

# Data Mining for Isotopic Mapping of Bioarchaeological Finds in a Central European Alpine Passage

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## ABSTRACT

Isotopic mapping has become an indispensable tool for the assessment of mobility and trade of the past. However, modeling and understanding spatio-temporal isotopic variation is complicated by the small number of available samples, potential mobility of the investigated samples, sample preservation quality, uncertainty of measurements, and so forth. In this work, we use data mining techniques to build an isotopic map (descriptive modeling) and to determine the spatial origin of new samples (predictive modeling). In particular, we propose a clustering-based isotope ratio model and a scoring function for the origin prediction of new samples. Our data was extracted from real animal finds from an Alpine passage that spans three countries (Germany, Austria, and Italy) and comprises a high variety of isotopes and geological characteristics. Our results and evaluation by domain experts show that it is possible to derive a model of the area for both descriptive and predictive purposes.

## 1. INTRODUCTION

Isotopic mapping has become a powerful tool for predicting the place of origin of a particular item. It is a popular method for solving Archaeology-related problems like determining the origin of archaeological finds, as well as analyzing the diet of individuals or entire populations, the climate of a region, and the migration patterns of people and their habitat [1, 5]. For example, in [6], isotopic mapping is used to predict the places of origin of ivory samples (from elephant teeth) in order to classify given samples as legally or illegally obtained. Typically, the items represent samples of living or dead creatures (humans, animals, sometimes even plants) such as bones, teeth, wood, etc.

The general idea behind isotopic mapping is that isotope measurements in different samples, reflect the environment

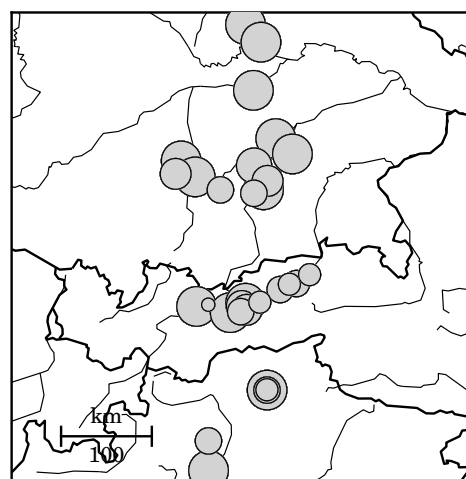


Figure 1: Spatial projection of the data set. Circle size indicates the number of samples at each location.

where the corresponding organisms were located in their lifetime. Isotope values in the organism of a given animal are the products of the metabolism of the animal. As such, the values are based on the food digested during the organism's life which in turn depends on geological processes of the environment. A common hypothesis is that there is a connection between isotopic measurements from skeletal remains of an organism and the geological isotopic fingerprints that are specific for the spatial catchment area where the organism mostly lived. Since the geological process on the globe differ considerably within surprisingly small regions, the surface of our planet can be divided into many small catchment areas each with a distinctive, characteristic geological isotope fingerprint. Isotopic mapping aims at defining small scale catchment areas featuring a homogeneous, characteristic isotopic fingerprint based on the observed characteristics of organisms that lived there (as the geological fingerprint is not directly applicable to the intended tasks).

In data mining terms, isotopic mapping aims at finding spatially coherent groups (clusters) of individuals with homogeneous isotopic features. The spatial extent of such

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a cluster represents a catchment area and the features of the individuals represent the characteristic fingerprint of this area. Based on this characteristic fingerprint, samples can be classified as either local (if its isotopic finger print matches the fingerprint of the catchment area where it has been found/obtained) or non-local. However, so far, the challenge of isotopic mapping has not caught too much attention in the computer science community and, thus, has been done mostly manually by domain experts.

One important thing to notice is that applying a spatial clustering algorithm (on the isotope attributes) is not feasible since we cannot expect a hard assignment between samples and locations due to migration and the effect of interfering variables on the metabolism. Due to the variability of this biological material, domain experts typically want the prediction of the location to be probabilistic, i.e., they want to know, given a concrete sample, for each catchment area the probability that the sample originates from this area.

At first glance, the problem of predicting the place of origin of an individual finding may appear as a simple classification task. However, in many applications we face the problem that the definition of the spatial extend of each catchment area is often not known, and, thus, we do not have a ground truth of classes. As a consequence, we cannot derive any class information from the spatial location of a sample that can be used in order to train a supervised classifier. Also, domain experts do not attempt to define catchment areas by hand (e.g. from geology, if known) since in this case they introduce a strong bias.

In this paper, we describe a new approach for isotopic mapping based on a pipeline of data mining algorithms which is applicable to multi-dimensional data. The approach evolved from a concrete use case: to investigate migration and trade in the past in the Alps using isotopic mapping of the remains of animals as part of a large interdisciplinary project (see acknowledgements). The task is to employ a data-driven approach to define the catchment areas and derive a characteristic isotopic fingerprint from these areas that can be used as predictive model. This enables archaeologists to evaluate the probabilities that a given finding originates from each of the catchment areas. In particular, it gives the domain expert a probability that a given sample is local or has moved to the place where it has been found. The proposed pipeline involves a clustering step in order to determine the catchment areas and a step that derives the isotopic fingerprints of each catchment area, and, finally a visual analytics step that enables the domain expert to locate a given sample through visually inspecting the isotopic map.

The remainder of this paper is organized as follows. We review related work in Section 2. A more detailed description of the use case and some basic concepts are introduced in Section 3. In Section 4, a new clustering-based method for isotopic mapping is presented and a predictive model for the domain expert is derived. We evaluate this approach on the data set from the sketched research project on migration and trade of people in the past in the central European Alps (see Section 5). Finally, some conclusions and future work directions are given in Section 6.

## 2. RELATED WORK

Isotopic analysis is a powerful tool for animal ecologists with a variety of applications like tracking animal migration, dietary reconstruction of animals, the use of water resources,

food web structure etc, e.g., [7]. Stable isotope ratios vary among food webs and are incorporated into the animal's tissue via its diet.

In [6], the authors study the problem of illegal elephant ivory trafficking by detecting the age and provenance of the ivory. Their dataset consists of 606 ivory samples from Africa and Asia. For the analysis, five different stable isotope ratios of carbon, oxygen, hydrogen and sulfur were used. For the determination of the origin of ivory, different neighborhood based classification models were employed, like nearest neighbor (NN) and  $k$ -nearest neighbors (KNN), whereas the Euclidean distance was employed as the distance function.

The importance of data mining [4] for natural sciences is constantly increasing as the domain scientists deal with larger datasets and higher data complexity. Classification, clustering, regression and other mining tasks are applicable to problems in these domains like species classification, grouping of findings and prediction. Data-driven exploration is different from the model-driven approaches that are typical in these domains and therefore this presents new opportunities for the Data Mining domain.

## 3. THE USE CASE: ISOTOPIC MAPPING OF BIOARCHAEOLOGICAL FINDS

The study area is the transalpine Inn-Eisack-Etsch passage across the German-Austrian-Italian Alps which has been used since prehistoric times and is of great archaeological interest. The spatial coverage of the region under investigation is shown in Figure 1; there are samples for the whole passage, although the sampling rate is low especially in the south. The overall goal of the project is the establishment of an isotopic fingerprint for bioarchaeological finds through isotopic mapping and its application to archaeological and cultural-historical problems of the Late Bronze Age until Roman Times.

The isotopic mapping is achieved using stable strontium  $Sr$ , lead  $Pb$ , and oxygen  $O$  isotopes from three species of residential vertebrates. The study population  $D$  consists of 218 animal findings including deer (48 samples), pigs (81) and cows (89). The data consists of spatial information on the location of the find (which is given by a latitude-longitude-pair associated with the archaeological site, not the particular find) and the ratios of oxygen ( $O$ ), strontium ( $Sr$ ) and lead ( $Pb$ ) isotopes in the find. The oxygen isotope  $^{18}O$  is given by its  $\delta$  value ( $\delta^{18}OPO_4$ ), whereas two measured strontium isotopes ( $^{87}Sr$  and  $^{86}Sr$ ) are expressed as their fraction  $\frac{^{87}Sr}{^{86}Sr}$ . and four lead isotopes  $^{204}Pb$ ,  $^{206}Pb$ ,  $^{207}Pb$ , and  $^{208}Pb$  are given as  $\frac{^{208}Pb}{^{204}Pb}$ ,  $\frac{^{207}Pb}{^{204}Pb}$ ,  $\frac{^{206}Pb}{^{204}Pb}$ , and  $\frac{^{206}Pb}{^{207}Pb}$ . So, in total 7 (partly redundant) isotopic ratios attributes and 2 spatial attributes are used for data description. From an analysis perspective the data set, although small, is extremely interesting and challenging because there will not be a perfect fit to a (previously unknown) ground truth for several, already discussed, reasons.

## 4. A CLUSTERING-BASED ISOTOPE RATIO MODEL FOR ISOSCAPING

The challenge for the data analysis part of the project is to build an isotopic map of the region based solely on the isotopic description of the samples that can be used for de-

iving probabilities about the origin of individual samples. Since there is no ground truth for the map, we first use *clustering* in order to derive the map components (catchment areas). We extract groups of samples with similar isotopic fingerprint in a data-driven way, explicitly not considering the spatial information of the samples. Rather, the spatial information is later used for the visualization. In particular, we chose to use a mixture model approach, where the components of the model are probability distributions reflecting the data distributions of the clusters. In particular, we use a Gaussian Mixture Model, which assumes that the data points are generated from a mixture of a finite number  $k$  of Gaussian distributions with unknown parameters. The reasons for this choice are that (i) it is a rather generic clustering model, especially if nothing is known about the ground truth beforehand, and (ii) due to the use of probability distributions it is able to capture variations and outliers (at least to some degree).

## 4.1 Isotopic mapping

Let  $D = \{o_1, o_2, \dots, o_n\}$  be a set of observations (samples) where each observation  $o_i \in D$  is described by  $d$  isotopic ratios, i.e.  $o$  is a  $d$ -dimensional feature vector  $o_i = (o_i^1, o_i^2, \dots, o_i^d)$  neglecting the spatial information. Let us assume that the isotopic data were generated according to a Gaussian Mixture Model with  $k$  components and each cluster  $1 \leq i \leq k$  can be modeled as a  $d$ -variate Gaussian with mean  $\mu_i$  and standard deviation  $\Sigma_i$ . The problem of determining these  $k$  Gaussians is two-fold: we need (i) to assign the points in  $D$  to the  $k$  clusters and (ii) to learn the Gaussian distribution parameters for each cluster. The well-known Expectation-Maximization (EM) algorithm [2], offers as solution to this problem by alternating between an *expectation step* and a *maximization step*. In the E-step, the model is fixed and an estimation of instance to clusters probabilities is made given this model. In the M-step, based on the assignments of the previous step new parameters from the model are computed so as the log-likelihood is maximized. These two steps are alternated until convergence.

The model of the isotopic map is a Gaussian Mixture Model learned from our dataset  $D$  through the EM algorithm. The final model  $M$  consists of  $k$  components/clusters:

$$M = \{(c_1 = (\mu_1, \Sigma_1)), (c_2 = (\mu_2, \Sigma_2)), \dots, (c_k = (\mu_k, \Sigma_k))\}$$

where each component  $c_i$  is described in terms of its mean and covariance,  $c_i = (\mu_i, \Sigma_i)$ , i.e.  $\mu_i$  is a  $d$ -dimensional vector and  $\Sigma_i$  a  $d \times d$  matrix.

As part of the model we also consider the probabilities according to which an instance was assigned to the different clusters. In particular, each observation  $o \in D$  is annotated with a cluster-distribution probability

$$o.\text{prob} = [o.\text{prob}^1, o.\text{prob}^2, \dots, o.\text{prob}^k],$$

with  $o.\text{prob}^j, 1 \leq j \leq k$  being the probability of instance  $o_i$  coming from component/cluster  $j$  and  $\sum_{j=1}^k (o.\text{prob}^j) = 1$ , that is the probabilities should sum up to 1. As we will show in the experiments, such a probability helps us understand better the topology of the isotopes. EM clustering is often used as a hard clusterer, by considering only the most probable instance assignment. However, for our problem, a soft assignment leads to much better insights on the data.

## 4.2 Applying the isotopic map

Based on the isotopic map, we use *nearest-cluster classification* in order to answer the question about sample origins. As our analysis shows that isotopic clusters are not well-separated spatially, we also propose a *cluster-spatial-location approximation* method, based on the spatial distribution of cluster members, in order to specify the origin of a new sample more precisely. We opt for classification instead of regression for the origin prediction task, due to the small size of our data set, the sparsity of the samples in the spatial domain and the other challenges mentioned above. Due to these issues, estimating the exact position of a new sample is more difficult than estimating a cluster (and an associated spatial distribution) the instance might belong to.

Although the primary goal of the isotopic mapping is to offer an understanding of the data w.r.t. their isotopic characteristics, it is also desirable to be able to assign new instances to their most probable clusters in the model subject to the following considerations: Given an observation  $o$  and its most probable cluster  $c$ , we can display the spatial distribution of all members of  $c$  over the area under investigation on a map. In our use case, we can visualize the spatial distribution of the members of  $c$  over all excavation sites in the alpine passage shown in Figure 1. This provides us with the information about which sites on the map contain members of the cluster  $c$ , i.e., the potential catchment area of  $c$ . These catchment area are not forced to be spatially coherent. However, if we further aggregate the number of instances of  $c$  at each site of the map, domain experts can use this data to get a feeling on how probable it is that  $o$  originates from a given site on the map.

Our prediction of the most probable cluster resembles the E-step of the EM algorithm, that is, for a given instance  $o = (o^1, o^2, \dots, o^d)$  and the extracted isotopic mapping model  $M$ , we estimate the probability of  $o$  being generated by the different components of  $M$ . The prediction is a cluster distribution vector:  $o.\text{prediction} = [o.\text{prob}^1, o.\text{prob}^2, \dots, o.\text{prob}^k]$  over the  $k$  different components of  $M$ . We pick that cluster  $c(o)$  for  $o$  which has the highest probability, i.e.,

$$c(o) \leftarrow \operatorname{argmax}_j \{ o.\text{prob}^j \}, 1 \leq j \leq k \quad (1)$$

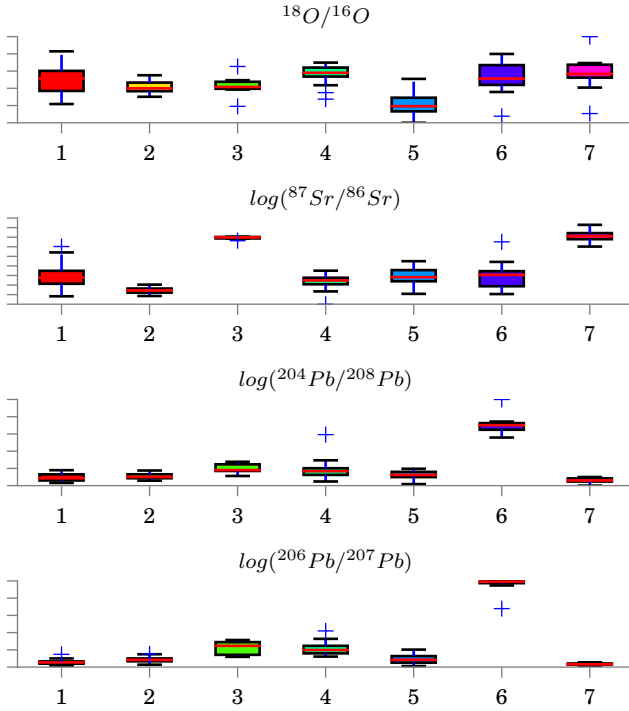
To summarize, the application of the isotopic mapping  $M$  for a given instance  $o$  is facilitated through clustering and visual analytics as follows: (i) Determine the most probable cluster  $c(o)$  from  $M$  by Eq. 1. This is the *nearest-cluster classification* step. (ii) Display the map of the area under investigation and aggregate for each location  $l$  on the map the instances of  $c(o)$  at  $l$  (e.g., as a heat map). This is the *cluster-spatial-location approximation* step.

## 5. EXPERIMENTAL EVALUATION

We evaluate our approach on the dataset introduced in Section 3. The preprocessing of the data is discussed in Section 5.1. The extracted isotopic mapping is presented in Section 5.2 and the origin prediction results in Section 5.3.

### 5.1 Data Preprocessing

We apply pre-processing to make the data easier to handle algorithmically. In a first step, all values are transformed into pairwise fractions of isotopes. As the oxygen isotope ratio is given in  $\delta$ -notation, we initially transform it back to the



**Figure 2: An isotopic description of the isotopic mapping model components (clusters).** For each isotopic ratio feature, the cluster distribution of its values is depicted. The cluster color is preserved across the different charts.

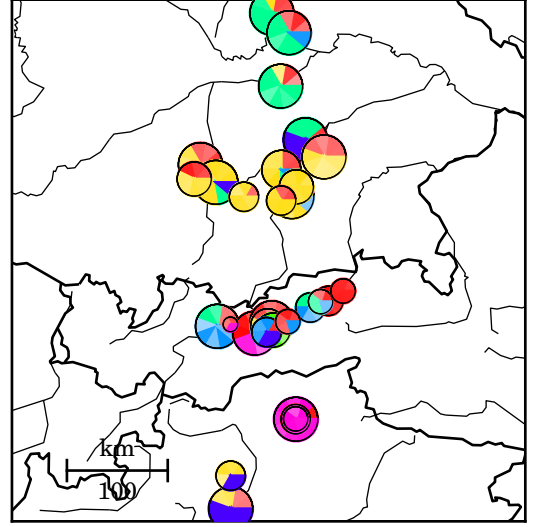
original  $^{18}\text{O}/^{16}\text{O}$  fraction. Strontium is already given as a single fraction, which we retain. Lead isotopes  $^{204}\text{Ld}$ ,  $^{206}\text{Ld}$ ,  $^{207}\text{Ld}$ , and  $^{208}\text{Ld}$  are measured as five pairwise fractions. We dismiss all but two, which retain all isotopes to reduce redundancy. We arbitrarily chose to group  $^{204}\text{Ld}$  and  $^{208}\text{Ld}$ , as well as  $^{206}\text{Ld}$  and  $^{207}\text{Ld}$ . We represented them as  $^{204}\text{Ld}/^{208}\text{Ld}$  and  $^{206}\text{Ld}/^{207}\text{Ld}$  to keep the skewed end towards zero. After standardizing all measurements to isotope fractions, we normalized the resulting values. Since we observed that the oxygen isotope ratio was approximately normally distributed, while the strontium and lead isotope ratios were skewed, we applied a logarithmic transformation to these ratios to counteract this effect.

## 5.2 Results of the Isotopic Mapping

The whole sample population was used to generate the isotopic mapping of the environment. Only the isotopic fingerprints of the instances was used for the descriptive modeling (clustering) part, the location information was omitted and used later to examine the spatial extension of the detected clusters.

The Expectation-Maximization algorithm implemented in Weka [3] was used for clustering. The choice of  $k$  was based on internal cluster quality measures, namely the silhouette coefficient, cohesion and separation, for which  $k = 7$  proved the best setting.

A per-isotope description of the clustering-based isotope ratio model resulted from  $k = 7$  is shown in Figure 2. For



**Figure 3: The spatial projection of the isoscaping model components.** Clusters are represented by color. The size of the circles at each location depicts the number of samples in the location.

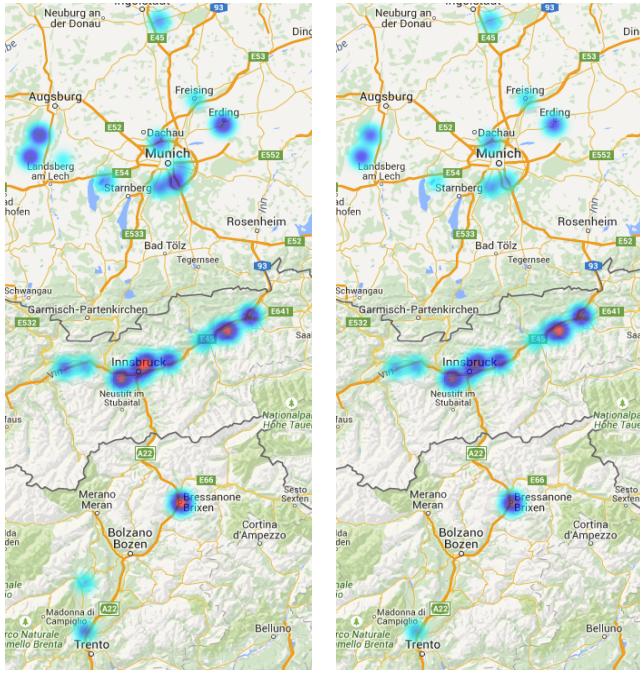
each of the  $d$  features (isotopic ratio), the distributions of its values within each cluster are depicted as box plots. Although only a single-attribute view in the clusters is provided by this figure, we can see that there is some variation in the values across the different clusters for all isotopes. The variation is lower for the oxygen feature, the mean value is very similar across the different clusters, only cluster 5 (light blue color) seems to differentiate significantly from the other clusters. Also, the range of oxygen values within each cluster is much larger compared to the ranges of the other isotopes. In addition, it is interesting to observe that each attribute contributes to the differentiation of different clusters so it seems necessary to consider all attributes simultaneously rather than focusing on only one of two.

The spatial projection of the clusters along the alpine passage under investigation is presented in Figure 3. Each of the different clusters is presented in a different color, the size of the circles corresponds to the population sample in the location. The “multi-colored” locations in the map indicate that the samples of those locations might belong to different clusters (note that the clustering takes place only in the isotopic space). It can be observed that the isotopic clusters are not spatially coherent and clearly separable. However, some of the clusters have a clear spatial “signature”. For example, the yellow cluster is mainly located in the middle Alps region, the green cluster is mainly in the north and the dark pink cluster is mainly in the south. The blue cluster is spread over the entire region.

## 5.3 Applying the Isotopic Mapping

### 5.3.1 Visually Analyzing the Map

The clustering model (EM clustering) is soft in its assignments. That is each instance is assigned a probability of belonging to each of the resulting clusters; the “hard-assigned” cluster to the instance is the one with the maximum prob-



(a) soft-view

(b) hard-view

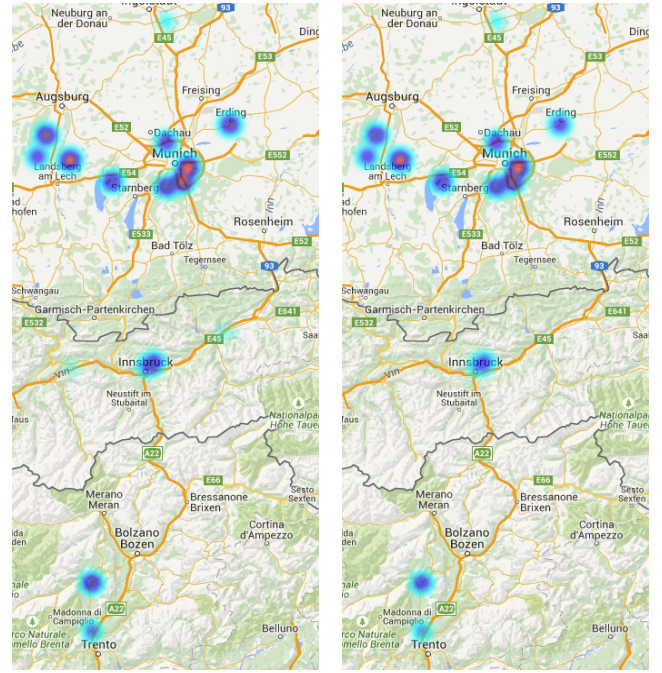
**Figure 4: Cluster 1 (the biggest one) spatially projected. More intense color indicates higher assignment probabilities to the cluster.**

ability. The highest probability though gives us an indication of how well an instance fits to its assigned cluster and at the cluster level, the assignment probabilities of cluster-members provide an indication of how tight the clusters are. A spatial projection of these probabilities, with higher probabilities being displayed by more intense colors, is shown below for two of the biggest clusters from Figure 3, cluster 1 (Figure 4, 68 cluster members) and cluster 2 (Figure 5, 61 cluster members), and the smallest one, cluster 3 (Figure 6, 7 cluster members).

For each figure, the right part shows the hard-view when only the instances with the highest probability of being generated by the cluster (c.f., Eq. 1) are aggregated at each location. The left part shows the soft-view when all instances and their probabilities to being generated by the cluster are plotted. It can be seen that especially when the number of cluster members is high and the members are not spread too strongly over the map, the proposed visualization gives a clear hint where a sample may come from. On the other hand, if the members of the cluster are spread over many locations, then the heat map does give a first impression but it is hard for a user to give an authoritative forecast on the place of origin. In the latter case, even though this seems somewhat unsatisfactory to computer scientists, to archaeologists multiple alternative hypotheses are acceptable. The visualization presented here was well-received by the domain experts.

### 5.3.2 Predicting Places of Origins

Although archaeologists are typically happy with the quite fuzzy visualization discussed above, we try to derive more profound predictions of the place of origin for a given sample.



(a) soft-view

(b) hard-view

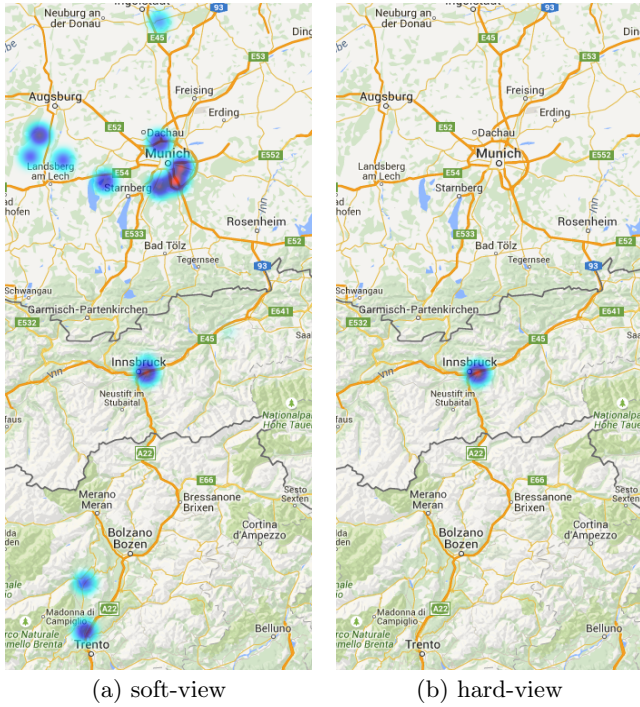
**Figure 5: Cluster 2 (the second biggest one) spatially projected. More intense color indicates higher assignment probabilities to the cluster.**

For this purpose, we employ a *nearest-neighbor-classifier* approach at the cluster level. That is, for a new sample  $s$ , we find its closest cluster minimizing the Mahalanobis distance of the isotopic fingerprint of  $s$  to each of the cluster centers  $\mu_i$ . This is a comparison in the isotopic space and since, as we saw previously, clusters are not well separated in the spatial domain, we further approximate the place of origin within the resulting clusters by considering where the spatial center of the cluster population is.

Since there is no ground truth of the exact classes of each instances and, in order to avoid bias and overfitting, we use two different experimental scenarios. In the first settings, called *scenario A*, we use the whole data set to build the isotopic mapping model and then we assign the observations to their closest cluster in the model using the proximity between the isotopic fingerprints of the observation and the cluster. We evaluate the spatial Euclidean distance between the true instance location and the predicted one (through clustering and cluster center location approximation). For this scenario, we use all instances during clustering as the ground truth labels come from the clustering itself. However, since testing instances are part of the model this approach is biased and subject to overfitting. Therefore, we also evaluate a second setting, called *scenario B*, where the data set is split into a training set and a testing set and only the training set is used for model building step (clustering). To evaluate, its quality we assign instances of the test set to their closest clusters (based on the isotopic part) and we check how far away the actual location of the test instances to the most probable location of the cluster is.

For the *scenario A*, i.e., when all instances are used for isotopic mapping, we achieved an overall score of 0.59. For





**Figure 6: Cluster 3 (the smallest one) spatially projected. More intense color indicates higher assignment probabilities to the cluster.**

the *scenario B*, we applied a 4-fold cross validation, that is, each time 3 of the folds were used for isotopic mapping (training) and the remaining 1 fold for testing. An overall average score of 0.60 was achieved for this scenario. The sheer numbers are not too impressive from a computer science point of view. But it shows on the other hand, that scenario A does not suffer significantly from overfitting. In addition, as outlined above, domain experts do not consider a hard classification as realistic due to the many origins of variability and uncertainty in the data.

## 6. CONCLUSIONS AND OUTLOOK

In this paper, we deal with the isotopic mapping and fingerprinting problem for the transalpine Inn-Eisack-Etsch passage across the German-Austrian-Italian Alps. The passage has been used since prehistoric times and is of great archaeological interest. We argue that due to the complexity of the data, simple models focusing on a single dimension or examining correlation between two dimensions, as it is typically used by domain experts, are not adequate. We follow a data-driven analysis path that does not include any background knowledge to build the model in order to avoid bias.

We propose a clustering-based isotopic mapping model and an origin prediction method for predicting the probability of an instance being generated by some model component. Our finding over real data, from animal findings in the Alps, suggest that our method offers a good “explanation” of the area under investigation and comprises a useful tool for domain experts not only for understanding the isotopic fingerprint of the area but also for locating the origin of unknown instances.

Future work includes better approximating of the spatial origin of each cluster and employing it for the origin prediction of new instances (now this is left to domain experts and is done by inspecting the heatmap of the closest cluster (c.f., Section 5.3.1) or is done naively by aggregating the location of cluster members (c.f., Section 5.3.2). Our results so far indicate that clusters of features have no separate spatial extent, on the contrary we can see overlaps and clusters scattered all over the place. An approach to spatial separation of the clusters, through e.g. some members re-positioning in other clusters, that would not significantly hurt their isotopic fingerprint (i.e., the model in the isotopic domain) might be a solution to the spatial overlap of the clusters issue.

The number of data points analyzed is quite small (218 data points) and scattered over only a few sites. This is particularly problematic when the goal is to build a model of the covered areas (isotopic fingerprinting) and use these models for origin prediction of future samples. Moreover, the samples might be subject to isotopic errors due to measurement device errors, bad preservation etc, but also to spatial errors due to migration and trading in the past or due to environmental factors. As part of our future work, we plan to model uncertainty of different types and incorporate it in the mining model.

## Acknowledgement

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<http://www.en.for1670-transalpine.uni-muenchen.de>

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