown that, in this case, (classical) MDS is mathematically equivalent to Principal Component Analysis (PCA; Vermeesch, 2013). The advantage of PCA over plain MDS is that it provides two sets of coordinates: one representing the rows and one representing the columns of the input data. This feature will be used in Section 3 of this paper.
3. *Count data* such as the petrography or heavy mineral composition of sediment are stored in *tables of integers*, in which rows correspond to samples and columns to lithologies or minerals. Pairwise comparison of samples of count data can be done using the Chi-square distance, which can handle zero values, unlike the Aitchison distance (Vermeesch, 2018b). It can be shown that MDS of Chi-square distance tables is equivalent to Correspondence Analysis (CA, Greenacre, 1984). Like PCA, CA also yields coordinates for the row and columns of the data tables, but these will not be discussed further here.
This paper adds a fourth class of data to this list:
4. *Varietal data* capture the variations in optical or chemical properties shown by an individual mineral or mineral group (Morton, 1985, 1991). This paper will focus on chemical properties, as measured by micro-analytical techniques such as electron, laser, or ion microprobe analysis. These data can be stored in *lists of compositional data tables*. Each table in a varietal data set contains the same number of columns (representing elements or isotopes) and a different number of rows (representing individual analyses in a sample).

Unlike distributional, compositional and count data, varietal data have hitherto not been associated with a “natural” dissimilarity measure. It is therefore not clear how varietal data can be analyzed by MDS. This is unfortunate because the complex structure of varietal data makes the need for multivariate ordination all the more pressing. This paper addresses this issue by proposing three mechanisms to compare varietal data (Sections 2–4). With these mechanisms in place, varietal data can be treated on an equal footing with other types of provenance data. Section 5 shows how varietal data can be combined with distributional, compositional, and count data using 3-way MDS and Procrustes analysis.

The methods discussed in this paper are illustrated with a data set from Colombia's Sierra Nevada de Santa Marta (SNSM). This data set comprises 17 samples of modern river sediment, characterized by 12 different provenance proxies, including three distributional data sets (detrital zircon, apatite, and titanite U-Pb ages); four compositional data sets (major and trace element composition of the sand and clay fraction); two data sets of counts (petrography and heavy minerals); and three varietal data sets (trace element compositions of detrital zircon, apatite, and titanite). The geological details of the data set are not relevant to the present discussion and are only

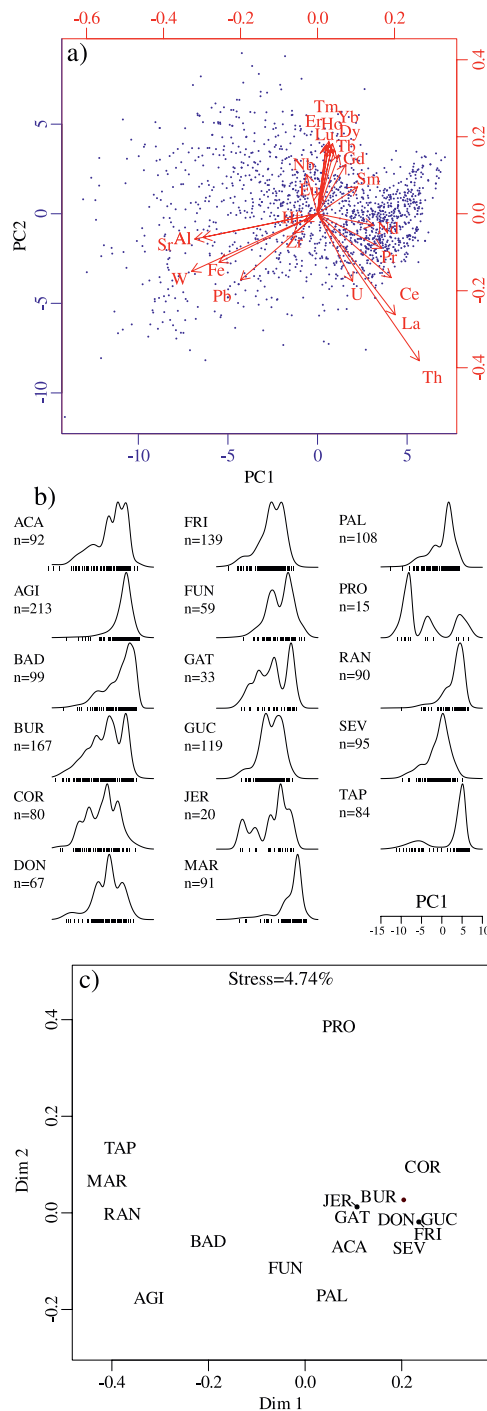


Figure 2. (a) Principal Component Analysis biplot of the pooled titanite geochemistry data. The blue dots mark 1,571 titanite analyses, which belong to 17 samples. (b) Kernel density estimates (bandwidth = 0.8) of the first principal component (PC1) of the 17 samples; (c) Nonmetric Multidimensional Scaling (MDS) configuration of the 17 PC1 distributions, using the Kolmogorov-Smirnov statistic as a dissimilarity measure. MDS coordinates are located in the middle of the plot labels. The Kruskal Stress value suggests a “good” fit.

briefly mentioned in this paper. The reader is referred to a separate paper for further details about the field setting (Hatzenbühler et al., 2022).

2. Method 1: Treatment by Row

As explained in Section 1, varietal data are, in essence, lists of compositional data tables. Compositional data can be compared using the Aitchison distance and subjected to PCA. The dimension-reducing properties of PCA can be used to turn a varietal data set into a distributional data set:

1. Pool all the samples together to create one large compositional data set, that is, a single table in which each row represents an analysis and each column represents an element or isotope.
2. Subject this data table to compositional PCA (Aitchison, 1983). Return the first principal component, which accounts for the largest proportion of the overall variance, and discard the other principal components.
3. Parse the first principal component vector into different samples. This results in a list of vectors or, in other words, a distributional data set. This can then be analyzed by MDS with the usual Kolmogorov-Smirnov statistic.

Figure 2 applies the treatment-by-row strategy to the titanite chemistry data from the SNSM. Figure 2a shows the first two principal components of the pooled titanite compositions on a biplot. Only the first of these components (PC1) is used for subsequent distributional analysis. It is dominated by Pb, Fe, W, Sr, and Al, which are associated with negative loadings (red arrows in Figure 2a), and the light lanthanides (La, Ce, Pr, and Nd) and actinides (U and Th), which are associated with positive loadings. PC1 accounts for 51% of the total variance among the 25 components. This means that 49% of the variance is discarded, including the 19% that is associated with PC2. It is a sacrifice that is needed to turn the varietal data set into a distributional one.

The distributions of PC1 are shown as kernel density estimates (KDEs) in Figure 2b. It is the shapes of these distributions that are used as a secondary provenance proxy. Inspecting the KDEs by eye shows some clear groupings. Samples TAP, MAR, RAN, and AGI are all characterized by sharp unimodal PC1 distributions that are dominated by positive values, which suggest that these samples are enriched in rare earth elements relative to Pb, Fe, W, and Al. In contrast, samples such as SEV, GUC, COR, and FRI are characterized by broader PC1 distributions that are shifted toward more negative values. This suggests that these samples are enriched in Pb, Fe, W, and Al relative to the rare earths in comparison with samples SEV, GUC, COR, and FRI.

A more objective comparison of the PC1 distributions is achieved by MDS analysis, using the KS-statistic (Figure 2c). As expected, samples SEV, GUC, COR, and FRI cluster closely together on the MDS map, opposite to samples MAR, TAP, AGI, and RAN. This grouping makes geological sense, as SEV, GUC, COR, and FRI were collected from river catchments that drain metamorphic lithologies (migmatite, gneiss, and metadiorite), whereas samples MAR, TAP, AGI, and RAN were collected from catchments that drain igneous lithologies (Hatzenbühler et al., 2022).

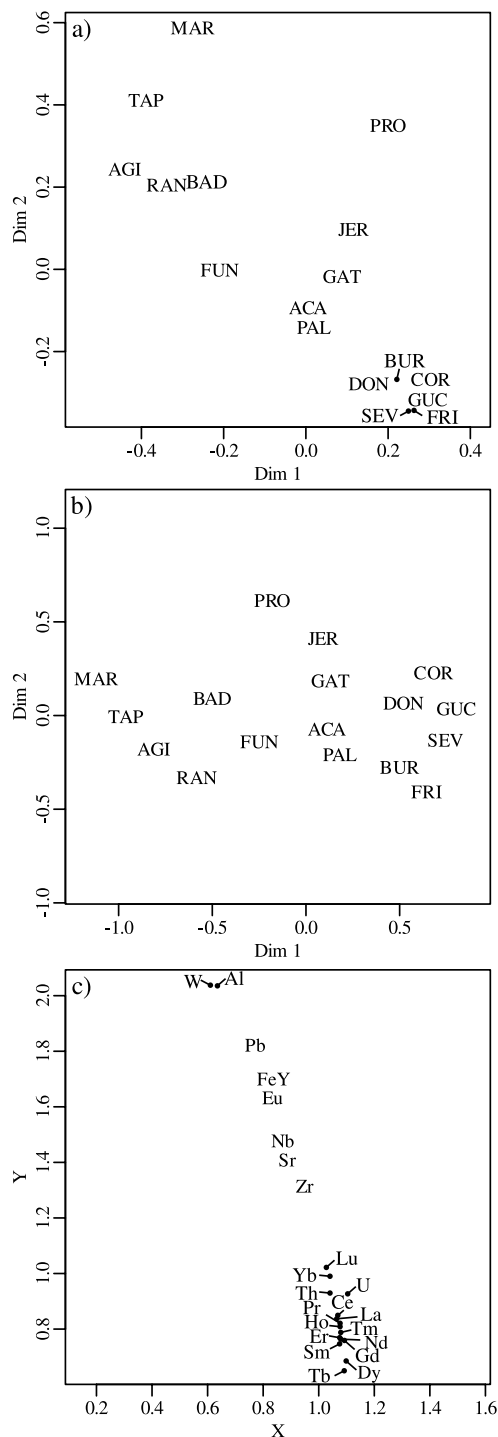


Figure 3. (a) Procrustes analysis of the 25 Multidimensional Scaling (MDS) configurations that are obtained by breaking the titanite chemistry data up into 25 distributional data sets; (b) Group configuration of a 3-way MDS analysis of the 25 dissimilarity matrices extracted from the same titanite geochemistry data set; (c) Source weights of the 3-way MDS analysis, showing the stretching factors that are associated with each of the 25 components. These can be combined with the group configuration to yield 25 “private spaces” (Arabie et al., 1987; Vermeesch & Garzanti, 2015).

3. Method 2: Treatment by Column

The treatment-by-row approach turns the varietal data into a single distributional data set. An alternative approach is to turn it into multiple distributional data sets:

1. Break the compositional data table of each sample up into its components (columns) and treat each of these components as a distributional data set. In other words, a varietal data set comprising n samples and m components (e.g., elements) can be turned into m distributional data sets containing n samples (each in turn containing a variable number of analyses).
2. Compute the dissimilarity matrices of all the distributional data sets and stack them together to form a multidimensional array of size $n \times m \times m$.
3. Subject the stack of dissimilarity matrices to Procrustes analysis or 3-way MDS (Carroll & Chang, 1970; Gower, 1975; Vermeesch & Garzanti, 2015). For Procrustes analysis, this produces a similar set of coordinates as Method 1. For 3-way MDS, it produces two sets of coordinates: one for the rows (samples) and one for the columns (components). In this respect, 3-way MDS is somewhat similar to PCA.

Applying the treatment-by-column approach to the SNSM data, Figure 3a shows the output of a Generalized Procrustes Analysis GPA (Gower, 1975). It uses affine transformations to obtain a single set of coordinates from the 25 compositional MDS configurations. The results in Figure 3a look remarkably similar to the MDS configuration of Figure 2c despite the completely different mechanism behind it. In both cases, samples SEV, GUC, COR, and FRI cluster closely together in an opposite corner from samples MAR, TAP, AGI, and RAN. The only major difference between the MDS (Figure 2c) and GPA (Figure 3a) configurations is the 45° clockwise rotation of the latter with respect to the former. This is expected since GPA is rotation invariant.

One limitation of GPA is the fact that all compositional information is lost in the visualization. This issue is addressed by 3-way MDS, as shown in Figures 3b and 3c. Together, these two pieces of graphical output display both the row names and the column names of the varietal data set. The “group configuration” of the samples (Figure 3b) is similar to the output of the GPA and (2-way) MDS configurations of Figures 2c and 3a: once again, samples SEV, GUC, COR, and FRI plot separately from samples MAR, TAP, AGI, and RAN. However, the 3-way MDS configuration (Figure 3b) is less similar to the GPA configuration (Figure 3a) than the GPA configuration is to the 2-way MDS analysis (Figure 2c).

The great appeal of 3-way MDS lies in the combination of the group configuration with the source weights, which are shown in Figure 3c. These weights show the relative importance that the two dimensions of the group configuration attach to the 25 compositional variables. Pb, Fe, W, and Al plot at the upper left end of the subject weights. They are associated with light horizontal weights (x -coordinates of 0.7–0.8) and heavy vertical weights (y -coordinates of 1.7–2.0). The rare earth elements (except Eu) plot at the opposite end of the subject weights and are associated with comparatively heavy horizontal weights (x -coordinates of 1.0–1.1) and light vertical weights (y -coordinates of 0.7–1.0). Note that the grouping of the elements is in good agreement with the loadings of the first principal component (Figure 2a).

The weights tell us that the horizontal dimension (Dim 1) of the group configuration (Figure 3b) is controlled by variability in the rare earth composition, whereas the vertical direction (Dim 2) is controlled by variability in the Pb, Fe, W, and Al concentrations.

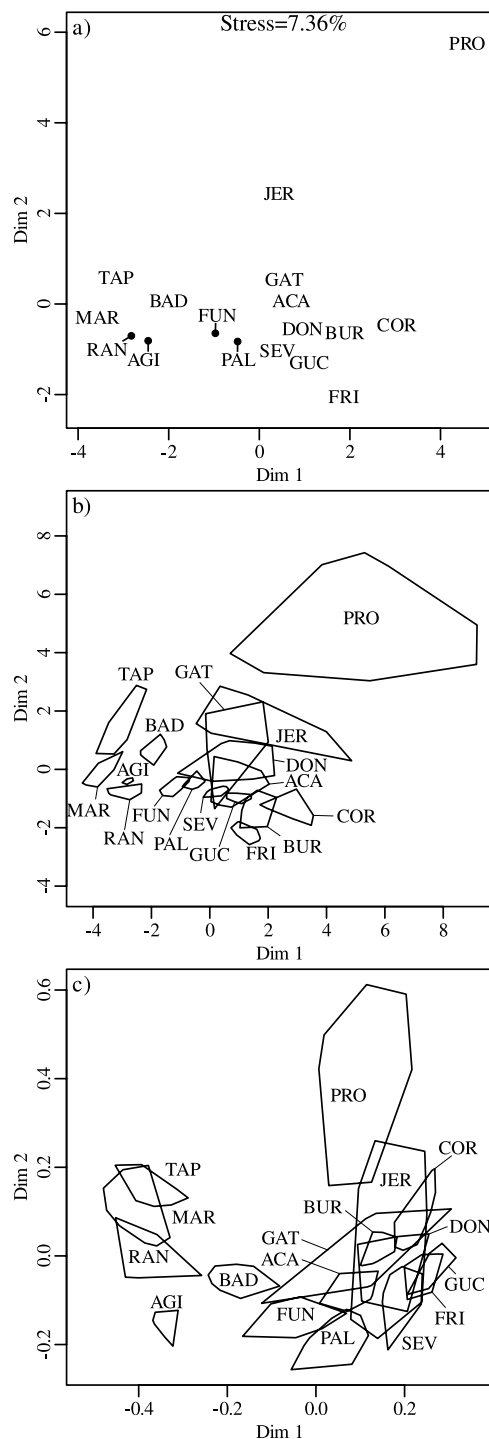


Figure 4. (a) Nonmetric Multidimensional Scaling (MDS) configuration of the titanite data using the Wasserstein-2 distance (method 3). Although the Kruskal Stress value is higher than for Figure 2a, this does not necessarily mean that the configuration is less informative than that of method 1. The higher stress values just means that it was more difficult for the MDS algorithm to fit the dissimilarity matrix to a 2-dimensional configuration of points. The fit still qualifies as “good.” (b) Uncertainty regions of the MDS configuration, obtained by constructing the convex hull of 20 bootstrapped replicates of each sample. (c) Bootstrapped uncertainty regions for the treatment-by-row results of Figure 2c.

4. Method 3: Wasserstein-2 Distance

Thus far we have seen how varietal data can be turned into distributional data, either by treating the compositions of each sample by row (method 1, Section 2) or by column (method 2, Section 3). In this Section, rows and columns will be treated jointly, using the principles of optimal transport (OT). OT is a burgeoning field of mathematics that is concerned with the constrained allocation of limited resources to achieve the greatest effect (Villani, 2021).

The “Wasserstein- p ” distance (W_p) is a key concept in the field of OT. A classical metaphor for the W_p -distance is the minimum amount of work that needs to be done to transform a pile of earth into a different pile of earth with the same volume but different location and shape. Based on this analogy, the W_p -distance is also known as the “earth mover’s distance.” Distributional data can be treated as 1-dimensional “piles of earth.” In this case, the W_1 -distance between two samples simply equates to the area between their respective empirical cumulative distribution functions (ECDFs):

$$W_p(A, B) = \left(\int_0^1 |F_A^{-1}(x) - F_B^{-1}(x)|^p dx \right)^{\frac{1}{p}} \quad (1)$$

where A and B are two distributional data sets, F_A and F_B are their respective ECDFs, and F_A^{-1} and F_B^{-1} are the corresponding quantile functions. The W_2 -distance is slightly less intuitive than the W_1 -distance but is nevertheless preferred because it mathematically behaves like a Euclidean distance. The W_1 and W_2 distances fulfill the metric requirements and can therefore be subjected to both classical and nonmetric MDS.

Lipp and Vermeesch (2022) show that the W_2 -distance produces results that are often equivalent and sometimes better than those obtained by the KS-statistic. Thus, we could substitute the KS-statistic for the W_2 -distance in Sections 2 and 3. Alternatively, it is also possible to apply the W_2 -distance directly to the varietal data, without conversion to distributional data, by generalizing Equation 1 from one to two dimensions:

$$W_p(A, B) = \left(\min_{\pi \in \Pi} \int c(x, y)^p d\pi(x, y) \right)^{\frac{1}{p}} \quad (2)$$

where π is the “transport plan,” that is, a probability distribution (a member of the function space Π) in which $d\pi(x, y)$ is the amount of material that is transported from location x to y ; and $c(x, y)$ is the “cost” associated with this transport. Given two compositional tables (X_A and X_B , say) of size $n_A \times m$ and $n_B \times m$, respectively the “cost matrix” is obtained by computing the Aitchison distance between each row of table X_A and each row of table X_B . This results in a matrix of size $n_A \times n_B$. The OT plan is obtained from this cost matrix by linear programming (Villani, 2021), the principles of which go beyond the scope of this paper.

Computing the W_2 -distance for all sample pairs in a varietal data set yields a square dissimilarity matrix that can be analyzed by MDS. For the SNSM titanite data set, this yields a configuration that looks broadly similar to the results obtained by methods 1 and 2 (Figure 4). Notable exceptions are samples PRO and JER, which are significantly further removed from the bulk of the data set than they are in Figures 2c, 3a, and 3b. This behavior is likely a consequence of the small number of analyses in these two samples (20 for JER and 15 for PRO, see Figure 2b), as confirmed by the uncertainty regions

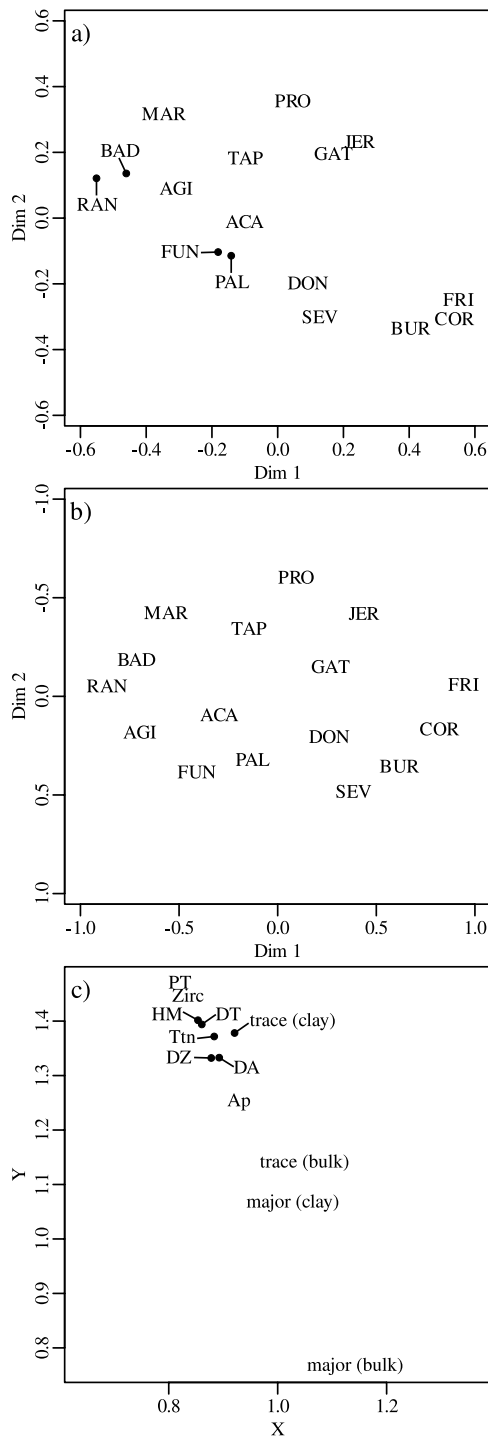


Figure 5. (a) Procrustes analysis and (b) group configuration of a 3-way Multidimensional Scaling (MDS) analysis of the 12 provenance proxies from the Sierra Nevada de Santa Marta, using method 3; (c) the source weights of the 3-way MDS analysis. DA, DT, and DZ stand for U-Pb age distributions of detrital apatite, titanite, and zircon, respectively; Ap, Ttn, and Zirc for the varietal apatite, titanite, and zircon data; PT and HM for petrography and heavy minerals; and major and trace for the chemical composition of the bulk sediment and clay fractions.

of Figure 4b, which correspond to the convex hull of 20 bootstrapped replicates for each sample. Repeating the same procedure for method 1 produces uncertainty regions that are, on average, larger than for method 3 but more uniform in size. This suggests that the “treatment-by-row” approach is less precise than the Wasserstein approach, but also less “heteroscedastic”.

The advantage of method 3 over the other two methods is that it makes full use of the entire data set, including any covariance structure that may be embedded therein. The disadvantage is that the compositional information is lost in the process of calculating the cost matrix. Therefore, method 3 acts more like a “black box” than method 1 and certainly more than method 2.

5. Combining Varietal Data With Other Provenance Proxies

Section 3 showed how Procrustes analysis and 3-way MDS can be used to combine multiple dissimilarity matrices together and extract a single configuration of samples from them. The same techniques can also be used to combine varietal data with other provenance proxies. In principle, this can be done using any of the three methods. However, in practice, methods 1 and 3 are the most sensible choices for the following reason.

There are 12 provenance proxies in the SNSM data set, including three varietal data sets, where the titanite, apatite, and zircon compositions comprise 25, 22, and 8 compositional variables, respectively. Using methods 1 or 3, each varietal data set yields its own dissimilarity matrix so that the entire multi-proxy data set involves 12 dissimilarity matrices. In contrast, using method 2 would yield $14 + 25 + 22 + 8 = 69$ dissimilarity matrices. This would cause several problems. First, fitting 69 matrices would be computationally difficult. Second, any 3-way MDS results would be difficult to interpret as the map of source weights would be overcrowded. Third, model 2 would give excessive weight to the varietal data compared to the other provenance proxies, with the titanite compositions being represented 25 times.

Although both methods 1 and 3 are viable ways to combine varietal data with other types of provenance data, method 3 is arguably the most sensible option. This is because its main disadvantage (namely the limited interpretability of the resulting MDS configurations) is nullified by the fact that the MDS configurations are not actually presented in the Procrustes map or the 3-way MDS configuration.

Figure 5a presents the results of Procrustes analysis for the combined SNSM data set, in which each varietal data set was subjected to method 3. It represents 12 multivariate data sets in a single scatterplot that shares many characteristics with the MDS plots of the titanite data set alone. Once again, samples SEV, COR, and FRI plot in close vicinity to each other and separately from samples MAR, TAP, AGI, and RAN. Note that sample GUC is missing from the Procrustes configuration. That is because this sample is missing from the data set of major element concentrations in clay.

Although the Procrustes map effectively summarizes the salient similarities and differences between the samples in the full SNSM data set, it does not provide any clues as to what causes these differences. The output of the 3-way MDS analysis addresses this issue. Figure 5b shows the group configuration. It fulfills a similar role to the Procrustes map of Figure 5a and has a similar appearance. However, the clustering of the different samples is less distinct in the group configuration than it is in the Procrustes map.

Figure 5c shows the source weights of the 12 provenance proxies. It reveals that samples that are separated along the horizontal dimension (such as FRI and RAN) have different bulk compositions and similar distributional and varietal characteristics. In contrast, samples that are separated along the vertical dimension have comparatively similar bulk compositions but differ in their distributional and varietal provenance proxies. One possible interpretation of these trends is that the horizontal dimension is controlled by lithology, whereas the vertical dimension is controlled by the geological evolution of the source terrane(s).

6. Implementation in ‘provenance’

All the algorithms described in this paper have been implemented in a free and open R package called `provenance` (Vermeesch et al., 2016). `Provenance` comes with a query-based user interface that does not require any knowledge of R. The following paragraphs, however, will focus on the command line interface. Version 4.1 of the package adds a new `varietal` data class, which can be populated from a `.csv` input file using the `read.varietal` function:

```
library(provenance)

Ttn <- read.varietal(fname="Ttn_chem.csv", snames=3)
```

where `Ttn_chem.csv` is a compositional data table containing the concatenated compositions of all the samples. The column names of this table specify its components, whereas the row names consist of an alphanumeric prefix corresponding to the sample name, followed by a unique identifier for each analysis. The `sname` argument either specifies a vector of prefixes or the length of the prefix. The output of the `read.varietal` function consists of a list containing the input table, a vector of sample names (in this case the prefixes extracted from the row names), the name of the data set, and the dissimilarity measure (KS for Kolmogorov-Smirnov by default). The `varietal` data object can be passed on to several other functions of the `provenance` package. To subject the `varietal` data to (2-way) MDS using method 1 (treatment-by-row):

```
plot(MDS(Ttn, method="KS"))
```

where the output of the `MDS` function is nested as input in the overloaded `plot` function. To analyze the titanite chemistry data by method 2 (treatment-by-column), using Procrustes analysis:

```
plot(procrustes(Ttn))
```

and using 3-way MDS (Carroll & Chang, 1970, a.k.a. “Individual Differences Scaling” or INDSCAL):

```
plot(indscal(Ttn))
```

Method 3 requires linear programming, which is currently delegated to either the `transport` or `approxOT` package (Dunipace, 2021; Schuhmacher et al., 2022). Using the former:

```
plot(MDS(Ttn, method="W2", package="transport"))
```

To combine multiple provenance proxies by Procrustes analysis, for example, using titanite, apatite, and zircon chemistry (using method 3); titanite, apatite, and zircon U-Pb ages; heavy minerals and petrography; and the major and trace element compositions of the bulk sediment and clay fractions:

```
Ttn <- read.varietal(fname="Ttn_chem.csv", snames=3, method="W2")
Ap <- read.varietal(fname="Ap_chem.csv", snames=3, method="W2")
Zr <- read.varietal(fname="Zr_chem.csv", snames=3, method="W2")
DA <- read.distributional("DA.csv")
DT <- read.distributional("DT.csv")
DZ <- read.distributional("DZ.csv")
HM <- read.counts("HM.csv")
PT <- read.counts("PT.csv")
```

```
major_bulk <- read.compositional("Major_BULK.csv")
major_clay <- read.compositional("Major_CLAY.csv")
trace_bulk <- read.compositional("Trace_BULK.csv")
trace_clay <- read.compositional("Trace_CLAY.csv")
proc <- procrustes(Ttn, Ap, Zr, DA, DT, DZ, HM, PT,
                  major_bulk, major_clay, trace_bulk, trace_clay)
plot(proc)
```

Note that the dissimilarity measure (i.e., W_2) is added to the data by the `read.varietal` function, unlike the earlier example, which used the default KS method. Analyzing the same holistic data set by 3-way MDS:

```
plot(indscal(Ttn, Ap, Zr, DA, DT, DZ, HM, PT,
            major_bulk, major_clay, trace_bulk, trace_clay))
```

7. Conclusions

This paper introduced three different approaches to quantify the dissimilarity between different samples in varietal data sets. These approaches can be used to populate dissimilarity matrices, which can be analyzed by MDS.

Methods 1–3 produce reassuringly similar results for the titanite chemistry data of the SNSM. This suggests that even though the three methods each consider different parts of the data set, they all retain the key intersample similarities and differences. Comparable results are obtained for the other provenance proxies, which confirms that varietal data do carry a robust and reproducible provenance signature. The consistency of the results obtained from a single data set with the combined data set of all the provenance proxies further lends credence to the conclusions drawn from the multivariate ordination analyses.

In principle, method 3 is the most powerful of the three approaches because it directly converts varietal data to dissimilarity matrices and jointly considers all the compositional information that is stored in the varietal data. In contrast, methods 1 and 2 require the conversion of the varietal data to distributional data. Some information is lost in this additional step. For method 1, only the information contained in the first principal component is retained. For method 2, the connection between the various columns of the compositional data members of the varietal data structure is lost, including any constant sum constraint.

Despite these limitations, methods 1 and 2 also offer some advantages over method 3. Whereas the connection between the MDS configuration and the compositional data variables is lost in the process of calculating the Wasserstein-2 distance, this connection is partially retained in method 1 and nearly completely in method 2. Thus, the results of methods 1 and 2 are easier to verify and interpret than those of method 3.

For example, in the case of the titanite chemistry data from the SNSM, samples MAR and COR plot on opposite sides of the MDS configuration (Figure 4), and it is not immediately clear which compositional variables cause these differences. However, inspection of PC1 in method 1 (Figure 2a) or, more directly, the subject weights in method 2 (Figure 3c) reveals that these trends reflect differences in the W-Al-Pb-Fe versus actinides and light rare earth abundances.

At first glance, the Procrustes analysis (Figure 3a) does not seem to offer any advantage over 3-way MDS. However, it is useful to repeat the caveat that was previously raised by Borg and Groenen (2005), which is that the source weights of a 3-way MDS analysis are sensitive to noise and are not as stable as the user might wish. Thus it is important not to overinterpret the results of 3-way MDS.

Inspection of Figures 4b and 4c also suggests that the W_2 distance is more sensitive to small sample fluctuations than the KS-distance. This is clearest for samples PRO and JER, which contain only 15 and 20 titanite analyses, respectively. Although the W_2 results are, on average, more precise than the corresponding KS results, the difference in precision between small and large samples is greater for the W_2 -distance than the KS-distance. This explains the distant location of PRO and JER on the MDS configuration of Figure 4a.

The limitations of method 3 become less important when it is used to combine varietal data with other provenance proxies (Section 5). The full SNSM data set contains no fewer than 126,408 measurements, spanning 12 dimensions worth of information. It is impossible to capture the full richness of data sets like this in a few simple scatterplots such as Figure 5. However, the internal consistency of the SNSM results and their sensible geological interpretation suggest that the approaches described in this paper are capable of separating geologically meaningful signals from noise. Further applications will be needed to confirm if this applies in other geological settings as well.

Data Availability Statement

All the data and software introduced in this paper are publicly available on the Comprehensive R Archive Network (CRAN, <https://CRAN.R-project.org/package=provenance>) and on GitHub (<https://github.com/pvermees/provenance/>, <https://doi.org/10.5281/zenodo.7699060>). The raw data files can be found at <https://github.com/pvermees/provenance/tree/master/inst/SNSM/>.

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