

## **Chapter 2**

# **Geometric morphometrics in archaeology**

# 1. Introduction

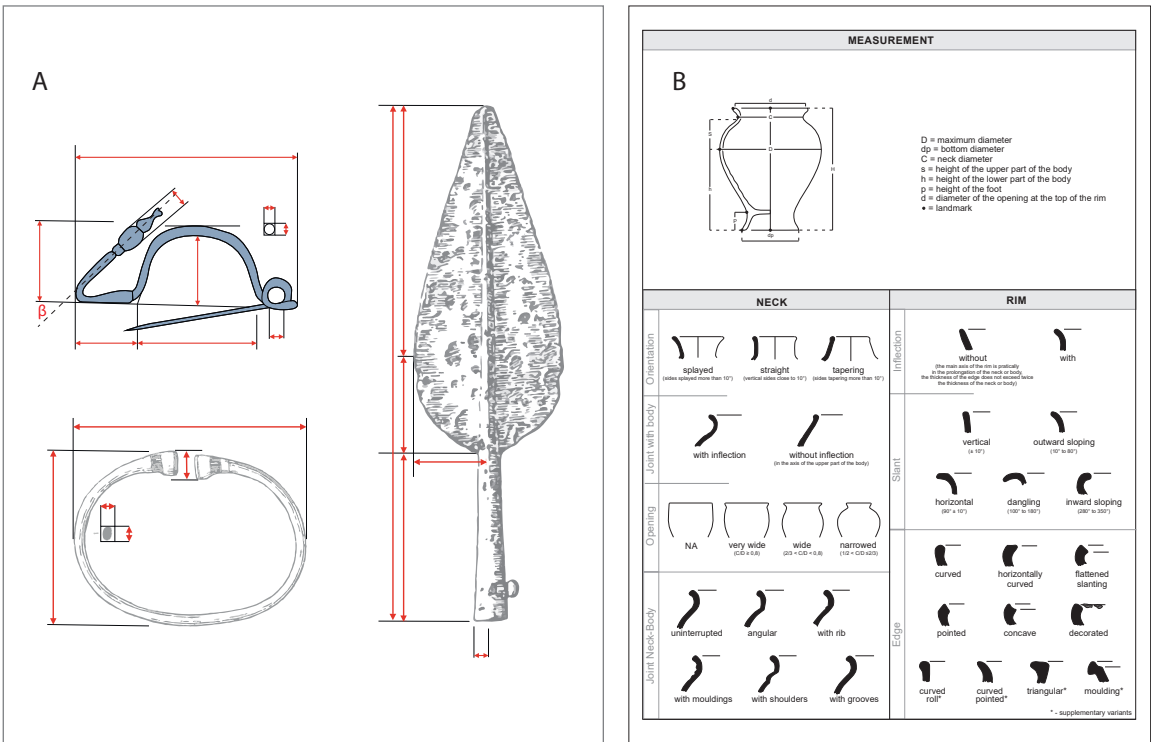
The goal of this chapter is to provide a brief introduction to morphometrics and its applications for the study of artefact shape in archaeology, from the acquisition to the statistical analysis of shape data. The focus here is not the evolution of morphometrics as a scientific methodology, although a brief history of its development is presented. This chapter can thus serve as an overview of the literature on the use of geometric morphometrics in archaeology. More information about traditional and modern morphometrics, especially in the context of life sciences, can be found elsewhere (Rohlf 1990; Bookstein, 1991; Lestrel, 1997, 2000; Adams et al., 2004; Zelditch et al., 2004; Slice, 2005; Reyment, 2010).

## 1.1. Traditional morphometrics

Morphometrics is often considered as the study of shape variation and its covariation with other variables (Bookstein, 1991; Dryden and Mardia, 1998; Adams et al., 2004).

Traditional morphometrics, sometimes called multivariate morphometrics (Blackith and Reyment, 1971), is based on the study of shape, generally expressed by linear distances (length, width, height, etc.), angles, and/or ratios; or by a set of pre-defined categories (triangular, rounded, oval, etc.; Fig. 1). Morphological variables are usually treated by multivariate statistical analysis in order to identify any structuration pattern(s), and differences between samples, or to investigate relationships between shape and size (Marcus, 1990; Slice, 2005).

Interest in traditional morphometric analysis for archaeology greatly increased as advances in biometrics and numerical taxonomy were proposed and developed by biologists and statisticians in the 1960s and 1970s (e.g. Sokal and Sneath, 1963). Shape contained measurable information that could be used for computer-aided classifications and seriations of archaeological artefacts. Methods of “typometrics” (Djindjian, 1991, p. 74) were developed by researchers from the numerical taxonomy movement – many of them present at the “Anglo-Romanian Conference



**Fig. 1.** Traditional morphometrics in archaeology. A) Measurements. B) Descriptive system (set of pre-defined categories).

on Mathematics in the Archaeological and Historical Sciences in Mamaia (Romania)”, held in 1968 (Hodson et al., 1971). Their methods were rapidly adapted by the broader archaeological community and increasingly used to classify a wide range of artefacts, notably brooches (Hodson et al., 1966, 1971), lithic artefacts (Boutin et al., 1977; Monnier and Etienne, 1978; Vigneron, 1979), bronze axes (Vuaillat and Massonnie, 1974), and ceramics (e.g. Hardy-Smith, 1974; Orton, 1974; Shennan and Wilcock, 1975; for a general overview see Orton, 1980 and Orton et al., 1993).

## 1.2. Modern geometric morphometrics

The need to rethink traditional morphometrics arose in the 1980s when a series of problems appeared that could not be solved by approaches based on linear measurements, ratios and angles. For instance, it became evident that (i) it was not possible to assess the homology of measurements on objects without precisely defined homologous points, (ii) a set of measurements did not automatically express the spatial relationship existing between them (an object with a maximum height of 1 cm and maximum length of 0.5 cm can be an oval, or a teardrop, or another shape entirely), (iii) measurements taken from a single object were inter-correlated (if starting from the same point), and (iv) no definitive solution to remove the size effect and thus observe only the shape had yet been found. Other limitations were that (v) generating datasets required a considerable amount of time, (vi) the operator effect on data acquisition and/or treatment was rarely discussed or quantified, and that (vi) some scarce and/or incomplete objects were often removed from the study (e.g. Adams et al., 2004; Zelditch et al., 2004; Urbanová and Králík, 2009).

New-wave morphometrics stated that most of these limitations could be overcome by studying the shape of objects, expressed not as sets of measurements, but by means of geometric relationships. The key aspect of modern morphometrics lies in the definition of shape as “all the geometric information that remains when location, scale and rotational effects are filtered out from an object” (Zelditch et al., 2004, p. 11; Kendall, 1977). The basic idea behind this is that, if any two or more objects are positioned in space, observable differences between them are caused by four factors – differences in position, size, orientation, and shape. When the first three factors are removed from the equation, objects differ only by their shape.

Although the idea of shape is simple, a considerable amount of work was required to transpose theoretical considerations about shape into shape theory, expressed in terms of mathematics (notably geometry), physics, statistics, and computer graphics. These aspects were developed more specifically by F. J. Rohlf, F. L. Bookstein, N. MacLeod, D. E. Slice, L. Marcus, P. E. Lestrel, F. P. Kuhl, and G. R. Giardina, through a variety of methods known together as geometric morphometrics.

The common element for all these methods is that they represent the shape of an object in a quantitative continuous way, in the form of shape variables. These shape variables characterise the shape of the original object, just as its chemical composition characterises the elements that compose it. They can also express the amount and direction(s) of shape transformation needed to metamorphose the shape of a given object into that of another.

Modern geometric morphometric methods are nowadays widely applied in life and other natural sciences. Shape variables are generally used to investigate both shape variation in the samples studied, and its covariation with any other discrete (e.g. gender, type, region) or continuous (e.g. size, weight, time) variables.

Although modern geometric morphometrics has not yet become a mainstream technique for the analysis of archaeological artefacts, archaeology was nevertheless in the forefront of key events related to the birth and development of modern morphometrics. Kendall, who defined

the modern concept of shape (Kendall, 1977, 1981, 1984, 1986), largely contributed to research in archaeology, notably through the application of computational Seriation (Kendall, 1963, 1971) and Multidimensional Scaling (Kendall, 1971). Kendall claimed that his interest in shape theory “was prompted by a statistical topic on the fringes of archaeology” (Kendall, 1989, p. 87). One of the earliest demonstrations of modern morphometric analysis was the study of 52 megalithic stones located near Land’s End (England), in order to find out whether they were aligned linearly or randomly (Kendall and Kendall, 1980; Kendall, 1989).

Although the term, concept, and terminology of geometric morphometrics as defined and used in the life sciences were not initially applied to the study of archaeological artefacts, some morphometric methods were gradually adopted, as computational power increased. Many computer applications and artefact databases were developed during the 1980s. Outline-based morphometric methods could thus be used more easily (e.g. B-spline curves, Bezier curves, cubic splines, tangent representation, Fourier Analysis; Jones and Wilcock, 1974; Main, 1978, 1986, 1988; Leese and Main, 1983; Gero and Mazzullo, 1984; Hall and Laflin, 1984; Laflin, 1986), and several tools were developed to compare artefact outlines (e.g. Jičín and Vašíček, 1971; Orton, 1974, 1987; Wilcock and Shennan, 1975; Gero and Mazzullo, 1984). However, these studies did not overtly set out to inspect shape variation, but rather sought to identify the closest analogy to the artefact in question in a referential database. This enthusiasm for computer-based archaeology shifted during the 1990s to applications based on imaging and Geographic Information Systems (GIS), thus focusing less on artefact shape and more on spatial organisation (Conolly and Lake, 2006).

The use of geometric morphometric methods in archaeology remained chiefly the domain of the life sciences, and biological remains were the main object of investigation. Pollen was used to study and model plant domestication and diffusion (e.g. Bouby et al., 2005; Terral et al., 2010), while human and animal skeletons (mainly skulls, pelvises, and long bones) were used to investigate sexual dimorphism, age and differences between samples of different geographic and temporal origin (e.g. Bookstein et al., 2003; Bruner, 2004; Gunz et al., 2009; Ottoni et al., 2013; Cucchi et al., 2017; Weissbrod et al., 2017).

Archaeology in the 21st century has now adopted geometric morphometric methods for the study of archaeological artefacts. The most successful applications to date have been with lithic artefacts (e.g. Lycett et al., 2006; Costa, 2010; Eren and Lycett, 2012), ceramics (e.g. Saragusti et al., 2005; Karasik and Smilansky, 2011), brooches (Small, 1996; Dryden, 2000), statues (Buxeda i Garrigós and Gordaliza, 2011; Urbanová et al., 2011), and Bronze Age axes (Forel et al., 2009; Monna et al., 2013).

## 2. Role of morphometrics in the study of archaeological artefacts

Archaeology is largely based on the study of artefacts, i.e. the intentional products of our ancestors. By definition, artefacts are “dead” objects, inert, motionless, mute, found either buried or lying on the surface of the Earth. Archaeological knowledge is based on the analysis of these dead items, by observing their attributes and spatial relationships, identifying any meaningful structure, and then interpreting these findings in terms of current paradigms or memes in archaeology (Spaulding, 1960; Neustupný, 2007, 2010).

The key question here is how geometric morphometrics can contribute to the archaeological investigation of artefacts. Generally, geometric morphometrics focuses on the quantitative analysis of shape information. In archaeology, geometric morphometrics combined with other statistical techniques can be used for:

Objective	Research question	Statistics	Literature/Chapters
(Semi-)automatic data acquisition)	What is the best method?	normal vectors circle fitting profile fitting rim fitting	Halif, 1997, 1999; Halif and Flusser, 1997; Cao and Mumford, 2002; Kampel et al., 2005; Mara and Sablatnig, 2006; Mara et al., 2007; Karasik and Smilansky, 2008; Mara, 2009; Karasik, 2010; Han and Hahn, 2014
		-	Chapter 3
Creating morpho-typology	Are artefacts organised by shape?	PCA CA	Gilboa et al., 2004; Smilansky et al., 2004; Karasik et al., 2005, 2014; Saragusti et al., 2005; Grosman et al., 2008; Karasik and Smilansky, 2011
	How many groups exist? Can morpho-typology be automatically generated?	PCA/MBCA	Chapter 4 Chapter 5 (Wilczek et al., 2014) Chapter 6 (Wilczek et al., 2015)
Shape comparison between pre-classified artefacts	Is there any shape difference between groups? Can shape difference between groups be visualised?	PCA LDA MANOVA	Lycett et al., 2006; Adan-Bayewitz et al., 2009; Forel et al., 2009; Costa, 2010; Karasik, 2010; Grosman et al., 2011; Karasik and Smilansky, 2011; Charlin and Rolando, 2012; Eren and Lycett, 2012; Lycett and Von Cramon-Taubadel, 2013; Okumura and Araujo, 2014; Eren et al., 2015
		PCA MBDA LDA MANOVA SOM	Chapter 5 (Wilczek et al., 2014) Chapter 6 (Wilczek et al., 2015) Chapter 7
Identification of best analogy for complete artefacts	What is the closest analogy to a given artefact?	calculation of similarities between artefacts	Martínez-Carillo et al., 2009, 2010; Lucena et al., 2014
	To which group does this artefact belong?	MBDA	Chapter 6 (Wilczek, Monna et al. 2015)
Identification of best analogy for incomplete artefacts (fragments)	What is the closest analogy to a given fragment?	calculation of similarities between a fragment and artefacts or fragment	Sablatnig and Menard, 1998; Kampel et al., 2001; Adler et al., 2002; Kampel and Sablatnig, 2002; Maiza and Gaildrat, 2005; Karasik and Smilansky, 2011; Picolli et al., 2015
	To which group does this fragment belong?	calculation of similarities between a fragment and existing artefacts or “potentially existing” artefacts projection of a fragment into a morphospace of all possible fragments	Chapter 4
Assessing variability between classes of artefacts	Which class of artefacts presents the greatest variability?	coefficients of variation Mahalanobis distance	Eren and Lycett, 2012; Monna et al., 2013
		convex hull calculation	Chapter 5 (Wilczek et al., 2014)
Assessing symmetry, regularity, and deformation in artefacts	How symmetrical or regular is this artefact?	calculating residual distances between expected and observed shape	Karasik et al., 2010, 2014; Mara et al., 2004; Saragusti et al., 2005; Lycett et al., 2006; Mara and Sablatnig, 2006, 2007; Lycett, 2008
		idem	Chapter 3
Testing and visualising shape changes over (continuous) time	Are artefact shape changes related to time?	-	-
		MANCOVA Multivariate Regression	Chapter 7

**Table 1.** General overview of research questions and statistical methods in the literature (chapters dealing with the same topics are also indicated). PCA – Principal Component Analysis; CA – Cluster Analysis; MBCA – Model-Based Cluster Analysis; MBDA – Model-Based Discriminant Analysis; LDA – Linear Discriminant Analysis; MANOVA – Multivariate Analysis of Variance; MANCOVA – Multivariate Analysis of Covariance; SOM – Self-Organised Maps.

- (Semi-)automatic data acquisition;
- Creating morpho-typologies, i.e. typologies based solely on shape; if required, classification can also introduce other descriptors (e.g. decoration, composition, or mode of fabrication);
- Shape comparison between pre-classified artefacts;
- Identification of best analogy for complete artefacts and prediction of class (“automatic classification”) for complete artefacts;
- Identification of best analogy for incomplete artefacts (fragments) and prediction of class (“automatic classification”) for incomplete artefacts;
- Assessing variability between classes of artefacts, notably for comparison of level of standardisation between classes of artefacts;
- Assessing symmetry, regularity, and deformation in artefacts;
- Testing and visualising shape changes over (continuous) time.

The choice of method depends on the research question, data selection, and on the logical and methodological research design developed in response to this question (e.g. [Legendre and Legendre, 1998](#)). In the absence of a focused research question, applying morphometrics to data is unlikely to provide any meaningful answers.

The following table ([Table 1](#)) presents a general overview of several previously studied research questions from the literature, and the statistical methods used to answer them. In addition, chapters in this thesis that deal with the same topics are also indicated.

Results obtained with geometric morphometrics and statistics are based on mathematical concepts, and are therefore reproducible. The crucial question is to what extent the results obtained can be considered as objective. The degree of objectivity depends on the selection criteria, the choice of model and method, and the quality and quantity of the artefacts studied. The availability of artefacts is not a matter of choice, but rather the objective result of archaeological surveys and excavations. Choosing models, methods, and selection criteria is the responsibility of the research team, and such choices will pre-condition the objectivity of the results. Systematically recording the choices made and the reasons for those choices will enhance reproducibility and thus contribute to the objectivity of the study.

### **3. Applying geometric morphometrics to archaeological artefacts**

The workflow to analyse artefacts using geometric morphometrics can be summarised as follows. Once the research question and hypotheses have been defined, the appropriate shape data are acquired, and processed by the best adapted method to obtain shape variables. These shape variables are then analysed by statistical techniques to provide coherent scientifically based answers to the research question.

This section provides a general description of the methods used in the studies presented here.

#### *3.1. Data acquisition*

The initial step in archaeological geometric morphometrics consists in acquiring shape data, (i) directly on the artefact (positioned in a fixed coordinate system), (ii) from any 2D image (e.g. drawings, orthogonal photographs, etc.), or (iii) from 3D models (see [Fig. 2](#) for a general overview of 3D acquisition techniques). Artefact shape can be expressed as landmarks and/or outlines.



### 3.1.1. Landmarks

Most modern morphometric studies are based on the treatment of landmark data. Landmarks, or homologous points, are “discrete anatomical loci that are arguably homologous among all the individuals under analysis” (Benítez et al., 2014, p. 1) and are expressed by two- or three-dimensional Cartesian coordinates (e.g. Rohlf and Marcus, 1993; Slice, 1996). A set of landmarks on a given artefact is called a configuration. Three types of landmarks are often distinguished, based on the degree of precision with which each point can be located on the artefact (Bookstein, 1991). Landmarks of Type 1 correspond to the point where three structures meet. Landmarks of Type 2 correspond to the maxima of curvature. Landmarks of Type 3 correspond to the most external points on the artefact (Fig. 3).

The landmarks identified on the artefact: (i) should be homologous loci, (ii) should not alter typological positions relative to other landmarks, (iii) should provide adequate coverage of the morphology of the object, (iv) should be found repeatedly and reliably, and (v) should lie within the same plane (Zelditch et al., 2004).

A case study using landmarks on La Tène brooches is presented in Chapter 7.

### 3.1.2. Outlines

Identifying landmarks on archaeological artefacts is often problematic. Problems with artefacts arise (i) from their state of preservation, (ii) from their great variability in shape, due to many different factors (e.g. functional, chronological, stylistic, regional, and social differences in production), and (iii) from the absence of internal structure, as most artefacts are recorded in the literature in the form of external outlines. However, morphometric analysis can be performed on outline data. Outlines can be open or closed, i.e. with a beginning and end, or forming a continuous contour. Outlines are usually represented by an ordered set of discrete 2D/3D Cartesian, or polar coordinates or by what is known as chaincode (Slice, 2005).

Case studies using outlines can be found in Chapters 4 and 5 (ceramics), and 6 (Bronze Age axes).

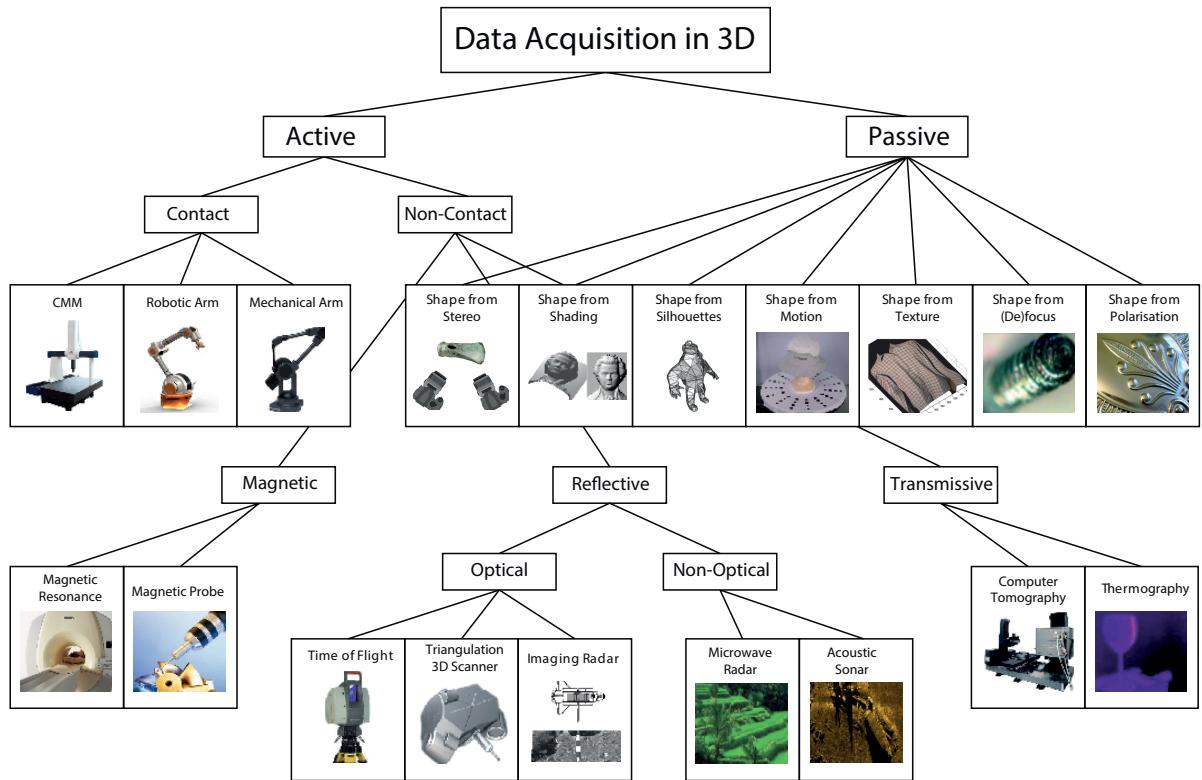
## 3.2. Processing

If two artefacts are positioned in space, differences between them are caused by size, position, orientation, and shape. In order to observe differences in shape alone, the first three factors must be removed to allow the artefacts to be superimposed. The distance between two or more objects can be minimised either by direct calculation or by optimisation. These minimised distances are usually called shape variables. Shape variables in outline-based methods are coefficients obtained by mathematical transformation.

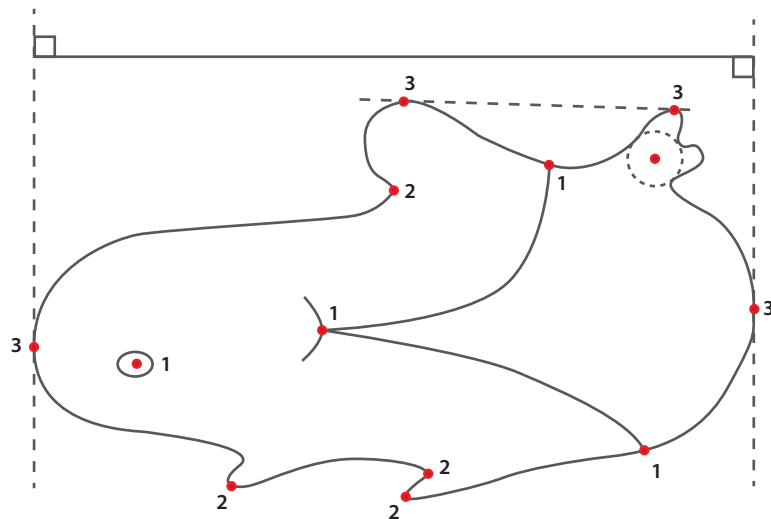
### 3.2.1. Size

To observe differences between artefact shapes, size correction must precede the calculation of shape variables. The commonest way to remove the size effect in landmark-based approaches is by scaling configurations by their corresponding centroid size, i.e. the sum of Euclidean distances between the centroid and every landmark in the configuration (Gower, 1971). In outline-based approaches, size can be removed by scaling: (i) relative to the perimeter (Schmittbuhl et al., 2003), or (ii) relative to the surface bounded by the outline (Sundberg, 1996; Hurth et al., 2003; Navarro et al., 2004). In the first case, the centred coordinates are divided by the perimeter length, in the second by the square root of the area bounded by the outline. In the case of very convoluted outlines, which have a longer perimeter than smooth outlines, it is not recommended to use the perimeter for size removal (Lestrel, 2000).

Several different methods of size removal for archaeological pottery are discussed in Chapter 5.



**Fig. 2.** General overview of 3D acquisition techniques (from Wilczek, 2013, Fig. 1; based on Curless, 1997, Fig. 1.1, 2000, Fig. 1; Lorient, 2009, Fig. 2.1, 2.2; Várady et al., 1997, Fig. 2; Vukašinović et al., 2007, Fig. 2).



**Fig. 3.** The three types of landmarks defined by Bookstein, 1991. 1. Point where three structures meet (Type 1), 2. Maxima of curvature (Type 2), 3. External points (Type 3). From Bookstein, 1991, Fig. 3.3.1.



### 3.2.2. Baseline registration

Landmark configurations or outlines with two homologous points can be superimposed directly by Baseline registration (Bookstein, 1984, 1986, 1991). The two homologous points are fixed at the ends of a baseline, defined arbitrarily, often as (0,0) and (1,0), resulting in Bookstein coordinates or Bookstein shape coordinates (Bookstein, 1996). If the points used for baseline registration are too close, results may be affected, especially regarding group differentiation (Slice, 2005).

A case study using baseline registration on archaeological pottery is presented in Chapter 5.

### 3.2.3. Procrustes superimposition

The most common landmark-based method for shape superimposition is Procrustes superimposition. The adjustment process in Procrustes superimposition, using the least-square approach, is based on landmark matching. Analysis is often performed in three consecutive steps: the first eliminates the effect of position, the second removes the effect of size, and the third removes the effect of orientation (Rohlf, 1990; Rohlf and Slice, 1990; Zelditch et al., 2004; Slice, 2005). In more detail:

- To remove the position effect, the centroids of configurations are translated to the origin of the coordinate system, ( $x=0$ ;  $y=0$ ; and in 3D,  $z=0$ ). Distances between configurations will then reflect differences in size, orientation, and shape.
- To remove the size effect, configurations need to be scaled to the same unit size (Gower, 1971), by dividing the coordinates of each landmark by the centroid size of the corresponding configuration. Distances between configurations will then reflect differences in orientation and shape.
- To remove the effect of orientation, the summed squared distances between corresponding landmarks are minimised. One configuration is fixed and labelled as reference ( $R$ ). The second configuration, labelled target ( $T$ ), is then rotated to minimise the distances between corresponding landmarks. The coordinates of the configurations aligned in this way are Procrustes coordinates. The sum of distances between corresponding landmarks (Procrustes distances) will then reflect differences in shape.

By removing position, size and orientation, the final dimensionality (degrees of freedom) of the shape space is  $2p-4$  for 2D data, and  $3p-7$  for 3D data, where  $p$  is the number of landmarks.

Procrustes superimposition uses the least-squares criterion, and is therefore sensitive to “outliers”, or imprecisely placed landmarks. The best-known problem is the Pinocchio effect: if one point is positioned at a great distance from the others, it will affect the alignment of all the other landmarks. For this reason, resistant fitting approaches were developed, using the median instead of the mean in alignment (Siegel and Benson, 1982; Rohlf and Slice, 1990; Slice, 2005).

Procrustes coordinates can be used to calculate the mean shape (Procrustes mean), which reflects the average shape of all the configurations. The vector of displacement between mean shape landmarks and each configuration (Procrustes residuals) can also be calculated. Mean shape and Procrustes residuals can be used to visualise differences between artefacts.

The most common method used to superimpose a set of objects is the General Procrustes Analysis (GPA), or General Procrustes Superimposition (GPS). The GPA consists in an iterative alignment process, in which one configuration is arbitrarily chosen as reference (mean shape). All configurations are then aligned with this reference. From these superimposed configurations, the new mean shape, i.e. new reference, and Procrustes distance are calculated. The process of fitting configurations to the reference continues until the difference in subsequently calculated Procrustes distances does not fall below an arbitrarily chosen threshold (Gower, 1975; Slice, 2005).

When the calculation of superimposition consists only in translation and rotation (without

size adjustment), the method is called Partial Procrustes Analysis. If the points can be mirrored in the analysis, the method is called Reflection Procrustes (Urbanová, 2009). If only two forms are superimposed, the analysis is called Ordinary Procrustes Analysis (OPA).

A case study using GPA on La Tène brooches is presented in Chapter 7.

#### 3.2.4. *The Iterative Closest Point algorithm*

Superimposition is also widely used in computer vision for 3D model alignment. The Iterative Closest Point (ICP) algorithm is used for this purpose (Besl and McKay, 1992; Turk and Levoy, 1994; Zhang, 1994; Fitzgibbon, 2003; Szeliski, 2011; Pomerleau et al., 2013). The difference between Procrustes analysis and ICP is that the ICP algorithm does not necessarily require landmarks for alignment. Any other features, such as non-corresponding point sets (point clouds), triangle sets (meshes), line segments (polylines), curves, or surfaces can be used (Besl and McKay, 1992).

The basic tenets of ICP are similar to Procrustes analysis, i.e. minimising distances between objects by modifying their position, size and orientation. An artefact (target) is given a set position in the coordinate system and another artefact (source) is iteratively scaled, translated and rotated in order to minimise the distance between them (Besl and McKay, 1992).

The use of ICP to identify the best analogy for pottery fragments is presented in Chapter 4.

#### 3.2.5. *Fourier analysis (harmonic or spectral analysis)*

Many outline-based geometric morphometric methods use Fourier descriptors calculated through Fourier analysis (Lestrel, 1997). Fourier analysis consists in transforming the original outline, expressed by (i) Cartesian coordinates, (ii) polar coordinates, (iii) tangent angles, or (iv) by chaincode (Claude, 2008), into an infinite series, called harmonics. Three types of Fourier Analysis are often presented in the literature: conventional Fourier analysis (FA), Elliptic Fourier Analysis (EFA) and Discrete Cosine Transform (DCT).

##### *Conventional Fourier Analysis*

Conventional Fourier Analysis transforms an outline by a trigonometric function into a set of harmonics, which can be represented as circles. Each harmonic is represented by two Fourier coefficients, which can serve as shape variables. Harmonics are ordered hierarchically, so that lower harmonics (i.e. larger circles) express overall shape, while higher harmonics (smaller circles) express local outline features. By summing harmonics (i.e. sets of coefficients), the shape of the artefact can be reconstructed by harmonic synthesis (inverse Fourier transformation). The greater the number of harmonics in the transformation, the more precise the reconstruction of the outline.

The Nyquist frequency criterion limits the number of harmonics to no more than half the number of points along the outline (Lestrel, 1989, 1997; Lestrel et al., 2005).

##### *Elliptic Fourier Analysis*

Elliptic Fourier Analysis (EFA), as proposed by Kuhl and Giardina (1982) decomposes an outline into a set of harmonic ellipses by separating the x and y coordinates, which are then expressed as a function of a third variable ( $t$ ). Elliptic analysis can be used on both 2D and 3D outlines.

Case studies using EFA can be found in Chapters 4 and 5 (ceramics), and 6 (Bronze Age axes).

##### *Discrete Cosine Transform*

Another Fourier-based method is Discrete Cosine Transform (DCT; Rao and Yip, 1990), originally developed for audio, video and image data compression. It is used to decompose an open outline into a set of Fourier harmonics, expressed by pairs of coefficients, which can be treated as shape variables (Dommergues et al., 2007; Forel et al., 2009).

Case studies using DCT on ceramics can be found in Chapters 4 and 5.

### 3.2.6. Other outline-based methods

Other outline-based methods used to transform open outlines into sets of shape variables are Tangent transform (e.g. [Main, 1978, 1986](#); [Karasik and Smilansky, 2011](#)), Polynomials (e.g. [Monna et al., 2013](#)), Bezier curves (e.g. [Engel, 1986](#); [Rohlf, 1990a, 1990b](#)), and Spline methods (e.g. [Evans et al., 1985](#); [Lafin, 1986](#); [Hlaváčková-Schindler et al., 2001](#); [Kampel and Sablatnig, 2002](#)), such as Basis Splines (B-splines), Cubic Splines, Parametric Cubic Splines, and Bell-shaped Splines (for a general overview see [Rohlf, 1990](#)).

### 3.3. Post-processing

#### 3.3.1. Investigation of shape variability – Principal Component Analysis

Principal Component Analysis (PCA) is the most frequently used multivariate method in geometric morphometrics. The main purpose of PCA is to reduce the dimensionality of the initial shape data, by replacing the original shape variables with Principal Components or Axes. These Principal Components (PC) are linear combinations of the original shape variables, and are mutually independent ([Jolliffe, 2002](#)). Principal Components are ordered in relation to the variance of the shape data they account for. A relatively low number of PC (from 3 to 10) is often sufficient to represent most (e.g. 90%) of the shape information in the dataset, and can thus be adequate for data interpretation.

In geometric morphometrics, the space thus defined by PCA is sometimes termed morphospace. The mean shape occupies the centre of the morphospace, around which all artefacts are distributed, based on their shape similarities.

In morphometrics, PCA is generally used to (i) transform original shape variables into linear combinations, (ii) inspect shape variation between artefacts, and (iii) identify shape-related organisation of artefacts. When the distribution of artefacts in a PCA-based morphospace represents spatially distinct classes, PCA can also serve to (i) create a classification, (ii) differentiate between classes, and (iii) integrate newly found artefacts into an existing classification.

#### 3.3.2. Classification

##### *Cluster Analysis*

Cluster Analysis (CA) is a generic family of methods designed to identify clusters (i.e. discrete loci) in a corpus of artefacts, based on discontinuities in the data ([Legendre and Legendre, 1998](#)). Cluster Analysis is the statistical technique most frequently used in archaeology for the creation of typologies (see e.g. [Orton, 1980](#); [Djindjian, 1991](#); [Baxter, 1994, 2003](#)). Clusters are formed based on similarities between artefacts. Results of hierarchical cluster analysis are usually represented as a dendrogram showing the distances between clustering artefacts.

##### *Model-based cluster analysis*

Model-Based Cluster Analysis (MBCA) is a modern classification method using probability models. The main difference between hierarchical and model-based clustering is that clusters are not defined by the similarities (i.e. distances) between artefacts, but rather by their shape. The advantage of model-based clustering over other classification techniques is that it allows (i) easier determination of the optimal number of clusters, (ii) a wide range of classification designs, (iii) more robust treatment of outliers, and (iv) probability values to be used to classify artefacts ([Fraley and Raftery, 1998, 2002](#); [McLachlan and Peel, 2000](#)).

In model-based clustering, the data are supposed to form groups, defined by the mean (corresponding to location) and the covariance (corresponding to shape, size and orientation). These parameters are usually estimated by a two-step iterative Expectation-Maximisation (EM) algorithm ([Dempster et al., 1977](#)).

The optimal classification model in MBCA and the number of typological groups are usually

determined by the Akaike or Bayesian Information Criterion (AIC, BIC; [Akaike, 1973](#); [Schwarz, 1978](#); [Wehrens, 2011](#)).

### 3.3.3. Investigation of differences between classes

Differences between classes can be investigated when membership is known in advance. Several statistical methods can be used to investigate differences between classes: (i) (Multivariate) Analysis of Variance, (ii) Linear Discriminant Analysis, or (iii) Canonical Variate Analysis.

#### *(Multivariate) Analysis of Variance*

Shape expressed by original or PCA-transformed shape variables is continuous in nature. The most appropriate statistical tests used to compare shape differences between groups are One-Way Analysis of Variance (ANOVA), Hotelling's  $T^2$  test, and One-Way Multivariate Analysis of Variance (MANOVA).

One-Way ANOVA tests if any difference exists between the means of two or more classes on one continuous dependent variable. The F statistic used for ANOVA calculation is the ratio between the variance explained by the categorical variable, and the variance that is unexplained. One-Way ANOVA in geometric morphometrics is generally used to compare differences between classes, based on size, or the selected Principal Component (e.g. [Gharaibeh, 2005](#)).

Hotelling's  $T^2$  tests if any difference exists between the vectors of the means of two classes on several continuous variables (e.g. shape expressed by a set of shape variables, or by a set of Principal Components; [Hotelling, 1931](#); [McLachlan, 1992](#); [Reyment, 2010](#)).

One-Way MANOVA has the same purpose as Hotelling's  $T^2$  test, but can be used to compare more than two groups.

The results of One-Way ANOVA and MANOVA indicate whether three or more classes differ statistically. Further information about which class differs significantly from the others can be obtained by additional post hoc multiple comparison procedures, such as LSD, Bonferroni, or Tukey.

The assumptions when using these methods are (i) the independence of observations, (ii) normally distributed data, (iii) the equality of variance, and (iv) the absence of outliers. A MANOVA also requires an adequate sample size (i.e. the number of artefacts within each class is higher than the number of dependent variables). In the case of assumption violation, differences between classes can be tested by using non-parametric alternatives: for example, Kruskal-Wallis ANOVA for One-Way ANOVA ([McKnight and Najab, 2010](#)), Two-group permutation test for Hotelling's  $T^2$  ([Urbanová, 2009](#)), or Non-parametric One-Way MANOVA for One-Way MANOVA ([Anderson, 2001](#)).

#### *Linear Discriminant Analysis*

The purpose of Linear Discriminant Analysis (LDA), is to optimally separate two or more classes of artefacts. Discrimination is achieved by identifying a linear transformation that maximises between-group variation while minimising within-group variation. The linear discriminant function calculated from an initial dataset can be used to classify newly found artefacts ([McLachlan, 1992](#)).

The LDA can be calculated only when the class for all artefacts is known in advance (*a priori*), and each object can be a member of only one class. Although LDA also assumes multivariate normal distribution, this technique remains reasonably robust even when the assumption of normality is not satisfied ([Klecka, 1980](#); [Lestrel, 2000](#)).

#### *Canonical Variate Analysis*

Canonical Variate Analysis (CVA) in geometric morphometrics serves as a powerful exploratory method to visually represent differentiation between classes of artefacts in a multidimensional space ([Lestrel, 2000](#)). Although based on the same principles as (M)ANOVA (i.e. maximising

between-group variation while minimising within-group variation), CVA calculation involves procedures that alter the multidimensional space, and thus do not allow statistical hypothesis testing (Zelditch et al., 2004).

## 4. Conclusion

This chapter has introduced all the morphometric and statistical methods that will be applied in the case studies presented in Chapters 4 to 7. It can thus serve as an overview of the literature on the use of geometric morphometrics in archaeology and provide a sound basis for the development of future morphometric applications.

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