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Using Fordisc software to assign obsidian artifacts to geological sources: Proof of concept

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ABSTRACT

In recent years, source provenance studies employing portable X-ray fluorescence (pXRF) technology have become commonplace in archaeology; however, they are not without critiques. Concerns center on the capability of instruments to produce valid results and researchers' abilities to accurately interpret those results and make correct source assignments. In this paper, we focus on the latter issue with a look towards statistical means of assigning artifacts to obsidian types using data provided by pXRF spectrometers. Using a sample of 677 obsidian artifacts from the northwestern Great Basin, we evaluate the ability of various approaches (principal components, cluster, and discriminant function analyses) to correctly assign artifacts to particular obsidian types. These multivariate methods generally work well to separate artifacts into different groups (i.e., obsidian types); however, they are less well-suited to assign individual artifacts to an obsidian source or type. We therefore tested the ability of the statistical program Fordisc, commonly used in forensic anthropology, to assign individual artifacts to specific geochemical obsidian sources or types. Our results indicate that Fordisc made accurate source assignments. Furthermore, because Fordisc provides probability values for different possible matches, it offers an advantage over other methods.

1. Introduction

Applications of portable X-ray fluorescence (pXRF) technology to address archaeological questions have increased dramatically in recent years and many academic institutions and cultural resource management (CRM) firms now possess units. Although relatively expensive to purchase, pXRF instruments offer numerous benefits: (1) a non-destructive method to determine trace elements; (2) the ability to conduct in-field analyses (important when artifacts may not be collected); (3) the ability to characterize large numbers of artifacts in a relatively short amount of time; and (4) the elimination of commercial lab fees (Shackley, 2011, 2012). Their rapid and widespread adoption by researchers lacking previous experience in geochemical characterization techniques has led some experienced analysts to express concern that some applications of pXRF technology have "no real foundation in science" (Shackley, 2012:2). Such concerns primarily center on issues related to *repeatability* (agreement between measurements collected under identical conditions at different times), *reproducibility* (agreement between measurements collected at different times under different conditions), *accuracy* (agreement between measurements collected using different instruments; for example, between pXRF and conventional wavelength-dispersive [WDXRF] and energy-dispersive [EDXRF] systems), and *validity* (the ability to collect and analyze data to differentiate raw material types and assign artifacts to those types) (Newlander et al., 2015).

In this paper, we focus on the latter topic – validity – and how trace element data may be used to assign artifacts to geologic sources of raw material. We briefly review the range of approaches that analysts may use when making source assignments. We then present a novel method of data analysis that draws from the subfield of forensic anthropology. In this approach, we use the computer program Fordisc to assign artifacts to obsidian types. Analysts typically use Fordisc to help in establishing the biological profile for a set of unknown skeletal remains. To the best of our knowledge, our study represents the first time that Fordisc has been used in a source provenance study. Fordisc is easy to learn and use, provides custom-order discriminant functions, allows flexibility in analyses, and generates probabilities for individual group assignment as well as model performance. Although our sample of artifacts is small and we recognize potential limitations to the approach, using Fordisc to make source assignments represents an improvement over, or alternative to, other means of comparing univariate and bivariate trace element data.

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2. Source provenance studies and source assignment practices

Source provenance studies are a routine component of many archaeological projects. Such studies use various techniques (e.g., XRF, neutron activation analysis, inductively coupled plasma mass spectrometry) to determine trace elements in artifacts (e.g., ceramics, obsidian and chert tools) and match their source profiles or signatures to those of geologic sources of raw material (e.g., clay, temper, stone and glass outcrops). Source provenance data help researchers calculate the distances and directions that artifacts (or the raw materials used to produce them) were conveyed. In turn, this information is used to interpret how and where prehistoric populations traveled (e.g., Jones et al., 2003; Shackley, 1990, 1996, 2002; Smith, 2010), how groups organized their lithic technology (e.g., Smith et al., 2013), and whether raw materials were obtained via exchange or procured directly (e.g., Beck and Jones, 2011; Kelly, 2011; King et al., 2011).

There are a number of ways that researchers can compare and correlate trace element data collected from artifacts and geologic sources. The simplest is to analyze elemental data one variable at a time to identify similarities and differences between source samples and an artifact. However, these univariate methods may result in the misclassification of an artifact's source (Glascock et al., 1998). An improvement is to compare two variables at a time, typically through the use of graphical methods (e.g., bivariate scatterplots or ternary diagrams). Combinations of various trace element data are displayed and artifacts are visually compared to geological reference sources. Scatterplots may be generated using widely-available programs such as Microsoft's Excel or IBM's SPSS, although this can be time-consuming and could potentially lead to incorrect source assignments. More sophisticated graphical methods, such as those available through the free GAUSS software developed by the Archaeometry Laboratory at the University of Missouri Research Reactor (MURR), may also be used. The GAUSS program allows analysts to generate multiple bivariate scatterplots of various trace element combinations and quickly calculate confidence ellipses. In many cases, especially involving regions where only a few obsidian types were available, this approach may be sufficient to correctly assign artifacts to geological sources (Glascock et al., 1998). In other cases, including regions where chemically distinct obsidian types are numerous, bivariate scatterplots or other basic graphical methods may be inadequate to differentiate raw material types (Glascock et al., 1998).

A variety of multivariate methods including principal components analysis (PCA), cluster analysis, and discriminant function analysis (DFA) may also be used to aid in source assignments; however, these methods have some shortcomings. Using diagnostic trace element data, cluster analysis assigns individual samples to distinct groups (i.e., obsidian types) based on any number of variables. There are many algorithms to calculate a cluster analysis but hierarchical techniques are most commonly used. In this method, dendrograms are created that graphically illustrate the arrangement of clusters and the distances between groups (Manly, 2005). While dendrograms may accurately characterize differences between members *within* clusters, Glascock et al. (1998) note that because cluster analysis generally assumes that trace elements are uncorrelated, it can misrepresent differences *between* clusters. Clearly, this is a problem when the ultimate goal is to assign artifacts to particular obsidian sources.

Principal components analysis is a multivariate statistical technique that linearly transforms a set of variables into a set of uncorrelated indices or components. An advantage of this approach is that if the variation can be adequately represented in a few components, large datasets can be effectively described with fewer variables (Manly, 2005). Principal components analysis can be used to identify patterns in the data and the components generated can be used in further analyses that require uncorrelated variables (e.g., cluster analysis); however, PCA is not a classification or distance statistic, which is ultimately what is needed to classify an unknown sample in provenance studies.

Discriminant function analysis is a means to address which variables separate two or more defined groups. In the case of source provenance data, the elemental variables would be used to predict group assignment (i.e., source). A common approach in DFA uses Mahalanobis distance as a means to calculate group centroids from which individual cases can be classified. Once a model is created, it is possible to allocate unknown individuals to one of the groups in the model, with the assumption that the reference sample is representative of the origin of the unknown artifact. The error rate of the overall model (i.e., the accuracy of the assignment of known individuals to the correct groups) can be used to evaluate individual assignment (Manly, 2005).

A major advantage of using multivariate statistical methods, rather than univariate or bivariate methods, is that they capture more of the sample variation in addition to providing some level of certainty (i.e., p values, probabilities, error rates) that the models are working correctly. However, as outlined above, they are not without problems, particularly in the case of assignment of an unknown artifact. For example, cluster and principal components analyses are not well-suited for the assignment of an individual artifact; rather, they explore similarities between already identified groups. Conversely, DFA can provide equations to be used to assign an unknown artifact to a reference sample. However, depending on the statistical package being used, the result does not necessarily provide probabilities of correct assignment of that individual artifact to an obsidian type; it only provides probabilities of the overall model performance. Moreover, calculating these equations can be cumbersome if done by hand and there are many possible source assignments.

Here, we offer an alternative approach: we explore the use of the computer program Fordisc to assign individual artifacts to obsidian types based on a reference sample. Fordisc is an interactive software package widely used by forensic anthropologists to estimate ancestry, sex, and stature of a set of unknown skeletal remains in a medicolegal context; however, because it offers the ability to import databases to be used within its statistical framework, it can be used on any type of continuous data including the elemental composition of obsidian artifacts.

3. Materials and methods

To evaluate Fordisc's utility in assigning artifacts to particular obsidian types, we used a sample of 677 artifacts from various sites in the northwestern Great Basin currently housed at the University of Nevada, Reno (Table 1). These artifacts were previously characterized by the Northwest Research Obsidian Studies Laboratory (NWROSL) in Corvallis, Oregon. Over the past decade or so, NWROSL staff characterized the artifacts using either a Spectrace 5000 EDXRF (pre-2012) or ThermoElectron QuanX EC EDXRF spectrometer (2012–2016). They determined the concentrations of various trace elements (e.g., Ti, Mn, Fe_2O_3, Zn, Ga, Rb, Sr, Y, Zr, Nb, Ba) in each artifact and compared them

Table 1
Sample distribution of obsidian sources used in this study.

Sample	N
Badger Creek	15
Beatys Butte	111
BSPPFM	20
Buck Spring	59
Cowhead Lake	14
Coyote Spring	19
Craine Creek	32
Horse Mountain	35
MLGV	357
Tank Creek	15
Total	677

Table 2
Distribution of sample in test and training sets.

Sample	Training set	Test set
Badger Creek	1	14
Beatys Butte	18	93
BSPPFM	0	20
Buck Spring	9	50
Cowhead Lake	1	13
Coyote Spring	1	18
Craine Creek	0	32
Horse Mountain	2	33
MLGV	27	330
Tank Creek	1	14
Total	60	617

to geochemical profiles of obsidian samples collected from various geologic sources. In some cases, artifacts were assigned to "unknown" obsidian types, meaning that although they possessed clear distinct profiles, the geographic origin/distribution of the source material was unknown. In other rare cases, artifacts possessed source profiles that could not be used to differentiate one geochemical type of obsidian from another. We excluded these problematic artifacts from our study.

We used an Olympus Delta DP-6000 GeoChem Analyzer (herein referred to as the pXRF unit) attached to an Olympus Portable WorkStation to determine the trace elements of artifacts previously characterized by the NWROSL; in other words, we reanalyzed and recharacterized artifacts that were previously correlated with known obsidian sources. The pXRF unit emitted two X-ray beams (10 keV and 40 keV) set to run for 60 s each using the default geochemical calibration setting provided by INNOV-X. We collected trace element data for each artifact using a laptop connected to the pXRF unit; data were automatically exported into an Excel file after each characterization session.

We then culled the data to only include variables for rubidium (Rb – Z = 37), strontium (Sr – Z = 38), yttrium (Y – Z = 39), zirconium (Zr – Z = 40), and niobium (Nb – Z = 41). These are often referred to as the mid-Z elements, or those elements with an atomic number (Z) between 19 and 41. Mid-Z elements can be detected with little background effect, making their error rates predictable (Shackley, 2011). These data were then subjected to various multivariate statistical analyses including PCA, hierarchical cluster analysis, and DFA to evaluate their suitability to make source assignments. These analyses were conducted using SPSS 23.0.

Finally, we tested the ability of the statistical program Fordisc to assign the artifacts in our sample to specific obsidian types. We used the custom database function in Fordisc to test its ability to assign artifacts

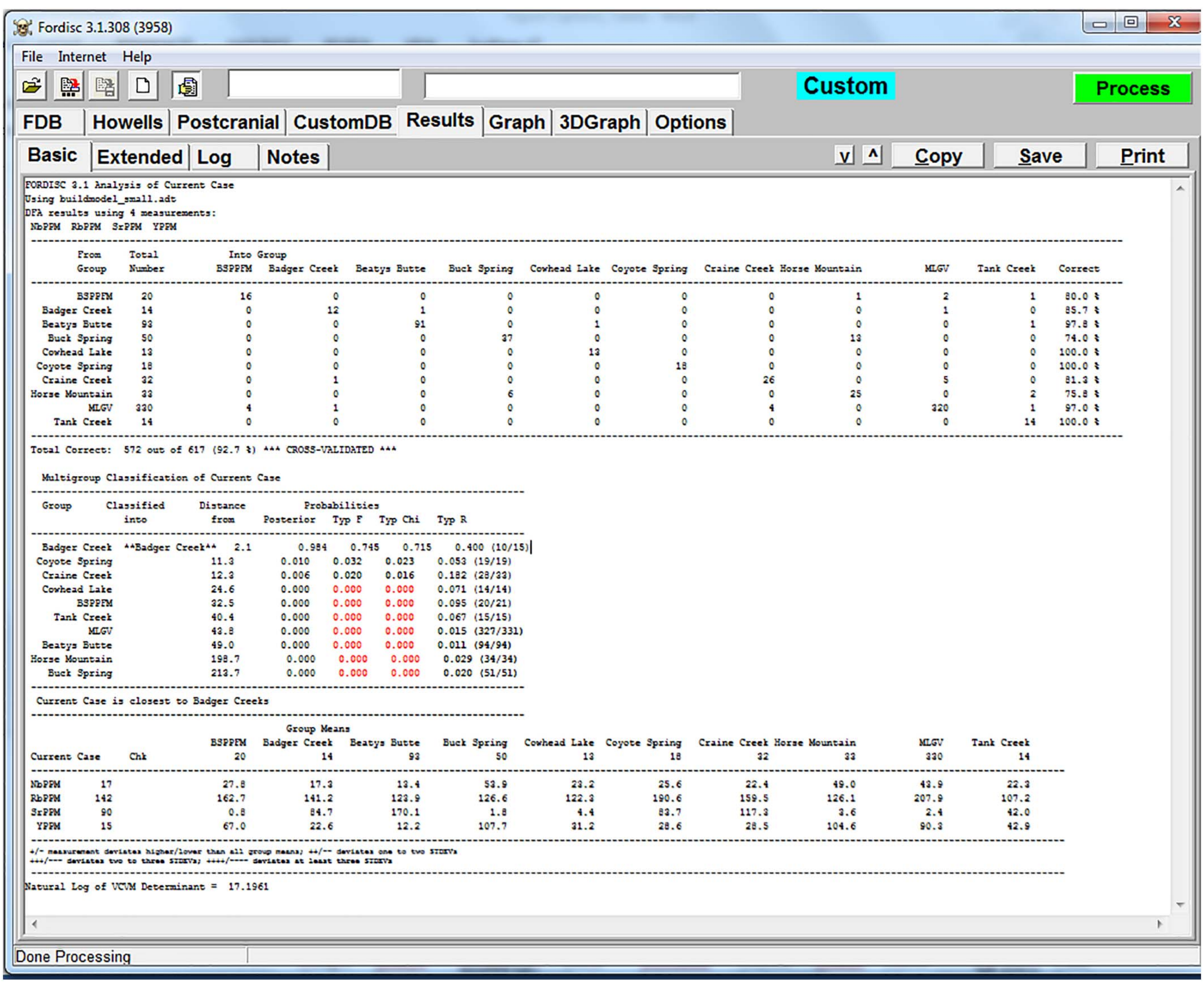

Fig. 1. Sample of Fordisc output for source provenance.

to obsidian types. A modest hold-out (i.e., training) sample (n = 60) was separated from the complete sample of 677 artifacts used to create the model (Table 2). The test sample (n = 617) was then imported into Fordisc to create a custom reference sample. Data on each individual obsidian artifact from the hold-out/test sample was then input into Fordisc to calculate its source provenance based on the reference sample (i.e., test sample).

Fordisc employs a type of DFA called linear discriminant function (LDF). The original variables are converted to LDF scores using the Mahalanobis distance. When more than two groups are included in analyses, a canonical variates analysis (CVA) is employed to accommodate multiple dimensions. As with other statistical applications, there are several assumptions inherent in LDF, including: (1) multivariate normality; (2) equal variance-covariance matrices across groups; and (3) equal prior probabilities. An advantage of this approach is that there is no assumption of independence of variables because the CVA linearly transforms the original data into uncorrelated variables. Further, Fordisc provides a test of matrix equality, the Kullback test, in the extended results tab. The extended results also identify outliers in the reference sample that can then be excluded in further analyses under the 'options' tab (Jantz and Ousley, 2005).

Researchers can input data from an artifact into Fordisc and the program calculates a source (i.e., group) assignment. Fig. 1 illustrates an example of the output. The box on the top shows model performance based on how well it classified the reference sample using cross-validation, or leave-one-out technique. In this case, the model was correct in 92.7% of the cases. This table can also be used to calculate the positive predictive value for the case in question, which is important for understanding model performance for an individual case and not the model as a whole (Klepinger, 2006).

The second box ("Multigroup Classification of Current Case") indicates the classification of the unknown sample into each of the reference groups. The Mahalanobis distance is provided as well as the posterior and typicality probabilities. The posterior probability is the relative probability that the unknown artifact belongs to each group. These probabilities will add up to 1 for all of the groups (Jantz and Ousley, 2005). Typicality probabilities are calculated based on the Mahalanobis distance and indicate the probability that the unknown artifact belongs to each group. The typicality probabilities are calculated three ways based on the F distribution, the chi distribution, and ranked distances (Ousley and Jantz, 2012). In this case, the artifact was assigned to the Badger Creek obsidian type, with a posterior probability of 0.984 and typicality probabilities ranging between 0.715 and 0.984. The final box shows the input data for the current case and how it varies from the mean values for the various source samples. Fig. 2 provides an example of the graphical output provided by Fordisc for the artifact. The graph shows the first two canonical variates accounting for 89.6% of the total variation. The black "X" represents the artifact being analyzed.

Table 3
First two components in principal components analysis.

Variable	Component	
	1	2
Sr	− 0.912	0.244
Zr	0.893	0.319
Rb	0.760	0.611
Nb	0.923	− 0.292
Y	0.952	− 0.270

4. Results

Multivariate statistical analyses were conducted on the entire dataset of 677 obsidian artifacts. Table 3 and Fig. 3 show the results of the PCA. The data show clear clustering in multivariate space, although, there is some overlap of Tank Creek and Cowhead Lake as well as Buck Spring and Craine Creek. Using the first two components from the PCA, we conducted a hierarchical cluster analysis based on the squared Euclidean distance for each artifact. This analysis resulted in a large dendrogram of 677 artifacts (data not shown due to large size)

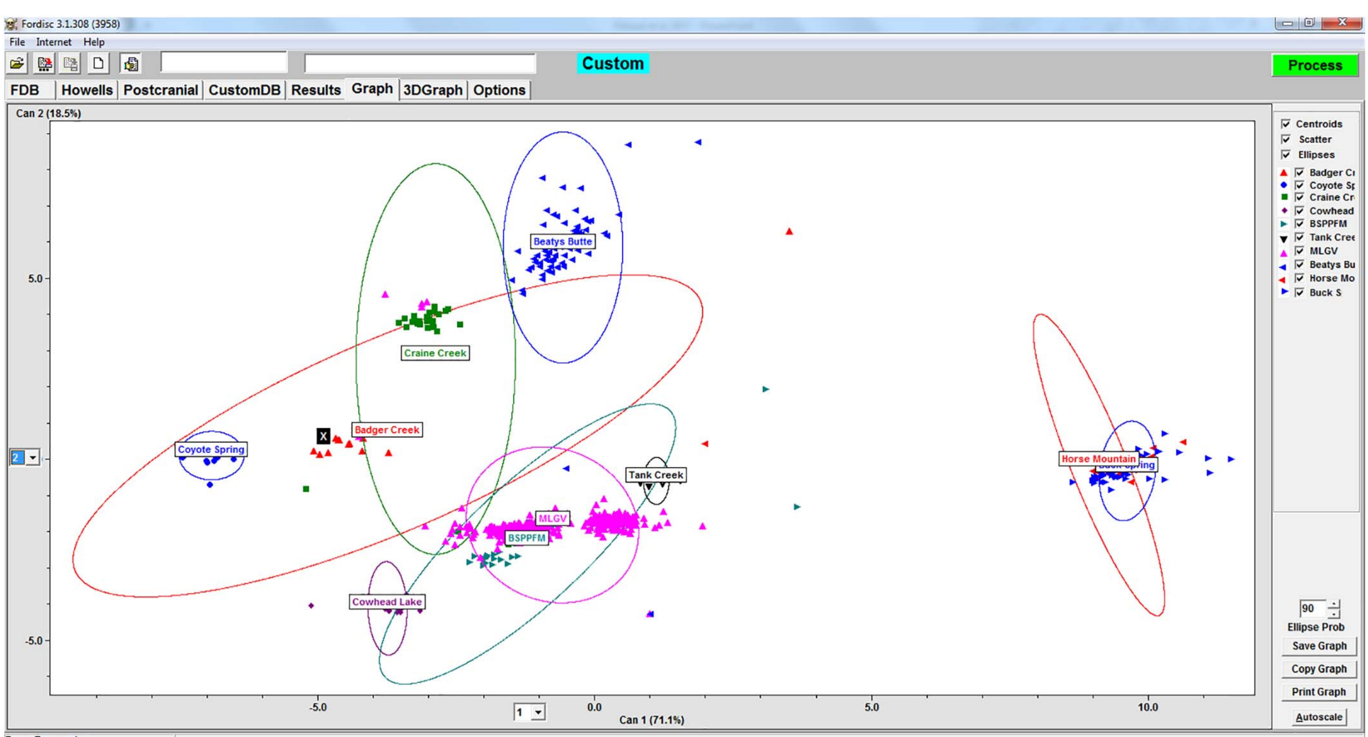

Fig. 2. Sample of Fordisc graphical output.

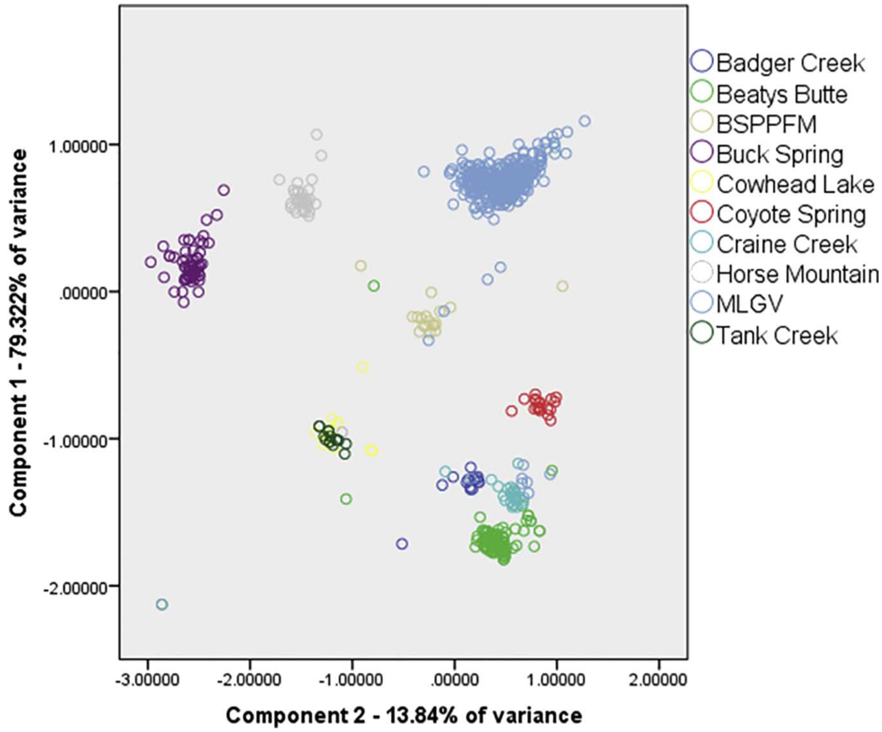

Fig. 3. Scatterplot of first two components of all data in the principal components analysis.

with 12 clusters largely divided by known source. Samples from Coyote Spring, Craine Creek, Beatys Butte, Horse Mountain, Bordwell Spring/ Pinto Peak/Fox Mountain (BSPPFM), and Buck Spring clustered clearly by individual group. Samples from Badger Creek were clustered throughout the different groups. As Fig. 3 shows, Tank Creek and Cowhead Lake also clustered together. The extra clusters in this analysis were the result of a few outlying data points in the dataset. We also ran DFA on the entire dataset in SPSS (Table 4). The model correctly classified artifacts into one of 10 groups 95.7% of the time on the original dataset. When the data were cross-validated, the model was correct 95.6% of the time. These results are far superior to those that would be expected by chance, which would only be 10% with 10 groups.

Finally, we analyzed data using the custom database function in Fordisc. For each artifact in the test sample, all possible source locations and variables were used. The sample sizes were large enough to accommodate the five variables, so over-fitting the model was not a concern and step-wise analyses were not employed. In this test, 57 out

Table 4
Results of discriminant function analysis on entire dataset.

		Predicted group membership									
		Badger Creek	Beatys Butte	BSPPFM	Buck Spring	Cowhead Lake	Coyote Spring	Craine Creek	Horse Mountain	MLGV	Tank Creek
Original %	Badger Creek	86.7	0	0	0	0	0	0	0	6.7	6.7
	Beatys Butte	0	97.3	0	0	0.9	0	0	0	0	1.8
	BSPPFM	0	0	85	0	0	0	0	0	15	0
	Buck Spring	0	0	0	100	0	0	0	0	0	0
	Cowhead Lake	0	0	0	0	100	0	0	0	0	0
	Coyote Spring	0	0	0	0	0	100	0	0	0	0
	Craine Creek	3.1	0	0	0	0	0	81.3	0	15.6	0
	Horse Mountain	0	0	0	0	0	0	0	94.3	0	5.7
	MLGV	0.3	0	1.4	0	0	0	1.7	0	96.4	0.3
	Tank Creek	0	0	0	0	0	0	0	0	0	100
Cross-validated %	Badger Creek	86.7	0	0	0	0	0	0	0	6.7	6.7
	Beatys Butte	0	97.3	0	0	1.8	0	0	0	0	0.9
	BSPPFM	0	0	80	0	0	0	0	0	15	5
	Buck Spring	0	0	0	100	0	0	0	0	0	0
	Cowhead Lake	0	0	0	0	100	0	0	0	0	0
	Coyote Spring	0	0	0	0	0	100	0	0	0	0
	Craine Creek	3.1	0	0	0	0	0	81.3	0	15.6	0
	Horse Mountain	0	0	0	0	0	0	0	94.3	0	5.7
	MLGV	0.3	0	1.4	0	0	0	1.7	0	96.4	0.3
	Tank Creek	0	0	0	0	0	0	0	0	0	100

Table 5
Results of test sample in Fordisc analysis.

	Badger Creek	Beatys Butte	Buck Spring	Cowhead Lake	Coyote Spring	Horse mountain	MLGV	Tank Creek	Crain Creek	Correct - N	Correct %
Badger Creek	1	0	0	0	0	0	0	0	0	1/1	100
Beatys Butte	0	17	0	1	0	0	0	0	0	17/18	94.4
Buck Spring	0	0	9	0	0	0	0	0	0	9/9	100
Cowhead Lake	0	0	0	1	0	0	0	0	0	1/1	100
Coyote Spring	0	0	0	0	1	0	0	0	0	1/1	100
Horse Mountain	0	0	0	0	0	2	0	0	0	2/2	100
MLGV	0	0	0	0	0	0	25	0	2	25/27	92.6
Tank Creek	0	0	0	0	0	0	0	1	0	1/1	100
Correct N	1/1	17/17	9/9	1/2	1/1	2/2	25/25	1/1	0/2		
Correct %	100	100	100	50	100	100	100	100	0		

of 60 artifacts (95%) were correctly classified (Table 5). Posterior probabilities ranged from 0.55 to 1.00, with an average value of 0.99.

5. Discussion

Our results show that multivariate statistical analyses can easily distinguish the source samples employed in this study. However, these methods can be more difficult to employ when trying to assign individual artifacts to an obsidian type. In such cases, Fordisc provides several advantages. First, it is extremely flexible with many options available including the ability to choose which sources and variables will be used in custom analyses. Second, it is fairly easy to use and does not require cumbersome calculations. Third, it provides probabilities (both posterior and typicality) for the sample in question as well as the performance of the model. Finally, Fordisc provides a summary table that allows for the calculation of the positive predictive value. Such outputs provide researchers with a broad sense of how well an unknown artifact fits that particular source assignment.

As with all statistical analyses, Fordisc should be used carefully and researchers should ensure that they understand the statistics being employed and the limitations inherent within them. A common criticism of Fordisc is that even if the unknown sample (i.e., the obsidian of which an artifact is made) is not represented in the reference sample (i.e., known obsidian types), the program will still provide a result (Elliott and Collard, 2009; Williams et al., 2005). Such an outcome is a valid concern that holds true for any statistical approach. Therefore, it is important to consider the applicability of the reference sample being used. One way to assess the suitability of the reference sample is to carefully consider the typicality probabilities that Fordisc provides. These probabilities indicate how appropriate the reference sample is for the unknown sample under analysis. As a general rule of thumb in forensic anthropology, if multiple typicality probabilities are < 0.05 then measurements should be checked for accuracy and the model should be scrutinized. If typicality probabilities are < 0.01, then the unknown artifact is very unlikely to be a part of that source group and the results are probably unreliable (Ousley and Jantz, 2012).

Other issues to consider when using Fordisc include the number of variables employed (i.e., number of elements) and the number of artifacts in the reference samples (i.e., the number of artifacts in each group). A conservative standard is that the reference sample of each group should be at least three times larger than the number of variables employed. To avoid overfitting of the model and ensure that not too many variables are used, a step-wise analysis may be employed (Jantz and Ousley, 2013). Another way to check if the model is overfitting is to look at the bottom of the output page and at the result for the "Natural Log of the VCVM Determinant" (see Fig. 1), where VCVM stands for Variance-Covariance Matrix. Any value not equal to 0 generally indicates that the model is not overfitting and there is sufficient variation based on the sample sizes and variables used in the analysis (Ousley and Jantz, 2012).

The guidelines outlined here are good practice in forensic anthropology when biological data (e.g., craniometrics) are involved; however, they may not always be of concern to archaeologists seeking to use XRF data to assign artifacts to particular obsidian types. As multivariate statistical analyses show, those data separate quite easily because the variables often vary considerably between geochemical types. This is not necessarily true for human skeletal data, which is more confined in expression. Additionally, sample sizes also tend to be much larger in source provenance studies than in forensic anthropology. Therefore, some of the standard considerations of applying Fordisc in forensic anthropology are likely not applicable to source provenance studies. For example, overfitting can generally be avoided with large samples of artifacts. Additionally, rules on typicality probabilities can be slightly relaxed. Specifically, to confidently assign an artifact to an obsidian type the typicality probability should be > 0.05; however, if the typicality is < 0.01 for the other groups in the same analysis then that does not necessarily indicate that artifact is too atypical of the entire reference sample for source assignment, rather it is just atypical of that particular reference sample. If the typicality probabilities are low for all of the groups, then this indicates that the reference samples are not appropriate for the artifact. In such cases, either a broader reference sample should be used or a source assignment should not be made.

6. Conclusions

Statistical analyses have become an integral part of anthropology. In this paper, we outlined various statistical methods that can be used in source provenance studies. We view multivariate methods as an improvement over univariate or bivariate methods, and Fordisc offers a relatively easy way to input data and perform such analyses without substantial coding or statistical knowledge. Fordisc can improve the validity of source assignments by providing reported probabilities, model performance, and positive predictive values; however, it does not obviate the need to periodically analyze international standards and report the results in order to establish validity (Shackley, 2010). Furthermore, a major drawback of Fordisc is that it can be expensive to purchase and in many senses the charge is a means to gain access to the skeletal reference data sample used in forensic anthropology. As the skeletal reference sample is obviously not needed for source provenance studies in archaeology, a similar statistical method to that used in Fordisc could be created in the free R or other such statistical programs, which would not require the purchase of Fordisc. Archaeologists could then incorporate their own reference samples based on known geological sources. Regardless of the program used, the ultimate goal of our paper has been to highlight an easy, user-friendly approach that researchers may use to increase confidence in making source assignments, including those involving obsidian artifacts.

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