Research Article

A brief review of shape, form, and allometry in geometric morphometrics, with applications to human facial morphology

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Abstract

We briefly and informally review the concepts of size, shape, and form and how they are estimated in geometric morphometrics using Procrustes analysis. We demonstrate how deformation grids and reconstructed shapes or forms can be used as powerful tools to visualize shape and form differences. Complex patterns of individual or group differences can be studied effectively by ordinations of shape space or form space. Allometry, the statistical relationship between size and shape, is estimated in geometric morphometrics by regression of the Procrustes shape coordinates on centroid size. We illustrate these methods by an application to human face shape. We reveal shape cues to body size in the adult male face, partly resembling ontogenetic allometry. Facial allometry might thus be an important confounding factor in studies of face perception and human mate choice.

During the last two decades, geometric morphometrics became the state-of-the-art method for statistical shape analysis in biology (Rohlf and Marcus, 1993; Bookstein, 1996; Adams et al., 2004; Mitteroecker and Gunz, 2009; Klingenberg, 2010). In this paper we briefly and informally review the concepts of size, shape, and form, and how they are estimated in geometric morphometrics. We further discuss how the classic concept of allometry is analyzed in contemporary geometric morphometrics and illustrate this by an application to human facial form. In the Appendix we provide some algebraic details on the visualization of shape and form differences.

Size and shape

It is a common practice in morphometrics to distinguish between the size and the shape of a biological structure. The *shape* of an object are the geometric properties that are invariant to translation, rotation, and scaling. In other words, the shape of an object is unaffected by changes in the position, the orientation, and the size of the object. Two objects have the same shape if they can be translated, rescaled, and rotated to each other so that they match exactly. For instance, the shape of a rectangle, which can be described by the ratio of the two different side lengths, does neither depend on the size of the rectangle, nor on its position and orientation. By contrast, the term *form* refers to the geometric properties invariant only to translation and rotation. Hence, form can be considered as "size-and-shape" (e.g., Dryden and Mardia 1998). The form of a rectangle (measured, for instance, by the two side lengths or by one side length together with the ratio of side lengths)

does not depend on the position and orientation of the rectangle, but both on its size and shape.

The size or scale of different objects is easy to quantify when the objects all have the same shape. For a set of rectangles, all of the same shape, any side length or diagonal length would be an equally suitable size measure. But whenever shape varies, size is an ambiguous concept and no unique quantification exists. For a set of rectangles varying both in size and shape, a single side length as size measure would be affected both by changes in shape (ratio of side lengths) and by changes in scale. Composite size measures, such as functions of the sum or of the product of the side lengths, may be less affected by shape changes than single measurements. Ultimately, it is up to the researcher to decide, based on biological considerations, whether a single measurement or a composite variable is the most useful size measure.

In contrast to classical morphometric approaches based on linear distances and angles, geometric morphometric methods are based on the Cartesian coordinates of measurement points, so-called *landmarks*. Landmarks have a position (two or three coordinates) and a name, expressing some sort of homology across all measured specimens (Bookstein, 1991). Since the geometry of the measured landmark configuration is preserved by the set of landmark coordinates, geometric morphometrics allows for effective visual representations of statistical results as actual shapes/forms or shape/form deformations (e.g., Bookstein 1991, 1996; Rohlf and Marcus 1993; Zollikofer and Ponce de Leon 2002; Adams et al. 2004; Zelditch et al. 2004; Slice 2007; Mitteroecker and Gunz 2009).

The most common measure of size used in geometric morphometrics is *centroid size* (CS): the square root of the summed squared distances between all landmarks and their centroid (Fig. 1). The centroid of a landmark configuration is the average (arithmetic mean) of all land-

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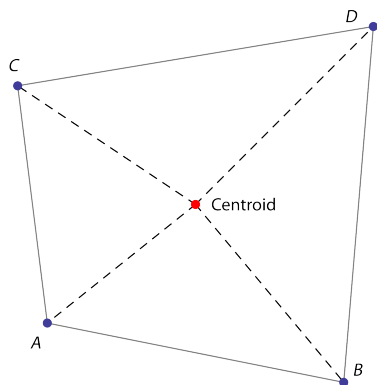*Email address:* philipp.mitteroecker@univie.ac.at (Philipp Mitteroecker)

Figure 1 – A configuration of four landmarks (A-D) with their centroid, which is equal to the average landmark position. Centroid size, the size measure used in geometric morphometrics, is equal to the square root of the summed squared distances between the landmarks and their centroid (square root of the summed squared lengths of the dashed lines).

marks. Centroid size is a composite size measure based on all landmarks and is proportional to the square root of the summed squared interlandmark distances. It has been shown to be uncorrelated with shape for small isotropic variation at each landmark (Bookstein, 1991; Dryden and Mardia, 1998). Isotropic variation (independent, identically distributed circular variation at each landmark) is the usual null-model corresponding to pure noise. It is an important property of a statistical method that pure noise does not induce an apparent "signal" (in this case a correlation between size and shape). Real biological data, however, may deviate considerably from isotropy and hence CS usually is not unrelated to shape.

The raw landmark coordinates do not only comprise information on size and shape of the landmark configurations, but also on their position and orientation. Landmark coordinates hence are not directly suitable for statistical analysis. The most common approach for separating shape from size and the "nuisance parameters" position and orientation is Generalized Procrustes Analysis (Gower, 1975; Rohlf and Slice, 1990). This method comprises three steps: translating all landmark configurations to the same centroid, scaling all configurations to the same centroid size, and iteratively rotating all configurations until the summed squared distances between the landmarks and their corresponding sample average is a minimum (Fig. 2). The coordinates of the resulting superimposed landmark configurations are called *Procrustes shape coordinates* as they only contain information about the shape of the configurations. (Note that scaling the configurations to unit CS resembles the usual approaches to size correction but is not the actual least-squares solution; it has thus been referred to as partial Procrustes fitting. Also, CS is slightly modified in the course of tangent space projection. For more details see Rohlf and Slice 1990; Dryden and Mardia 1998; Rohlf 1999).

The standardization for position, scale, and orientation is based on all landmarks. Alternatively, Procrustes analysis may be based on just a subset of landmarks, for example when some landmarks are known to vary in the sample or are subject to some treatment, whereas the other landmarks are relatively stable (e.g., Bookstein et al. 1999). When the registration is based on two landmarks only, the resulting shape coordinates are called two-point shape coordinates or Bookstein shape coordinates (Bookstein, 1991). Alternatives to the commonly used least-squares oriented Procrustes analysis are maximum likelihood Procrustes analysis (Theobald and Wuttke, 2006) and robust Procrustes analysis based on medians instead of means ("Resistant Fit"; Slice 1996).

Shape space and form space

Mathematical spaces are widely used in the sciences to represent relationships between complex objects (e.g., Stadler et al. 2001; Mitteroecker and Huttegger 2009). In a *shape space* the shapes of different objects are represented by single points, related by some notion of dis-

tance or proximity (as a measure of shape difference). The mathematical properties of the shape space for landmark configurations, usually referred to as Kendall's shape space, have been studied intensively (e.g., Kendall 1984; Bookstein 1991, 1996; Goodall 1991; Small 1996; Dryden and Mardia 1998; Rohlf 1999; Slice 2001). For p landmarks in k dimensions, it is a nonlinear Riemannian manifold of dimension $pk - k - k(k-1)/2 - 1$, which can be approximated locally by a Euclidean space of the same dimension, a so-called tangent space. Marcus et al. (2000) showed that the Euclidean approximation of shape space is appropriate for most biological data sets. The metric on Kendall's shape space is *Procrustes distance*, which is approximated by the Euclidean distance between two sets of Procrustes shape coordinates (square root of the summed squared distances between the corresponding landmarks after Procrustes superimposition). Procrustes distance is a measure of shape difference between two landmark configurations. It is zero only if the configurations have the same shape, and larger than zero otherwise. Standard multivariate methods, such as principal component analysis, can thus be applied to Procrustes shape coordinates in order to yield a low-dimensional representation (a so-called ordination) of shape space.

Figure 3a shows the first two principal components for the Procrustes shape coordinates of the landmark configurations in Fig. 2. Each point in this plot corresponds to the shape of one landmark configuration; the plot thus is a low-dimensional representation of shape space. The principal component loadings (eigenvectors of the covariance matrix of Procrustes shape coordinates) can be visualized by deformation grids ("relative warps"; Bookstein 1991).

A space relating the forms of different objects is called *form space* or *size-and-shape space* (or simply size-shape space). For landmark configurations, form space can be constructed in two principal ways: first, by standardizing the raw landmark configurations for position and orientation as in the usual Procrustes analysis, but not standardizing for size (e.g., Dryden and Mardia 1998, chapter 8), and second, by augmenting the Procrustes shape coordinates with the natural logarithm of centroid size (ln CS) as an additional variable (Mitteroecker et al., 2004a). The log transformation guarantees that for isotropic landmark variation the distribution in size-and-shape space is isotropic as well. Either set of variables can be used for principal component analysis (PCA) and other statistical analyses, and the Euclidean distance in these spaces can be interpreted as a measure of form difference. Both approaches yield similar results for small variation in size and shape, but they may differ if shape variation is large. We recommend constructing form space by augmenting the Procrustes coordinates by ln CS, following Mitteroecker et al. (2004a), because size is explicitly represented by centroid size in this approach and the loadings or coefficients
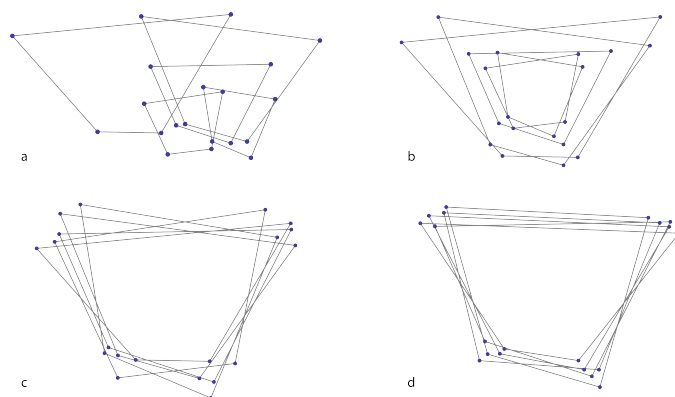

Figure 2 – Procrustes superimposition consists of three steps: translation, scaling, and rotation. As an example, take five configurations of four landmarks each. The raw landmark configurations in (a) are translated so that they all have the same centroid (b). The centered configurations then are scaled to the same centroid size (c) and iteratively rotated until the summed squared distances between the landmarks and their corresponding sample average position is a minimum (d). The resulting landmark coordinates are called Procrustes shape coordinates because variation in position, size, and orientation is removed.
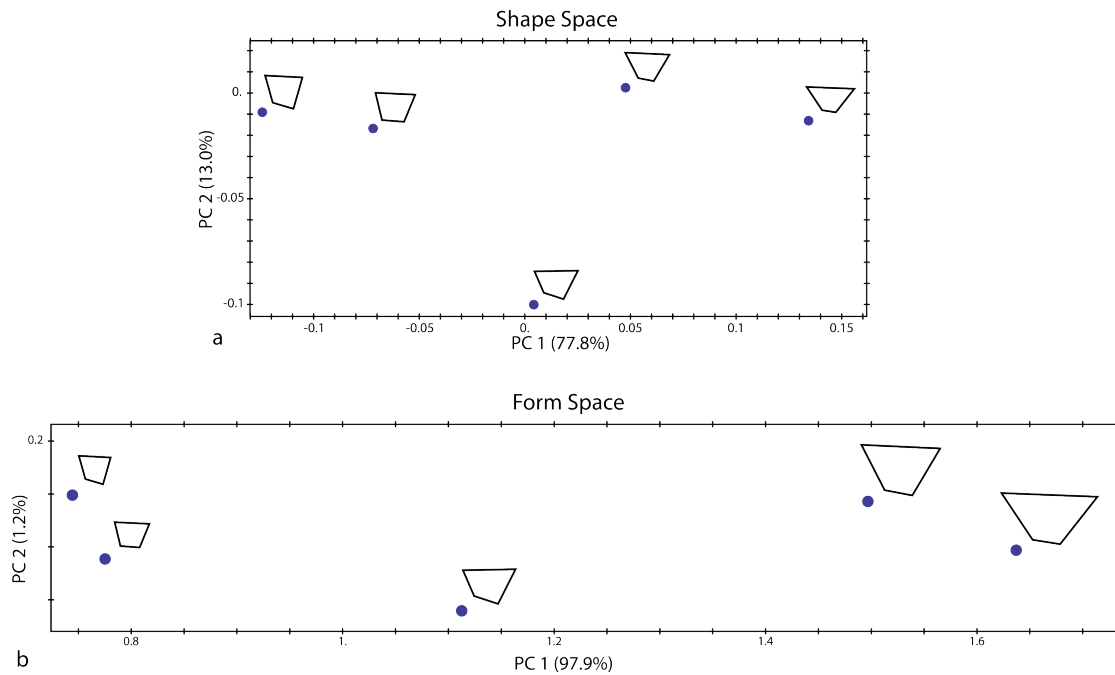
Figure 3 – (a) The first two principal components (PCs) of the eight Procrustes shape coordinates for the landmark configurations shown in Fig. 2. This plot is a low-dimensional representation of shape space, in which every point represents one shape. The actual shapes are drawn next to the corresponding points. (b) The first two PCs of the Procrustes shape coordinates and the natural logarithm of centroid size (nine variables in total). This plot is a low-dimensional representation of form space: every form is represented by a single point. The forms (scaled shapes) are drawn next to the corresponding points. Note that differences in size and allometric shape are closely aligned with PC 1 of form space (ln CS has a loading of 0.97 on the first eigenvector). The first PC thus accounts for a larger fraction of variance in form space than in shape space.

for size and shape, resulting from statistical methods such as PCA or multivariate regression, can directly be compared and interpreted.

In Fig. 3b, the first two PCs of form space (Procrustes shape coordinates plus ln CS) are shown for the landmark configurations in Fig. 2. This plot is a low-dimensional representation of form space. The forms are drawn next to the corresponding points. Note that these configurations are the same as those in Fig. 3a, but scaled to their original size. See the Appendix for more details on the visualization of principal components in form space.

Allometry

Allometry is the statistical association between size and shape (Mosimann, 1970), or as formulated by (Gould, 1966, p. 587) with a stronger emphasis on causality, "the study of size and its consequences". Allometry has been an influential concept in biology and morphometrics since Huxley's seminal treatise "Problems of Relative Growth" in 1932 (for reviews see, e.g., Gould 1966, 1977; Klingenberg 1998). Huxley's original version as well as its multivariate generalization by Jolicoeur (1963) were based on multiplicative growth models for size measurements such as bone lengths and other linear distances, areas, organ weights or volumes. Allometry was thus expressed as a power function between traits, or equivalently, as a linear relationship between the log-transformed traits. Logarithmic transformation of variables is also common as a way of overall size correction and to account for different units (e.g., Gould 1966; Bookstein et al. 1985; Marcus 1990).

Geometric morphometric studies of allometry require a methodological approach that differs in several aspects from the classic allometry studies. Procrustes shape coordinates are shape variables, not size variables, and they have no natural zero point (they are on interval scales, not ratio scales) and hence cannot be log transformed. Allometry is thus expressed as a – usually linear – function of the Procrustes shape coordinates, estimated by multivariate regression of the shape coordinates on centroid size or the logarithm of centroid size (Fig. 4; see also Bookstein 1991; Dryden and Mardia 1998; Klingenberg 1998; Monteiro 1999; Mitteroecker et al. 2004a). Note that in the classic approach to allometry a constant linear slope between two size variables indicates a constant size ratio, i.e., isometric size increase, whereas a constant linear slope between a shape variable and a size variable indicates

allometric size increase. The vector of regression coefficients resulting from the multivariate regression of the shape coordinates on CS describes how shape changes in response to one unit size increase. This coefficient vector, or an arbitrary multiple of this vector, can be visualized as a shape deformation.

Statistical significance tests for allometry, i.e., for the dependence of shape on size, usually are multivariate tests based on all shape coordinates (or a subset of shape coordinates). Since allometry is computed as a multivariate regression of the shape coordinates on CS, significance levels can be computed either by the usual multivariate parametric methods (e.g., MANOVA) or by resampling tests, which do not require normally distributed variables (e.g., Good 2000; Mitteroecker and Gunz 2009; Bookstein in press).
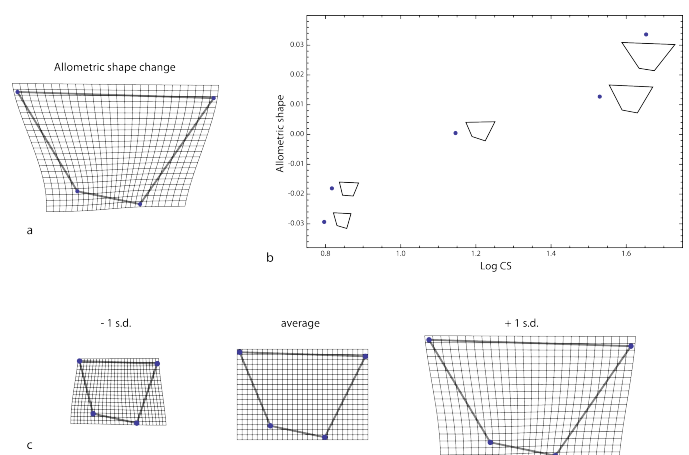

Figure 4 – (a) The multivariate regression (shape regression) of the Procrustes shape coordinates on ln centroid size is visualized by a TPS deformation grid. It represents the allometric shape change that corresponds to a size increase of 2 standard deviations. (b) Scatter plot of allometric shape (scores along the vector of regression coefficients) versus ln CS. (c) Visualization of PC 1 in form space (Fig. 3b). The left grid corresponds to a deformation from the average form to -1 standard deviation (s.d.) along PC 1 and the right grid to a deformation from the average form to +1 s.d. along PC 1. Note that the configurations change both in shape and size along this direction in form space. The shape changes depicted in (a) and (c) are very similar.

In many morphometric data sets, allometry is the most dominant factor of shape and form variation within one group. Thus allometry often is closely aligned with the first (within-group) principal component in shape space and particularly in form space (Mitteroecker et al. 2004a; see also Fig. 4c). However, since this is not guaranteed to be the case for all data sets, the actual multivariate regression of shape on CS is the more direct and reliable method to determine allometry and should be preferred over the first PC in shape space or form space.

Similarly, it has become common practice in geometric morphometrics to plot principal component scores of shape versus CS in order to assess or test for allometry. But this approach is likewise not ideal because single principal components are not necessarily good representations of allometric shape, especially if the PCA is over multiple groups. Instead of plotting PC scores, the score along the allometry vector (vector of regression coefficients) can be plotted as an "allometric shape score" against CS or other variables (Fig. 4; see also the Appendix). Statistical tests for allometry, the dependence of shape on size, should not be based on selected PCs, but should be multivariate tests based on all shape coordinates or all principal components. Of course, statistical tests for the dependence of *form* on size make no sense, since form comprises both shape and size.

Ontogenetic allometry, the association between size and shape across different age stages, often is used as an estimate of a population's ontogenetic trajectory (average growth pattern), especially when the individual calendar ages are not known. *Static allometry*, the association between size and shape within a single age stage (usually in adults), has often been used to explain the coevolution of size and shape (i.e., *evolutionary allometry* – the association between size and shape across multiple species) and as a model for functional and behavioral adaptations (e.g., Gould 1966, 1977; Lande 1979; Cheverud 1982; Klingenberg 1998; Marroig and Cheverud 2005; Schaefer et al. 2004; Gunz 2012).

In the classic concept of allometry, a trait is considered as negatively allometric if it increases less in size than other traits or overall size do. The trait's relative size thus decreases with increasing overall size. A trait with positive allometry, by contrast, increases more in size than other traits do. For instance, head size, compared to body size, is negatively allometric during human growth, whereas limb length is positively allometric. The variables used in geometric morphometrics are the shape coordinates of the landmarks. Positive or negative allometry cannot be inferred from single shape coordinates (they are shape variables, not size variables, and depend on the actual superimposition). All shape coordinates must be visualized together in order to draw inferences about the relative size increase or decrease of specific parts described by the landmarks (see the example below).

Comparison of allometric relationships

When comparing two or more groups of individuals, the question might arise how allometry differs across the groups. In recent years, a large body of literature on the morphometric comparison of growth patterns and ontogenetic allometries arose, advocating different morphometric and statistical approaches (e.g., O'Higgins et al. 2001; Ponce de Leon and Zollikofer 2001; Zelditch et al. 2003; Mitteroecker et al. 2004a,b, 2005; Gerber et al. 2007; Gerber 2011; Adams and Collyer 2009; Piras et al. 2011; Gunz 2012; Collyer and Adams this issue; Sheets and Zelditch this issue).

A simple and effective way to compare ontogenetic or static allometry across groups is the visual comparison of deformation grids or of series of reconstructed shapes representing group-specific allometry (see Fig. 4 and the example below). Since these deformations can easily be described in qualitative morphological terms, the comparison of deformations often leads to useful biological inferences.

Growth patterns and allometric relationships can be compared in a more abstract way by assessing the geometry of the corresponding vectors in shape space or form space. This can be particularly effective when comparing more than two trajectories (see the example below), but the biological meaning of such quantifications, especially of single parameters such as the angle between two trajectories, is not

always clear (Mitteroecker et al., 2004b, 2005; Huttegger and Mitteroecker, 2011). Ordinations such as principal component analysis or between-group principal component analysis (Mitteroecker and Bookstein, 2011) can be useful to explore ontogenetic and allometric trends in different groups. Growth trajectories and allometric vectors can be plotted within a principal component plot, either as linear vectors or as nonlinear estimates such as local linear regressions (e.g., Bulygina et al. 2006; Coquerelle et al. 2011). Alternatively, multiple allometric vectors can directly be compared by principal component analysis (for examples see the analysis below and Schaefer et al. 2004).

Parallel ontogenetic trajectories or allometry vectors in two or more groups indicate that the groups have the same linear pattern of (relative) growth during the observed age periods, even if they differ in the initial or in the adult morphology. If the average morphology of a species differs from its ancestral average morphology mainly by the extension, truncation, or the developmental timing of an otherwise conserved ontogenetic trajectory, the underlying evolutionary process is referred to as *allometric scaling* or *heterochrony* (Gould, 1977; Alberch et al., 1979; Klingenberg, 1998; Mitteroecker et al., 2004a, 2005; Gerber et al., 2007).

Ontogenetic trajectories or allometry vectors differing in direction indicate different growth patterns or ontogenetic allometries. Many studies advocated the use of the angle between two trajectories in shape space as a measure of difference in allometry or growth. While this can be useful, one should be careful in interpreting angles without the starting positions of the trajectories. For example, the angle alone is not sufficient to distinguish between diverging, converging, or intersecting trajectories. Furthermore, if two or more pairs of trajectories deviate in different directions in shape space or form space, the angles may not be comparable in a biologically meaningful way because they also depend on the number and spatial distribution of landmarks (Huttegger and Mitteroecker, 2011).

Example: Ontogenetic and static allometry of male faces

In this empirical example we apply the methods described above to assess allometry in human faces. A large number of studies investigated how face shape leads to masculinity attributions and other social inference, such as dominance, attractiveness, or trustworthiness (e.g., Zebrowitz and Montepare 2008; Schaefer et al. 2009; Little et al. 2011). Head size and body height are positively correlated (e.g., Geraedts et al. 2011), and body height has been found to play an important role in studies of social inference and mate choice (Pawlowski et al., 2000; Courtiol et al., 2010). Therefore, human facial allometry – aspects of face shape reflecting body size – seems to be of central relevance to these questions. However, it has received surprisingly little attention in the literature.

Our sample comprises frontal photographs of 19 boys (age 6–11 years) and 25 men (age 17–33 years). A camera with a 200 mm lens was positioned at eye height, 3.5 m away from the face. The heads were adjusted according to the Frankfort Horizontal Plane, and a ruler was placed next to one ear. This careful procedure is a prerequisite for the reliable assessment of undistorted face shape and size (e.g., Schneider et al. 2012).

On each image we digitized 35 anatomical landmarks and 34 semilandmarks to describe overall facial form (see Windhager et al. 2011 for details). Semilandmarks are points on smooth curves, for which the exact location on the curve cannot be identified and hence is statistically estimated. We used the sliding landmark algorithm for this purpose, which minimizes the bending energy, a measure of local shape difference, between each individual and the sample average (Bookstein, 1997; Gunz et al., 2005; Gunz and Mitteroecker, this issue). This approach allows for the joint analysis of biologically homologous points (anatomical landmarks) and curves (represented by geometrically corresponding semilandmarks).

After sliding the semilandmarks, all 44 landmark configurations were superimposed by a Generalized Procrustes Analysis and symmetrized by averaging each landmark configuration with its relabeled
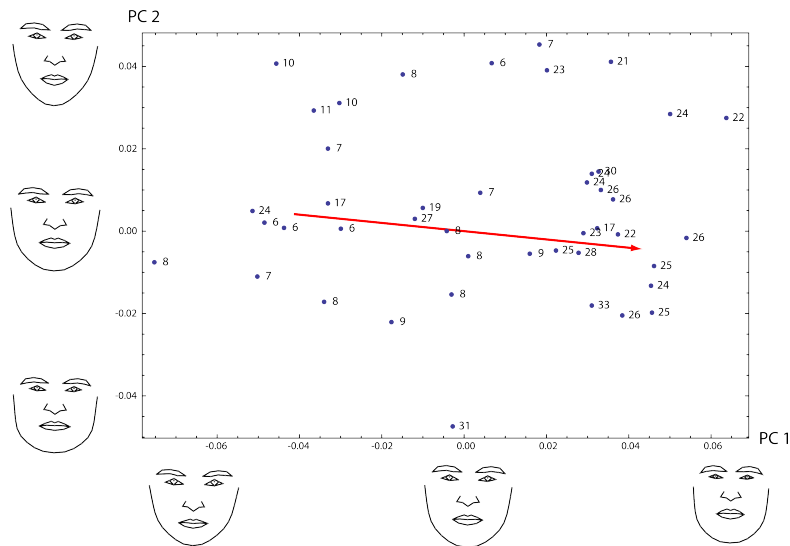
Figure 5 – Scatterplot of the first two principal components (PC) of face shape. The individuals are labelled by their age. The red arrow represents ontogenetic allometry – the regression of shape on ln centroid size. The facial reconstructions correspond to PC 1 scores of -0.7, 0, and 0.7 and to PC 2 scores of -0.5, 0, and 0.5, respectively. They visualize the shape differences associated with the first two PCs.

reflection (Mardia et al., 2000; Mitteroecker and Gunz, 2009). Figure 5 shows a scatterplot of the first two principal components (PC 1 and PC 2) of the resulting shape coordinates, accounting for 42% and 14% of total shape variation. The difference between juvenile and adult face shape is the most dominant factor of shape variation and hence is closely aligned with the first principal component of shape – a common finding in ontogenetic samples. The red arrow represents the coefficient vector for the regression of shape on ln centroid size, i.e., actual ontogenetic allometry, which is likewise aligned along PC 1. The three facial configurations visualizing shape differences along PC 1 show an overall elongation of the midface and the lower face, a relative decrease in eye size, as well as a thickening and lowering of the eyebrows. Shape changes associated with PC 2 reflect the differences between more gracile and more robust faces (Fig. 5) – a pattern known to correlate with prenatal testosterone exposure (Fink et al., 2005; Meindl et al., 2012).

Figure 6 shows the first two principal components of facial form (Procrustes shape coordinates augmented by ln CS). They account for 79% and 6% of total form variation, respectively. The shape differences corresponding to PC 1 are similar to the first PC in shape space (Fig. 5), but PC 1 in form space additionally comprises differences in size. As in most other morphometric datasets, PC 1 in form space accounts for a larger fraction of total variance and is even more closely aligned with allometry (the red arrow) than PC 1 in shape space.

Because facial growth comprises changes in both shape and size, facial form more closely reflects an individual's age than facial shape. The first PC in form space accounts for 71% of variance in age, whereas PC 1 in shape space accounts for 42% only.

Figure 7a contrasts ontogenetic allometry (the regression of shape on ln CS in the full ontogenetic sample) with static allometry (the regression of shape on ln CS in adults). Ontogenetic allometry, which is close to PC 1, reflects the relative size increase (positive allometry) of the lower face and the resulting decrease of relative eye size (negative allometry). A permutation test shows that ontogenetic allometry is statistically significant (Tab. 1). The pattern of static allometry is less pronounced and the regression is not significant, indicating a weaker allometric relationship within male adults and less variation in face size.

Behavioral biological theory primarily refers to sexual dimorphism separately in body size and in face shape, but face size is itself negatively allometric with respect to body size during human ontogeny (for our data, ln face CS and ln body height have a correlation of 0.47 and a slope of 0.14 in adults). We thus also regressed face shape on body height, both in the ontogenetic sample and in adults only. Furthermore, we regressed face shape on age in the two samples (Fig. 7b,c). All three ontogenetic regressions are very similar, reflecting the high correlation

between face size, body height, and age during ontogeny (the pairwise correlation coefficients range from 0.84 to 0.92). The static regression of shape on body height to some degree resembles the ontogenetic pattern, but the static regression on age seems to reflect another process—aging as opposed to growth. Static and ontogenetic regressions on body height as well as on age are all significant (Tab. 1).

Figure 8 shows a more abstract comparison of the three ontogenetic and the three static patterns of allometry. All six coefficient vectors, standardized to unit length, are subjected to a principal component analysis. The three ontogenetic regressions cluster together closely, reflecting the similar deformation grids in Fig. 7, whereas the static regressions are heterogeneous and differ from the ontogenetic ones.

Discussion

Size, shape, and form

In this paper we briefly reviewed the concepts of size, shape, and form, and how they are estimated in geometric morphometrics. The shape of a landmark configuration is what remains after position, orientation, and size have been filtered out. In geometric morphometrics, the shape parameters of a set of landmark configurations usually are estimated by Generalized Procrustes Analysis, and the scale of the configurations is quantified separately by centroid size.

Size and shape are classic geometric concepts, and it is a longstanding tradition in morphometrics to analyze and interpret variation in shape separately from variation in size. Yet every organism, and every part of an organism, has a certain form, i.e., a certain size *and* shape. Modern geometric morphometrics hence offers two modes of analysis: an analysis of shape separately from size, and the joint analysis of size and shape in a single form space. But when should one study the shape of objects, separately from size, and when their form? Form is the more comprehensive description of an object than shape alone; it should be used, for instance, in classification studies whenever groups of organisms differ both in size and shape. Discrimination and

Table 1 – Explained variance and statistical significance for the ontogenetic and static regressions of shape on the natural logarithm of centroid size (ln CS), body height, and age. The *p*-values were estimated by permutation tests using 1000 random permutations and the explained variance as the test statistic.

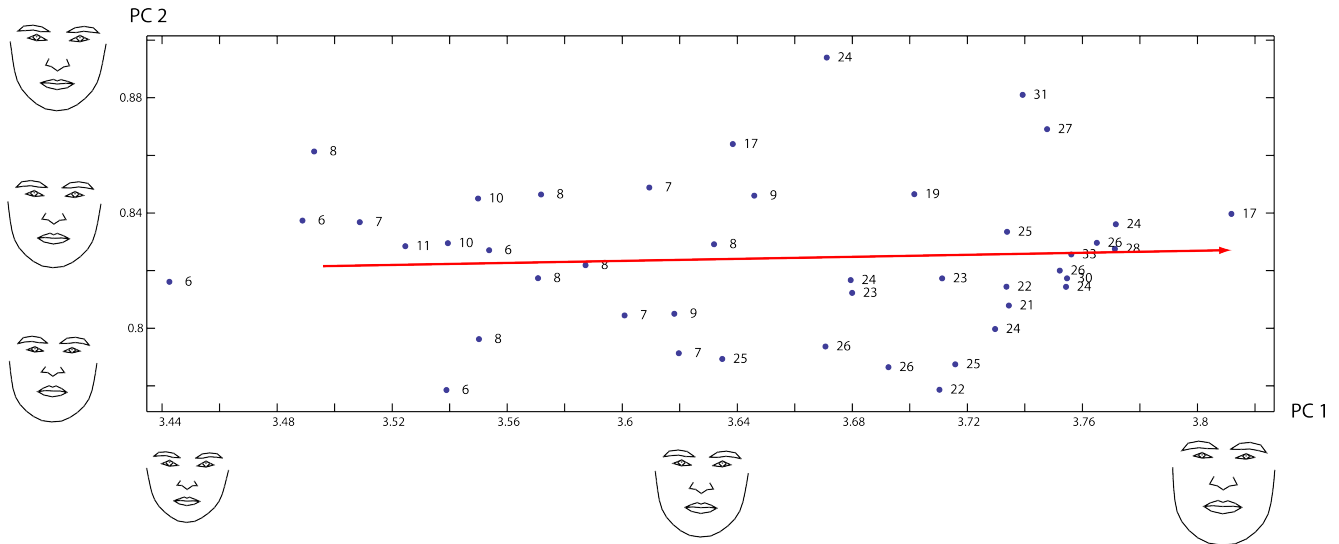| | ontogenetic regressions | | static regressions | |
	p-value	expl. var.	*p*-value	expl. var.
ln CS	*p*<0.001	22.4%	*p*=0.76	2.8%
body height	*p*<0.001	23.5%	*p*<0.001	7.8%
age	*p*<0.001	20.1%	*p*<0.001	7.0%

Figure 6 – Scatterplot of the first two principal components (PCs) of facial form (Procrustes shape coordinates augmented by ln CS). The individuals are labelled by their age. The redarrow represents ontogenetic allometry (allometric shape and size) – the regression of form on ln CS. The facial reconstructions visualize the form differences associated with the first two PCs and correspond to PC 1 scores of 3.44, 3.63, and 3.82 and to PC 2 scores of 0.78, 0.84, and 0.90, respectively.

classification based on form usually is more successful than based on shape alone (e.g., Mitteroecker and Bookstein 2011). Likewise, when predicting a variable, such as age in our example on facial morphology, form is the better predictor than shape whenever size is related to the variable as well. In most studies of growth and development, changes both in size and shape may be of scientific relevance and can be analyzed jointly.

When variation in shape is explained differently from variation in size, or when size differences are used as an explanation of shape differences (such as in studies of allometry), shape and size should be quantified and analyzed separately. In some studies, particularly on organisms with indeterminate growth, both geometric size and allometric shape might intentionally be neglected and removed from the data. When the size of the measured objects is not well preserved (e.g., because of unstandardized photographs), shape should of course be analyzed separately from size.

In general, it is a useful exploratory approach to contrast ordinations in shape space to that in form space. For example, ontogenetic trajectories that overlap or are parallel in shape space but differ in direction in form space indicate a dissociation of size and shape during ontogeny (e.g., Mitteroecker et al. 2004a, 2005; Gerber et al. 2007). An *a priori*

limitation of a morphometric analysis to either shape or size should be justified explicitly.

Geometric morphometrics offers powerful techniques for the visualization of both shape differences and form differences. Deformation grids and series of reconstructed shapes or forms can easily be interpreted within a biological context (e.g., Bookstein 1991). Ordinations and other multivariate statistical analyses of high-dimensional shape spaces or form spaces can be useful when comparing relationships between multiple groups, but meaningful biological interpretations of such analyses are more difficult (e.g., Mitteroecker et al. 2004b, 2005; Huttegger and Mitteroecker 2011; Bookstein in press). A careful ordination analysis, consilient with a biological explanation, can be more convincing than lists of geometric parameters and significance tests (McCloskey and Ziliak, 2009; Bookstein, in press). Furthermore, in contrast to deformation grids, most multivariate analyses and geometric parameters in shape or form space do not account for the spatial relationship among landmarks (they ignore the mean shape), even though the information is present in the shape coordinates. For example, all shape coordinates contribute equally to multivariate statistics such as covariance matrices or the angle between two trajectories, regardless of whether the landmarks are far apart or whether they almost have the same position (e.g., Mitteroecker 2009; Huttegger and
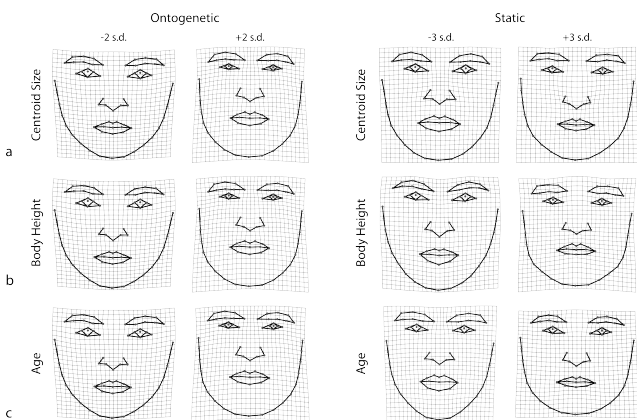

Figure 7 – Visualization of the ontogenetic and static shape regressions. (a) Facial allometry estimated via regressions of face shape on ln CS in the full ontogenetic sample (ontogenetic allometry) and in the subsample of adults (static allometry). The displayed grids are deformations from the mean shape to shapes corresponding to -2 standard deviations (s.d.) and +2 s.d. of centroid size. (b) Regression of face shape on body height in the full sample and in adults only. (c) Regression of face shape on age in the full sample and in adults only.
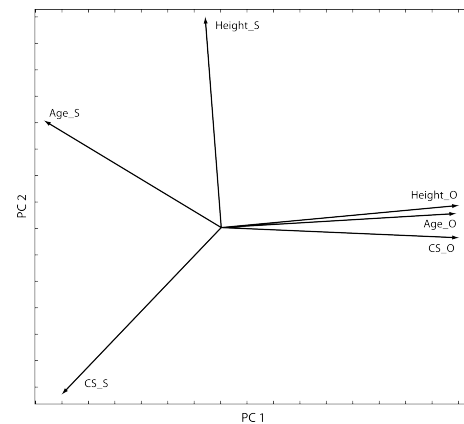

Figure 8 – Principal component analysis of the six shape regression vectors (standardized to the same length) shown in Fig. 7. The ontogenetic regressions are very similar and hence point into a similar direction in this ordination, whereas the three static regressions differ considerably, with the vector of the static regression on body heigh located closest to the ontogenetic ones.

Mitteroecker 2011). Further theoretical and statistical developments may lead to more powerful morphometric analyses.

Facial allometry

We have applied geometric morphometric methods to study ontogenetic and static allometry in human faces. Despite its obvious importance for studies in face perception and evolutionary psychology, facial allometry has received little attention in the corresponding literature. The ontogenetic relationship between body size, face size, and face shape is no big surprise since they all change considerably with age. But our results further reveal shape cues to body size in the adult male face, partly resembling ontogenetic allometry. Face size, by contrast, is less clearly and not significantly related to face shape in our adult sample.

This has far reaching consequences for several lines of face research. Shorter men on average have more childlike facial features than taller men, which in turn affect trait attributions and social stereotyping (Zebrowitz and Montepare, 2008). Facial allometry might thus be an important confounding factor in studies of facial masculinity, dominance, and the like.

We further found age-related shape changes in the adult male face, resembling the qualitative descriptions of Albert et al. (2007): the face becomes wide relative to its length and the lips become thinner, even after correcting for body weight. These are features typically associated with and perceived as mature and male, even in inanimate objects (Windhager et al., 2008).

Effects of aging on face shape differ from the subadult growth pattern, even in our sample with an adult age range from 17 to only 33 years. This may confound estimates of ontogenetic allometry and linear growth trajectories when pooling subadult individuals with adults of a large age range. ✎

Appendix

Here we give some details about the visualization of regression and principal component analysis in shape space and in form space. To our knowledge, the visualization in form space has not been published before.

Let $\mathbf{s}_i$ be a vector of the pk shape coordinates of the ith individual, where p is the number of landmarks in k dimensions, and $i = 1, \ldots, n$. Let further $\mathbf{a}$ be a vector of pk regression coefficients (resulting, for example, from a regression of the shape coordinates on CS in order to estimate allometry) or a vector of principal component loadings in shape space. The coefficient vector $\mathbf{a}$ can be visualized as a deformation grid between a reference shape, usually the mean shape $\overline{\mathbf{s}_i}$, and $\overline{\mathbf{s}_i} + f\mathbf{a}$, the reference shape plus a convenient multiple f of the coefficient vector $\mathbf{a}$. It is effective to contrast two deformations, one from the reference to $\overline{\mathbf{s}_i} - f\mathbf{a}$ and one from the reference to $\overline{\mathbf{s}_i} + f\mathbf{a}$ (such as in Fig. 7), or to present a series of reconstructed shapes, such as $\overline{\mathbf{s}_i} - f\mathbf{a}$, $\overline{\mathbf{s}_i}$, and $\overline{\mathbf{s}_i} + f\mathbf{a}$ (Fig. 5). Scores along the vector $\mathbf{a}$, that is, a variable reflecting allometric shape (Fig. 4), can be computed as the linear combination $\mathbf{a}'\mathbf{s}_i$. When $\mathbf{a}$ is scaled to unit length, the linear combination is equal to an orthogonal projection on the coefficient vector.

Vectors in form space, resulting from a regression of form on some variable or from PCA in form space, can be visualized as form deformations or series of reconstructed forms, comprising differences in both size and shape. When form space is constructed based on the pk coordinates of the centered and rotated – but not scaled – landmark configurations, the visualization can proceed as described above for shape, but now $\mathbf{a}$ might induce a change in size.

When form space is based instead on the shape coordinates (centered, scaled, and rotated configurations) together with the natural logarithm of centroid size ($pk + 1$ variables in total), the visualization is slightly more complex. A vector $\mathbf{b}$ of regression coefficients or of principal component loadings in form space consists of pk coefficients or loadings for the Procrustes shape coordinates and one for ln CS. Let $\mathbf{b}_{1\ldots pk}$ denote the elements of $\mathbf{b}$ corresponding to the shape coordinates and $\mathbf{b}_{pk+1}$ the element corresponding to ln CS. The visualization of $\mathbf{b}$ must be based on a reference form, which usually is the product $\overline{\mathbf{s}_i} e^{\overline{\ln \rho_i}}$, that is, the mean shape $\overline{\mathbf{s}_i}$ scaled by the mean size $\overline{\ln \rho_i}$, where ρ_i is the centroid size of the ith individual. Note that when size is measured by ln CS, the average shape must be scaled by the exponential function of the average ln CS, which is equal to the geometric mean of CS. The target of the deformation is $(\overline{\mathbf{s}_i} + f\mathbf{b}_{1\ldots pk})e^{\overline{\ln \rho_i} + f\mathbf{b}_{pk+1}}$, i.e., the shape $\overline{\mathbf{s}_i} + f\mathbf{b}_{1\ldots pk}$ scaled by $\overline{\ln \rho_i} + f\mathbf{b}_{pk+1}$. For the visualization of form differences the absolute size usually does not matter, just the relative size difference associated with some shape difference is presented. The reference and the target forms can thus be rescaled by the same size factor and the terms above can be simplified to $\overline{\mathbf{s}_i}$ for the reference form and to $(\overline{\mathbf{s}_i} + f\mathbf{b}_{1\ldots pk})e^{f\mathbf{b}_{pk+1}}$ for the target form.

In order to visualize allometry as a shape change together with the corresponding size change, one can add the vector of slopes resulting from the regression of the shape coordinates on ln CS to a reference form, and increase the scale of this reference form (measured as ln CS) by one unit. This is equivalent to regressing form (shape coordinates plus ln CS) on ln CS and to follow the procedure outlined above (the slope for ln CS would be 1). The same regression of form on ln CS (i.e., the regression slopes of shape on ln CS plus one element containing 1) can be used to project the vector of allometry (vector of regression slopes) into a PCA plot of form space (e.g., such as in Fig. 6).

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