

KOHONEN SELF-ORGANIZING MAPS TO UNRAVEL PATTERNS OF DENTAL MORPHOLOGY IN SPACE AND TIME

1. INTRODUCTION

This review paper relies on two studies we conducted on the classification of human dental morphological data by means of Artificial Neural Networks (ANNs). Analysed samples included Middle Pleistocene to Early Holocene populations across Europe, North Africa and the Middle East. At that time, our research was directed to the classification of a recently discovered dental sample (Tabun cave, Israel) that was compared to a reference database composed of a large number of different samples in order to confirm its belonging to the Neanderthal teeth morphotype (COPPA *et al.* 2007a). The reference database itself was published the same year (MANNI *et al.* 2007).

In spite of the very wide application of ANNs in the most diverse scientific disciplines, they have hardly ever been applied to physical anthropology. Prescher, Meyers and Graf von Keyserlingk (PRESCHER *et al.* 2005) found them suitable for the investigation of a large collection of samples concerning the human nasal skeleton. Corsini, Schmitt and Bruzek (CORSINI *et al.* 2005) and Buk, Kordik, Bruzek, Schmitt and Snorek (BUK *et al.* 2012) showed that ANNs make possible a more accurate inference of the age at death, a crucial yet still far from being solved issue in physical anthropology and forensic sciences. Mahfouz, Badawi, Merkl, Abdel Fatah, Pritchard, Kesler, Moore, Jantz R. and Jantz L. (MAHFOUZ *et al.* 2007) have shown that ANNs yield the best predictive accuracy and classification success rate, among a range of alternative methods, in sex determination according to the dimension of the proximal femur. Another study concerning sex determination, a major issue in anthropology and forensic disciplines, was about the analysis of high-resolution computer tomography images of the femoral patella (kneecap) (DU JARDIN *et al.* 2009).

To conclude this short list, ANNs have been combined with Geographic Information Systems (GIS) to predict the location of possibly productive fossil-bearing localities (ANEMONE *et al.* 2011). Our two studies (COPPA *et al.* 2007a; MANNI *et al.* 2007) confirm their usefulness in a variety of issues addressed by physical anthropologists, palaeontologists and forensic scientists (classification, prediction) and we advocate their further spread and dissemination in our discipline. This article may be a way to attract the attention of colleagues on ANNs and, in order to provide some insight, we will methodologically review our studies by stressing their advantages over other existing methods.

2. ARTIFICIAL NEURAL NETWORKS TO CLASSIFY HUMAN DENTAL MORPHOLOGY

In the studies we have mentioned (COPPA *et al.* 2007a; MANNI *et al.* 2007), we analysed dentitions of single individuals with the aim to display each of them as a single data point in a kind of multivariate representation. As a consequence, all the traits scored on each tooth of the maxilla and mandible of single individuals were coded as vectors having the components defined by a zero (0), or by a one (1), according to the presence or absence (established on the basis of selected breakpoints) of given morphological tooth traits listed in the *repertorium* of the ASUDAS system (TURNER *et al.* 1991; SCOTT, TURNER 1997) (see Fig. 1 for an example). Incomplete dentitions, dental wear and poor conservation often impeded the scoring of all traits, giving rise to missing data descriptors. This is commonplace in the study of anthropological collections of human remains, like bones and teeth, because samples or fragments of the samples can be missing or broken. Teeth, very resistant, are less likely to be broken but are often missing; either they were never recovered in burials or excavations, or they could not be easily attributed to the individual they belong to or – and this also often happens – because they can fall down and get lost in collection repositories. Nevertheless, given the chemical and physical properties of teeth, they are among the elements that best withstand taphonomic processes and they constitute one of the most abundant finds in archaeological sites (HILLSON 1986).

The statistical constraints of missing data preclude a number of multivariate analyses, namely Principal Component Analysis, Multidimensional Scaling, Mean Measure of Divergence, Multiple Correspondence Analysis, to mention only the most frequently-used ones. To overcome such limitation, a customary approach in dental anthropology, and one often applied by us in both micro-regional (CUCINA *et al.* 1999; VARGIU *et al.* 2009) and macro-regional (COPPA *et al.* 1998, 2001, 2007b, 2007c, 2011; CANDILIO *et al.* 2010) studies, consists in the merging of different samples into a single population vector by “averaging” available measures in individual samples, either by a mathematical average of real valued traits or by a majority-rule-consensus for discrete measures like the presence/absence ASUDAS system. In this way, the operational units are no longer the single individuals but groups of them, populations, that have no missing components and are statistically tractable (Fig. 2, case A). Another solution, to overcome missing components in vectors, is to consider only those morphological traits that are available in a large number of individuals, meaning that analysed vectors do not correspond to the whole set of traits defined by the ASUDAS system but only to a subset of it.

According to this *modus operandi*, the database is larger when only a few traits are accounted in vectors (Fig. 2, case B), and smaller when more

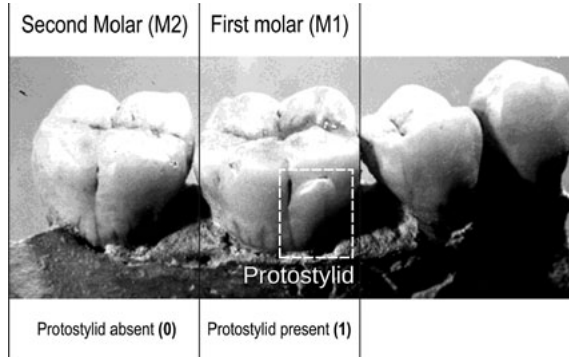


Fig. 1 – ASUDAS scoring system (TURNER *et al.* 1991; SCOTT, TURNER 1997) for the description of human dental morphology. Example of a dental trait scored on lower molars (the Protostylid) that can be either present (M1) or absent (M2). Our analyses were made according to 23 traits of this kind, thus giving rise to vectors having 23 binary descriptors.

traits are considered (Fig. 2, case C). In both cases (B and C) the final analysis will be a compromise based on a small number of traits (lack of statistical resolution) or on a low number of individuals (lack of geographical and historical resolution). The “population approach” – though very useful and often adopted – has its limitations as it decreases the sample size and rubs off individual variability. If this is not a major problem in archaeological contexts yielding a large amount of copious anthropological samples, it becomes a serious limitation in less productive sites, as the pooling of the samples “to fill the gaps” may lead to a disharmonic chronology, provenance, or even genetic asset of those included in a population.

To conclude, the analysis by single individuals should be regarded as the optimal one in many paleoanthropological and forensic contexts where the estimation of intra-population variability, in the identification of migrants, and in the identification of different subpopulations, as can be the case – this is just an example – in an ancient battlefield where two very distinct human groups, that had no previous contact before, are buried together in a same site. In such cases, a classification method able to cope with missing descriptors, in other words able to process single individuals, provides a much better insight into the past. This is why we turned to ANNs.

3. SELF-ORGANIZING MAPS (SOMs) AS AN APPLICATION OF ANNs

ANNs are machines or software whose architecture is modelled after the brain. They typically consist of hundreds of simple processing units,

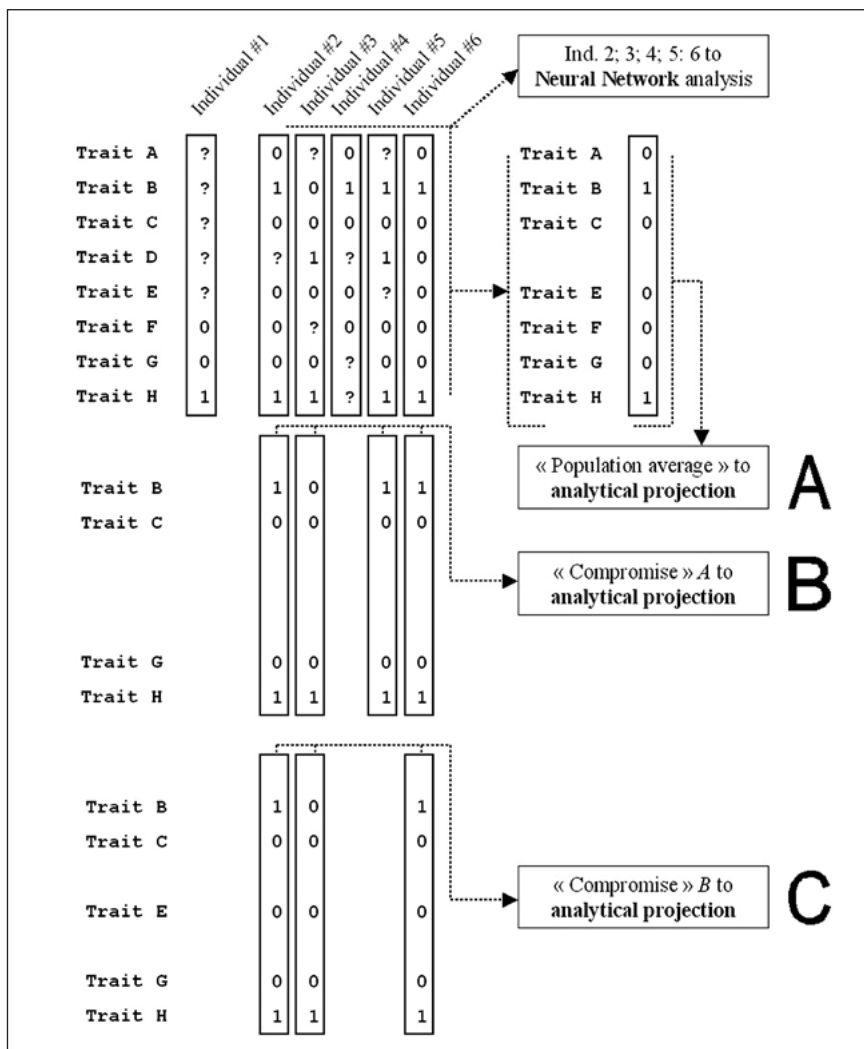


Fig. 2 – Examples of data vectors defined by eight dental traits (A; B; C; D; E; F; G; H). On the top of the figure a dataset of 6 individuals is displayed and the descriptors correspond to the presence (1) or absence (0) of a given dental trait. Missing measures are reported as “?”. As all vectors present missing descriptors, we visually suggest the various strategies that are generally adopted to analyze them. In analytical projections (like MDS or PCA), no missing data can be processed, therefore individual samples can be converted in a population vector whose descriptors correspond to a majority rule consensus concerning available descriptors (case A). Otherwise, a compromise between the number of individuals or the number of observations that are kept for the analysis has to be achieved. In B there are 4 individual vectors (#2; #3; #5; #6) with 4 traits (B; C; E; G; H); in C there are less individuals (#2; #3; #6) with more descriptors defining them (B; C; E; G; H). Artificial Neural Network analysis can be used to process the full set. Please note that the vector corresponding to “Individual #1” has been excluded from analyses due to its too many missing descriptors.

which are wired together in a complex communication network. Each unit or node is a simplified model of a real neuron which fires (sends off a new signal) if it receives a sufficiently strong input signal from the other nodes to which it is connected. The strength of these connections may be varied in order to reach different patterns of node firing activity that adjust the network to different classification tasks. In a similar way, the brain contains many billions of a very special kind of neurons that are organised into an intercommunicating network. Typically, each neuron is physically connected to many others and their connections are not merely *on* or *off*, since they can have a varying *strength* which allows the influence of a given neuron on one of its neighbours to be of different intensity (according to its distance from them). Many aspects of brain function, particularly the *learning process*, are closely associated with the adjustment of these connection strengths.

Even if ANN were inspired by the function of biological neurons, many of the software and hardware designs have become far removed from biological reality. At the beginning of their application, ANN were intended as a simulation of neurophysiological processes but, today, they are simply considered to be tools to solve problems. Popular applications concern discrete or real valued high-dimensional input, possibly noisy in the fields of phoneme recognition, image classification or pattern recognition. As an example, we will mention the automatic reading of ZIP codes by distributing machines in major post offices. Camera images of the addresses on the envelopes of the letters are analysed with ANN to recognise the written pattern (ultimately the handwritten ZIP code) and to assign it to reference models (numbers from 1 to 9, including the 0). This example concerns the morphology of written numbers and, after all, our application to teeth concerns morphology as well. ANN can be divided in two categories, *supervised* and *unsupervised*. In *supervised* applications a known dataset is used to train the network, meaning that the final classification of the items is expected to follow an expected categorisation (like the numbers in the ZIP codes).

The ANN can be trained in different ways until the final classification matches the classification expected (learning phase). Once that ANN provide the desired classification of a known database, a new database can be analysed and classified according to the categories (clusters) that the test database yielded in the training phase. Differently, when a desired classification is not known a priori, unsupervised learning has to be preferred. In this latter case there is no expected classification, and the ANN will provide the categorisation that best matches the variation of the data. In this latter case there is no need to use a test database and the data can be entered directly, though the classification output will differ if different datasets are used. In

both approaches, the supervised and the unsupervised one, data are clustered on the basis of similarity and correlation criteria.

We adopted a specific version of ANN: Self-Organizing Maps (SOMs) (KOHONEN 1982, 1984). SOMs are based on “competitive learning”, an adaptive process in which the cells in a neural network gradually become sensitive to different input categories (KOHONEN 1982, 1984). SOMs consist of a two dimensional array of neurons, fully connected, with no lateral connections, arranged on a square or hexagonal lattice (the map). Vectors can be different skull measures or, as in the case of this review article, discrete traits of dental morphology. In this process:

- 1) identical vectors will be mapped at the same position of the map;
- 2) slightly different ones close to each other;
- 3) very different vectors will be mapped far from each other.

The visual aspect of data representation obtained by SOMs is somewhat similar to a classical Multidimensional Scaling (MDS) or to a Principal Component Analysis (PCA) plot. SOMs are topology-oriented but the distances between mapped data points do not correspond to a MDS representation (MDS takes a set of dissimilarities – as in a distance matrix – and returns a set of points such that the distances between the points tend to be as close as possible to the dissimilarities), though they describe more accurately the neighbourhood of items (KASKI 1997). For this reason, SOMs should be preferred to MDS or PCA when all the different data (vectors) slightly differ one from another, as is often the case with paleontological data. A type of division of labour emerges in the network when different cells specialize to represent different data points. The SOM maps are divided into an arbitrary number of cells (5×5; 6×6; 7×7; etc.), according to user specifications and, once the analysis is done, each cell (neuron) corresponds to a cluster.

The degree of specialisation is enhanced by the competition among cells: when an input arrives, the neuron that is best able to represent it “wins” the competition and can continue the learning process. If there is ordering between the cells, i.e. when the cells are located on a discrete map, the competitive learning can be generalised. If not, the winning neuron and its neighbours on the map are allowed to learn: neighbouring cells will gradually specialize to represent similar inputs and the representations of input data will become ordered. This is the essence of the SOM algorithm (KASKI 1997). The SOM algorithm is very robust, as it is indicated by the fact that it can go through vectors having missing descriptors (KASKI 1997). With sets of vectors presenting missing descriptor values, only the available values will contribute to the learning process of the map, while the missing values will not. For an effective learning process, it is obviously advisable

to process vectors having only a few descriptors missing. Each cell of the map, indexed with i , represents a reference vector \mathbf{m}_i whose components correspond to synaptic weights. In the exploration of data, the cell (indexed with c) whose reference vector is nearest to the input vector \mathbf{x} , becomes the winner of the competition between all the different input vectors:

$$c_i = c(\mathbf{x}) = \arg \min \{ \|\mathbf{x} - \mathbf{m}_i\|^2 \} \quad (1)$$

Usually the Euclidean metric is used as a measure of $\|\mathbf{x} - \mathbf{m}_i\|^2$.

The winning unit (c) and its neighbours adapt to represent the data point even better by modifying their reference vectors towards the current data. The amount the units learn will be governed by a neighbourhood function h , which decreases with the distance of all units different from the winning unit on the map. If the locations of cells i and j on the map grid are denoted by the two-dimensional vectors \mathbf{r}_i and \mathbf{r}_j , respectively, then

$$h_{ij}(t) = h(\|\mathbf{r}_i - \mathbf{r}_j\|; t) \quad (2)$$

where t denotes time.

During the learning process, at time t , the reference vectors are changed iteratively according to the following adaptation rule:

$$\mathbf{m}_i(t+1) = \mathbf{m}_i(t) + h_{ci}(t)[\mathbf{x}(t) - \mathbf{m}_i(t)] \quad (3)$$

where $\mathbf{x}(t)$ is the data point at time t and $c = c(\mathbf{x}(t))$ is the index of the winning unit. In practice the neighbourhood function is chosen to be wide at the beginning of the learning process, to guarantee global ordering of the map, and decreases in width and height, during the learning process. Consisting in the winning selection by equation (1) and in the adaptation of the synaptic weights by equation (3), the learning process can be modelled with a neural network structure where the cells are coupled by inhibitory connections (KOHONEN 1993; KASKI, KOHONEN 1994). By virtue of its learning algorithm, the SOM forms a non-linear regression of the ordered set of reference vectors into the input surface. The reference vectors form a two-dimensional “elastic network” that follows the distribution of data.

4. EXAMPLE OF CLASSIFICATION

As we mentioned in the introduction, the purpose of the analysis (COPPA *et al.* 2007a) was the classification of a new dental sample (TBN-BC7) excavated in the Tabun cave (Israel) that could have been considered a new

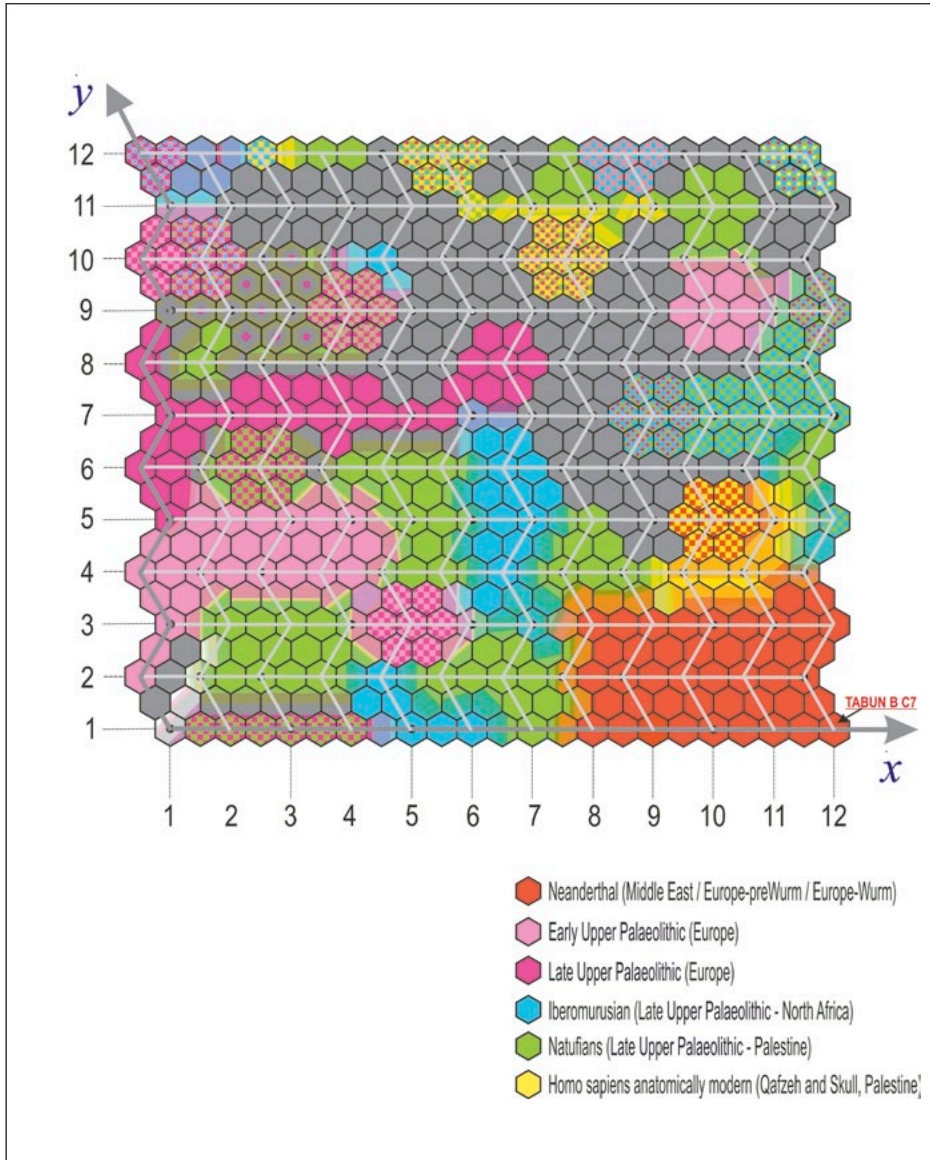


Fig. 3 – Example of a Self-Organizing Map (KOHONEN 1982) concerning the analysis of 126 dentitions from different geographic locations and periods. The map is a 12x12 lattice corresponding to 144 neurons. Several samples can be mapped to a same neuron (not shown). We display only the position of the sample Tabun BC7 that falls in an area whose neurons became specialized in the description of the Neanderthal teeth morphotype. The map has been colored according to time periods and geographical areas. Gray cells correspond to empty neurons, meaning that no inputs were linked to them in the classification process (redrawn from COPPA *et al.* 2007a).

Neanderthal specimen, though the issue was debated. Twenty-three dental morphological traits were scored on the Tabun BC7 dentition and compared to a reference dataset of 125 known samples belonging both to Neanderthals and to anatomically modern human specimens from Europe, Middle East, and North Africa, that is covering a large area around the location where the sample TBN-BC7 was discovered. The scoring values of the traits were dichotomised (presence/absence) and a first binary matrix (1/0) was obtained (similarly to the example provided in Fig. 1). When this database was processed with the Self-Organizing Maps algorithm the obtained map (whose size we set at 12×12 cells) displayed an ordered representation (Fig. 3).

Although the upper portion of the map shows an overlapping of dental features for individuals belonging to different periods and samples, this is not the case for Neanderthal samples, which are grouped in the lower right corner of the lattice (in orange). It should be noted that highly divergent samples, in all SOM maps, tend to be mapped at one extreme of the map, as is the case for Neanderthal teeth. The topology and shape of the Neanderthal area suggest that the range of variability of dental features of Neanderthals was different from, and non-overlapping with, the range of variation of the other reference samples and confirmed the belonging of the Tabun BC7 sample to the Neanderthal teeth morphotype.

5. CONCLUSIONS

We have successfully experimented the classification properties of Self-Organizing Maps (KOHONEN 1982, 1984), an application of Artificial Neural Networks (ANNs) and demonstrated how robust and reliable they are in processing databases heavily flawed by missing data, as it is the case of human dentitions excavated in an archaeological context. ANNs, and SOMs in particular, are capable of classifying the variation through time and space of ancient or degraded human biological material and must be regarded as an invaluable tool to assess ancestry in both archaeological and forensic contexts and to establish the phyletic relations existing between fossil remains. This is why ANNs will be particularly useful to assess if hybridisation occurred between Neanderthal populations, or other species of the genus *Homo*, and populations of anatomically modern humans, and to empirically measure the extent of it (DUARTE *et al.* 1999; DI VINCENZO *et al.* 2012; CONDEMI *et al.* 2013).

The classification that ANNs enable, by making tractable the morphological variation of past human populations at the individual level, will lead to a more accurate depiction of intra-population variation and, ultimately, to a better description of many demographic processes of the past, like migration and admixture. In a wider scale, computational archaeology may also benefit of such neuronal classifications. The computational analysis of artefact features

pioneered by Stephen Shennan, like ceramics or basketry that can be dissected in many computationally tractable features (SHENNAN 2001; JORDAN, SHENNAN 2003), may also benefit of this methodology. In fact, similarly to what occurs in anthropology, artefacts are often incomplete and missing data (pieces, attributes, features). A more widespread application of ANNs will certainly prove much convenient for the anthropological and archaeological community of scholars and we hope to have here contributed to their dissemination.

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ABSTRACT

The paper illustrates how the application of a specific version of Artificial Neural Networks, Self-Organizing Maps (SOMs), enabled a more accurate analysis of human dental morphology. SOMs enable the processing of individual samples (dentitions) because they can cope with missing data. In fact, in archaeological samples of human remains, teeth are often broken or missing making a complete set of morphological traits often impossible to achieve. Other classification methods like Principal Component Analysis, Multidimensional Scaling, Mean Measure of Divergence, Multiple Correspondence Analysis do not handle missing descriptors and incomplete data matrices have to be “filled in”, thus leading to a certain approximation in the outcome with a lack of geographical or temporal resolution, as many incomplete samples have to be merged into a virtual one that does not present missing descriptors. Our discussion about the proficiency of SOMs, and ANNs in general, in the exploration and classification of anthropological databases concerning morphology is based on a specific case study, that is the classification of a Neanderthal sample. Through this example we would like to attract the attention of anthropologists and archaeologists to a very flexible methodology that is seldom applied, despite being widely used in many other disciplines.