Analyzing shapes as compositions of distances

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Abstract

We propose to analyze shapes as "compositions" of distances in Aitchison geometry as an alternate and complementary tool to classical shape analysis, especially when size is non-informative.

Shapes are typically described by the location of user-chosen landmarks. However the shape – considered as invariant under scaling, translation, mirroring and rotation – does not uniquely define the location of landmarks. A simple approach is to use distances of landmarks instead of the locations of landmarks them self. Distances are positive numbers defined up to joint scaling, a mathematical structure quite similar to compositions. The shape fixes only ratios of distances. Perturbations correspond to relative changes of the size of subshapes and of aspect ratios. The power transform increases the expression of the shape by increasing distance ratios. In analogy to the subcompositional consistency, results should not depend too much on the choice of distances, because different subsets of the pairwise distances of landmarks uniquely define the shape.

Various compositional analysis tools can be applied to sets of distances directly or after minor modifications concerning the singularity of the covariance matrix and yield results with direct interpretations in terms of shape changes. The remaining problem is that not all sets of distances correspond to a valid shape. Nevertheless interpolated or predicted shapes can be backtransformated by multidimensional scaling (when all pairwise distances are used) or free geodetic adjustment (when sufficiently many distances are used).

Key words: Shapes, distances, compositions

1 Introduction

The statistical analysis of shapes is a great challenge. Shapes typically are expressed by the positions \mathbf{x}_i of special locations $i=1,\ldots,N$ on the shape typically called landmarks. However although the position can be expressed in Euclidean coordinates, like with compositional data, the resulting dataset can not be interpreted in a standard multivariate scale. Objects with translated, rotated and scaled landmarks are called similar. If no scaling is necessary the objects are called geometrically equivalent. In this article we will assume that two objects have the "same" shape, if they are similar.

Thus the main problem is to replace the coordinates with something invariant under similarity transforms. Different approaches have been proposed:

• Distances

A simple approach is to report distances between landmarks instead of coordinates. This works for equivalent shapes only and introduces some arbitrariness by the choice of the reported distances. Furthermore distances form strictly positive quantities and are therefore difficult to handle statistically.

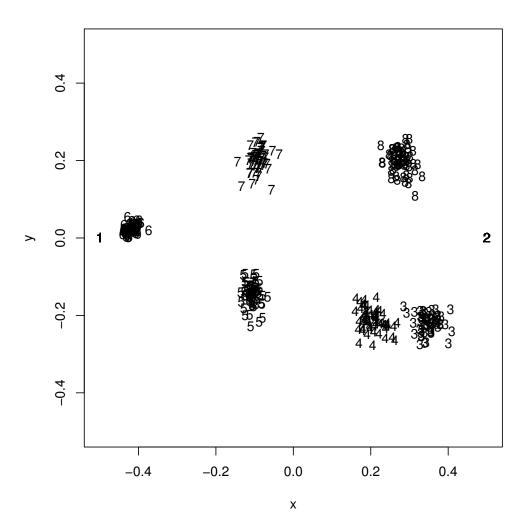


Figure 1: Positions of Bookstein coordinates of landmarks of the skulls of male and female gorillas from the dataset published in (Dryden& Mardia 1998). Landmark 1 corresponds to the tip of the nose and landmark 2 to the back of the head.

Bookstein coordinates

The idea is to fix two points and to move and scale each observed shape to fit at these to points (Dryden & Mardia 1998).

Problems with Bookstein coordinates are the arbitrariness of choosing the two points.

• Procrustes coordinates

The idea is to translate, rotate and scale each configuration to fit to the first configuration as good as possible in mean square error.

Again there is an arbitrary choice of the first configuration influencing the results.

2 Towards a compositional representation of shapes

2.1 Compositions of distances and angles

In my opinion a multivariate representation of shapes should have some nice properties. E.g. the components should be easy to understand and invariant under equivalence of similarity transformations and it should uniquely define the shape. Candidates are:

• Distances between landmarks

For general Euclidean configuration in any dimension the shape is (up to mirror) uniquely defined by all pairwise distances. The same is true for some subsets of distances. The distances between the landmarks are invariant under equivalency transforms. A scaling of the shape results in a similar scaling of all the distances. Thus scaled distances need to be considered as equivalent and thus the distances form $D = \binom{N}{2}$ -part compositions in the equivalence class formulation of (Barceló-Vidal et al.(2001))

• Angles between lines connecting landmarks

In the same way angles between connecting lines determine the shape of all connecting triangles, resultingly determine the relative length of all distances and thus specify the shape of the object in all dimensions. The same is true for some subsets of angles. Since the sum of the angles in each triangle are known to be 180^o the sum of all the angles is known to be $\binom{N}{3}180^o$. Thus the angles form a $D = \binom{N}{3}$ -part compositions in the sense of (Aitchison(1986)).

We will later see that the compositions of angles have some drawbacks, rendering them very specific to special situations. The proposal of this paper is therefore to analyze shapes as compositions of distances. We will justify this further by stating more properties and analyzing the resulting geometry in more detail. Afterwards we will show how to use this approach in practice.

It should be mentioned that not all compositions correspond to valid shapes. Simple restrictions for the composition of distances $d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|$ are given by the triangular inequality

$$d_{ij} \le d_{ik} + d_{kj} \forall i, j, k$$

and by the constant sum constraint

$$\alpha_{ijk} + \alpha_{jki} + \alpha_{kij} = 180^{\circ}$$

for angles

$$\alpha_{ijk} = \mathbf{acos} \frac{(\mathbf{x}_i - \mathbf{x}_j, \mathbf{x}_k - \mathbf{x}_j)}{\|\mathbf{x}_i - \mathbf{x}_j\| \|\mathbf{x}_k - \mathbf{x}_j\|}$$

where $\mathbf{acos} \ x \in [0, \pi)$ by definition. The proposed transform is thus not bijective.

2.2 Selected distances and subcompositional dominance

The compositions of distances or angels are very high dimensional. The manifold dimension of the configurations of N points with relative dimension d is $d(N-1) - \frac{1}{2}d(d-1)$. This is always positive since relative dimension d implies that N > d. The dimension of the corresponding compositional space of distances is $D-1=\binom{N}{2}-1=\frac{N(N-1)}{2}-1\geq d(N-1)-\frac{1}{2}d(d-1)$. It is thus often sufficient to use only a subcomposition of distances. However than the analysis depends on the chosen subcompositions and we are obliged to request that the analysis obeys the rules of subcompositional dominance (Aitchison(1986)), saying that the information in any chosen subcomposition should be visible as long as this subcomposition is part of the analyzed composition. Correspondingly selecting a subcomposition for the analysis explicitly throws away some information. It is easy to interpret which information is thrown away.

Example 1: We analyze the shape of crayfish. The crayfish can chance some of the distances by motion of its limbs. We would like to ignore these motion and use only distances between rigidly connected landmarks.

Example 2: We analyze the shape of gorilla skulls. We could find that the total length from the back of the head to the tip of the nose might be important in itself or only measured by some subdistances "from the back to the base" - back length, "from the back base to the front base" - base length, "from front base to the root of the nose" - position of nose, "root of nose to tip of nose" - length of the nose. Figure 2 shows four different possible minimal sets of distances defining the shape of a Gorilla skull based on the landmarks given in (Dryden & Mardia 1998).

An analysis of the composition in a Aitchison geometry would guarantee that all these subcompositions are handle consistently according to the principle of subcompositional dominance.

2.3 Subshapes, subcompositions and perturbation

Subshapes can be seen as subsets of points and the corresponding subsets of distances between these points. The subshape has the same shape if and only if the corresponding subcompositions of distances are equivalent. If a part of an object consists of two subshapes (e.g. the left and right scissor of the crayfish), there are three sets of distances in the part: Distances in the first subshape, distances in the second subshape and distances between both subshapes. If now both subshapes change their relative size but keep their inner shape, the resulting two subshape subcompositions would stay the same. The subcomposition containing only the distances in the two shapes is perturbed by a simple balance vector contrasting the two subshapes and the rest of the distances change on a nonlinear curve due to a complex shape change of the whole part.

Directional size changes of parts are expressed by a perturbation. E.g. for uniaxial extension the perturbing vector has high values in the for directions in the extension direction and gradually decreasing values in the segments with increasing angle to the extension direction. Since segments not parallel or perpendicular to the extension direction this angle changes during deformation. Thus the perturbing vector will also slightly change during deformation. However this is only a second order effect and important only with substantial changes of shape.

2.4 Singular compositions and singular shapes

A major difference between Aitchison geometry and Euclidean geometry is the handling of extremal compositions. The effect of this should be studied for shapes. The first concern here is on small subshapes (e.g. the nose of the gorilla) with small absolute variation. In case of classical shape analysis, based on coordinates, these small variations are more or less ignored. However the Aitchison distances in the subcompositions do not depend on the absolute size of the subshape, but only on change relative to size. The Aitchison geometry consequently honors shape changes in subshapes independent of the overall size of the subshape.

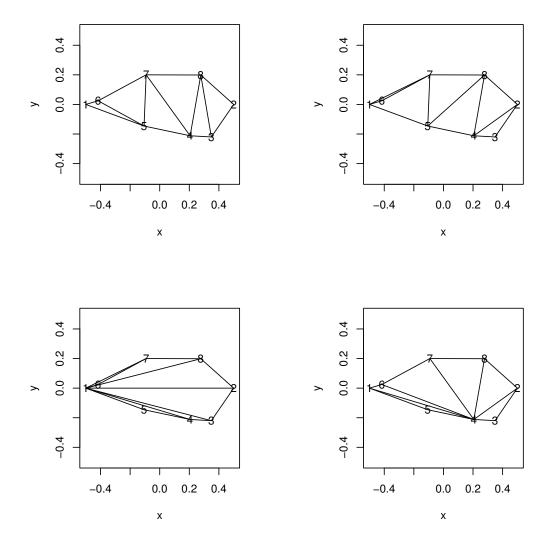


Figure 2: Four different minimal subsets of distances uniquely defining the shape.

Shapes correspond to extremal compositions of distances not modeled by the Aitchison simplex if and only if a distance becomes zero, which corresponds to the two points being equal. As for compositions, one can argue that in this case we look a qualitatively different shape.

Other extremal combinations of distances are given by the geometric constraint due to the triangular inequality $d_{ij} \leq d_{ik} + d_{jk}$. However the corresponding compositions are not considered extremal, which is in perfect coherence with the fact that these triangles in the mid of a bending path and are therefore not to be considered as extremal shapes.

2.5 Why are angular compositions not useful?

On the other hand angular compositions are extremal, when two segments originating from the same landmark get collinear. However this can easily happen during a sign change of curvature or even by change for connection lines of different subshapes. I therefore consider the angular compositional geometry in general as invalid for shape analysis. It could be valid, when all the selected segments have some physical meaning hindering them to be collinear. However perturbation of angles seams to have no meaning. The ratio of two angles is a mathematically flaw quantity, due to the circular geometry of angles. There is no easy effect of standard operations like local size change, uniaxial extension or bending. A good hint that Aitchison geometry might be invalid for compositions of angles is that there is no interpretation in terms of equivalence classes. We therefore discourage to use compositions of angles as representation of shape.

3 Technical prerequirements

3.1 Standard tools from compositional data analysis

The central idea of this paper can therefore be formulated as follows: Analyze shapes S as compositions of all or some selected pairwise distances $d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|$ between the landmarks \mathbf{x}_i . The analysis should be done in the Aitchison geometry (Aitchison(1986)) and following the principle of coordinates (Pawlowsky-Glahn(2003)) based on the centered log ratio transform and the isometric log ratio transform. The whole theory of compositional data analysis such as more explicitly cited and referenced in (Barceló-Vidal et al.(2001)) or (Boogaart&Tolosana-Delgado 2005) in this Proceedings is taken as granted and not further described here.

Thus the shape is identified with a composition

$$(d_k)_{k=1,...,D} = (d_{i_k j_k})_{k=1,...,D} = (\|\mathbf{x}_{i_k} - \mathbf{x}_{j_k}\|)_{k=1,...,D}$$

based on a chosen set of segments between landmarks:

$$S = \{(i_k, j_k) : k = 1, \dots, D\} \subset \{(i, j) : i < j\}$$

Based on our standard definitions (Boogaart&Tolosana-Delgado 2005) for compositions we define for shapes:

$$clr S := clr(d_k)_{k=1,...,D} = (\log d_k - \frac{1}{|S|} \sum_{l} \log d_l)_{k=1,...,D}$$

$$||S|| := ||(d_k)_{k=1,...,D}||_A = ||clr S||$$

$$ilr S := ilr(d_k)_{k=1,...,D} = Bclr S$$

$$(S, \tilde{S}) := (d, \tilde{d})_A = (clr S, clr \tilde{S})$$

3.2 Inverse Transforms

For application of the working in coordinates principle we need an inverse for the clr and the ilr-transforms. However not all compositions (e.g. a mean composition) correspond to a valid shape. This is a typical problem for all scales not homomorphic to an Euclidean space. E.g. in the statistics of directions (i.e. of unit vectors) the mean resulting direction is a vector of a norm strictly smaller than 1. However we can identify a direction of the mean by the unit vector with the smallest distance to the resulting mean.

A similar approach can be used here: A composition, which does not correspond to a valid shape, could be represented by a shape fitting "as good as possible" to the given set of distances. For a full set of distances such configuration could be calculated by multidimensional scaling (Cox(1994)). For incomplete sets of distances a best fitting configuration can be calculated by free geodetic adjustment(Caspary(1987)). Due to the relative geometry of the distances weighted adjustment should be used. The errors in long distances should be downweighted by the length of the segment. The adjustment must be a free adjustment since the configuration is determined only up to rotation and translation. For this reason a starting configuration is needed in a free adjustment, from which the final configuration inherits location and rotation. To ensure comparability the same starting configuration should be used for all backtransforms. To avoid further dependence on the starting configuration of the adjustment, the network of segments should be fully determine the shape and the adjustment should be iterated until convergence.

3.3 Triangular plots of triangles

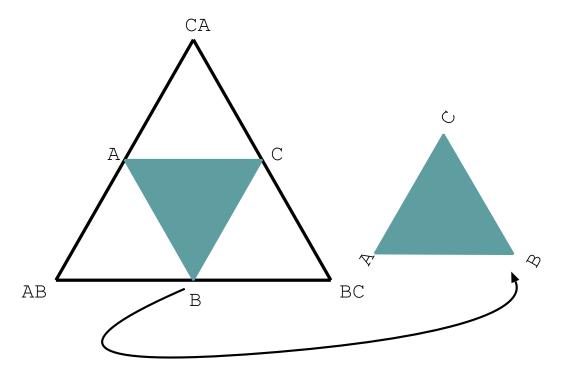


Figure 3: Illustration of the plot representing the triangle of possible compositions originating from the sides of a triangle.

For the subcomposition of three segments making up a triangle, the triangular inequality limits the possible values to the triangle given by the side mids of the triangle bounding the ternary diagram. Triangular subshapes can therefore be plotted into a upside down triangular plot. The plot is

explained in Figure 3. The triangles in the corners correspond to triangles with two equivalent points. The triangles on the sides of the triangle correspond to triangles with three collinear points. This is illustrated in Figure 4.

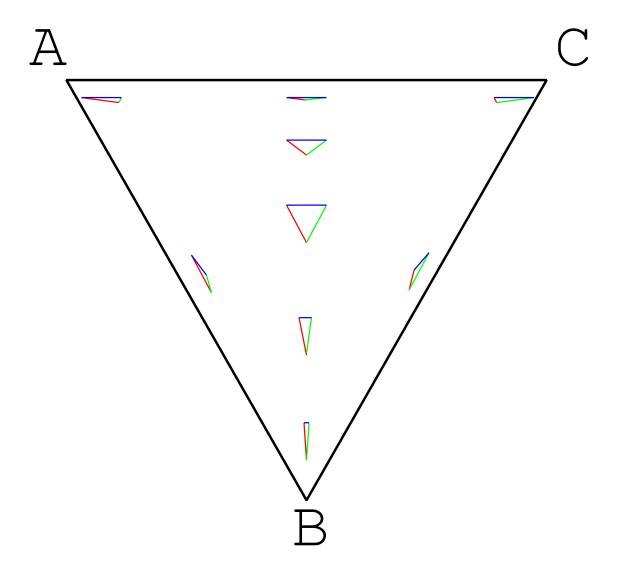


Figure 4: Illustration of the triangles represented by the different positions in the triangle of triangles.

3.4 Plotting perturbations

Not all compositions showing up during a shape analysis in this approach are really shapes. Many – e.g. principle components or linear model coefficients – are differences of shapes or shape changes, expressed by a composition to be used in a perturbation. To represent this compositions I invented a new plot, which uses a shape with all the connecting lines as a start point but shortens or lengths each segment around its midpoint according to its relative length in the perturbing composition. An example can be seen in Figure 8 for the display of principle components. A color code can be used to distinguish shortened and lengthened segments.

4 Multivariate analysis with compositions of distances

4.1 Mean shape

A big problem concerning shapes is the definition of a mean. The state of the art solution are mean Bookstein coordinates. However these means depend on the two selected points. The compositional approach offers an alternate solution by representing the mean by the mean of the corresponding compositions. However this mean composition does in the most cases not correspond exactly to a valid shape. However a corresponding optimal backtransform can be given by finding the best fitting shape through the free geodetic adjustment described in section 3.2.

Figure 5 shows that the variation of the adjusted coordinates obtained by forward and backward transform through the compositional approach, have a substantially smaller variation around the mean coordinates, than the Bookstein coordinates around mean Bookstein coordinates.

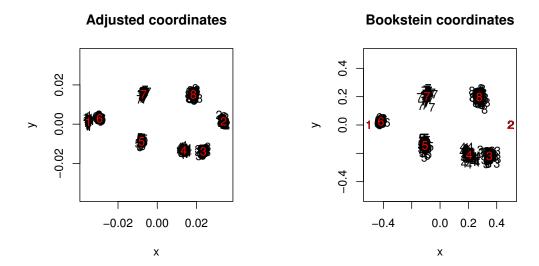


Figure 5: The mean shape of the gorilla skull is plotted in red and the dataset in black. The Bookstein coordinates reveal a substantially larger relative variation around the mean.

4.2 Variation of shape

The variance is typically not an object in the space itself but a matrix. Therefore we can define the variance of the shape as the variance of the corresponding composition,

$$\operatorname{var} S = \operatorname{var} \operatorname{clr} S$$

and the metric variance of the shape as the metric variance of the corresponding composition:

$$\operatorname{mvar} S = \operatorname{tr} \operatorname{var} \operatorname{clr} S$$

A similarly important object is the variation matrix of the shape to be defined as:

variation
$$S = \left(\operatorname{var} \log \frac{d_k}{d_l} \right)_{kl}$$

The variation matrix is a symmetric matrix and describes the variation of the ratio of lengths. Thus a small entry in the variation matrix corresponds to proportional distances.

4.3 Clusters of shapes

The Aitchison distance, like all other typical metrics on the clr-transform of compositions, induces a natural metric for shapes. This can be used for cluster analysis. To ignore specific aspects of the shape one can easily remove the corresponding distances from $\mathcal S$ by selecting a subcomposition. A simple application of this method is shown in Figure 6, which shows a separation of datasets of male and female gorillas in four major clusters of which two are mainly male and two are mainly female.

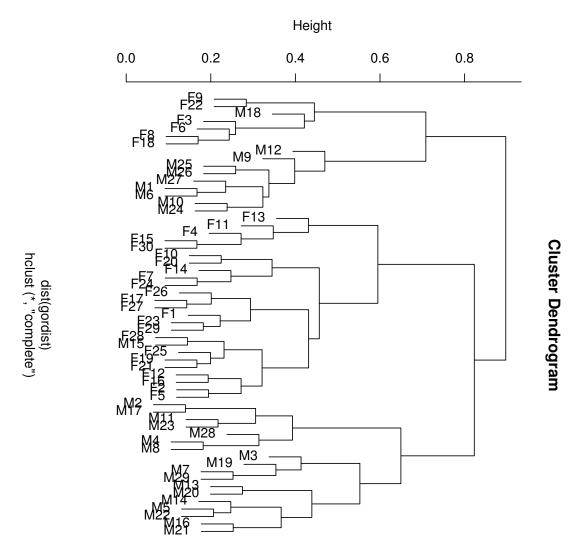


Figure 6: Dendrogram of a row mode cluster analysis of the gorilla dataset based on Aitchison distance and complete linkage. Gorillas with an F label are female. Gorillas with an M label are male. Based on four clusters male and female gorillas are nicely separated.

Discrimination analysis can be based on the clr transform. However one has to keep in mind that the multivariate normal distribution is a not valid model here and therefore only nonparametric discrimination analysis applies.

4.4 Finding undeformed subshapes by Q-mode cluster analysis

An other important question, when working with shapes, is the detection of undeformed subshapes. This would imply a clustering of points belonging to subshapes. However a point can belong to more than one subshape, e.g. when it is a link and even if a point behaves rigid in relation to some other points it will have a set of varying distances. However segments between landmarks can belong to one or zero rigid subshapes. Thus we could try to find cluster of segments with small relative variation. The variation of the relative length of segments is described by the corresponding entry of the variation matrix, which can serve as a distance of segments. Thus we propose to use a Q-mode cluster analysis based on the variation matrix (or its element wise square root) as a measure of distance. The results of such cluster Analysis is given in Figure 7.

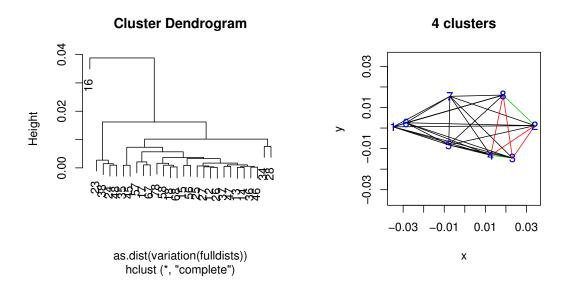


Figure 7: Dendrogram and clustering of the quantity mode cluster analysis based on variation as distance for the female gorillas. This can be interpreted as follows: black: overall shape of the front skull is constant. blue: the length of the nose varies, red: the height of the back skull and green: the length of the back skull vary.

However the interpretation might be somehow different from a classical cluster analysis. The cluster analysis tries to completely split the dataset in clusters. However in case of rigid subshapes not all distances will belong to a rigid subshape since many will connect landmarks from different rigid subshapes. These distances should not belong to any cluster and join lately. Only the clusters formed early at small distances can be interpreted rigid, especially, when they form cliques of landmarks. The joining distance has direct interpretation in terms of how rigid the subshapes are, since the have an interpretation in the variation of the log of the ratio.

4.5 Subcompositional balances

If rigid subshapes have been identified, we can try to analyses their relative behavior. Compositional balances, as introduced in (Egozcue, J.J. and V. Pawlowsky-Glahn (2005)), between the distances of different subshapes can be used to describe the relative size change of the subshapes. Balances of the connecting segments of subshapes and inner segments of the subshapes can describe changes in relative distance of the subshapes. Balances between upper and lower connecting lines can describe changes in relative rotation of the subshapes.

4.6 Principle component analysis for shapes

Principle component analysis based on Bookstein coordinates is a well known technique for shapes. However as illustrated in Figure 5 the compositional approach induces a different variation structure than the Bookstein coordinates. A more detailed view would reveal that the Bookstein variation is related to compositional variation somehow like the alr-variance to the ilr-variance. Which means that there is an artefact in the variation induced by the selected fixed landmarks, which looks like a nonorthogonal transformation. However principle components are totally based on the notion of orthogonality, which therefore really matters.

Accordingly the principle component based on the compositional approach, honoring all natural orthogonality and symmetry relations, can be seen as more well founded. The resulting principle components have to be interpreted in terms of perturbation and can therefore be plotted as the corresponding shape of the mean shape perturbed by the components or directly as a perturbation based on the mean shape as described in section 3.4. Biplot, screeplot and the first two principle components are plotted in Figure 8.

5 Conclusions

Based on the principle of working in coordinates the compositional approach to shape analysis provides new tools with direct application. The whole approach is not as straight forward as with the simplex, since the corresponding mappings go into a manifold and not into a full vector space. However combining the approach with approaches for statistics on manifolds allow interesting applications.

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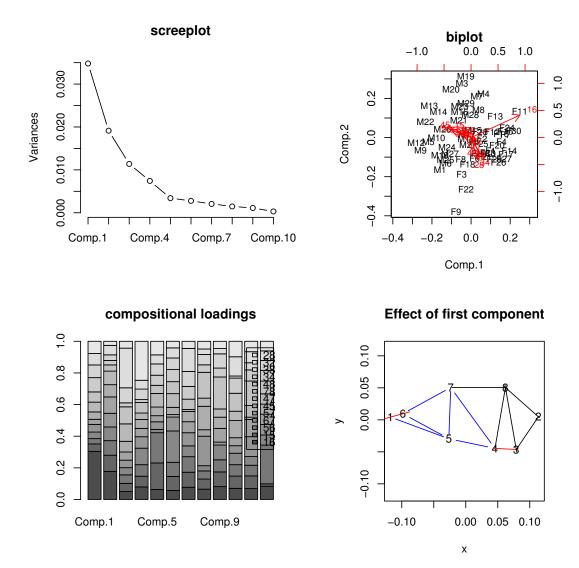


Figure 8: Results of the principle component analysis of the gorilla dataset based on Aitchison geometry. The first and second principle component clearly mark the difference between male and female gorillas. First principle component shows that female gorillas have a smaller forehead in relation to the length of the nose.

Appendix

Here is the R-code to generate the plots:

```
library(shapes)
library(compositions)
data(gorf.dat)
data(gorm.dat)
di \leftarrow matrix(c(1,6, 1,5, 5,6, 6,7, 5,7, 4,5, 4,7, 7,8,
                4,8, 3,4, 3,8, 3,2, 2,8),byrow=T,ncol=2)
row.names(di) <- paste(di[,1],di[,2],sep="")
fulldi <- diag(1:8);</pre>
fulldi <- cbind(c(row(fulldi)),c(col(fulldi)));</pre>
fulldi <- fulldi[fulldi[,1]<fulldi[,2],];</pre>
row.names(fulldi) <- paste(fulldi[,1],fulldi[,2],sep="")</pre>
todists <- function(X,di) {</pre>
  if( length(dim(X))<3 )</pre>
    dim(X) \leftarrow c(dim(X),1)
  erg <- t(apply(X,3,function(x) {</pre>
     sqrt(c((x[di[,1],]-x[di[,2],])^2 %*% rep(1,ncol(x))))
  colnames(erg) <- row.names(di)</pre>
  erg
}
plotCS <- function(X,...,di=NULL,which=1:d,xlim=range(X),</pre>
                     ylim=range(X),pch=paste(1:k),add=FALSE,col=par("col")) {
  if(length(dim(X)) == 2)
    dim(X) \leftarrow c(dim(X),1)
  n \leftarrow dim(X)[3]
  d \leftarrow dim(X)[2]
  k \leftarrow dim(X)[1]
  par(pty="s")
  if (add)
    points(matrix(c(aperm(X,c(1,3,2))[,,which,drop=FALSE]),
                   ncol=2),pch=gsi.getmod(pch,rep(1:k,n)),...,col=col)
  else
    plot(matrix(c(aperm(X,c(1,3,2))[,,which,drop=FALSE]),
                   ncol=2),pch=gsi.getmod(pch,rep(1:k,n)),...,
                    xlim=xlim,ylim=ylim,col=col)
  if(!is.null(di))
    segments(c(X[di[,1],which[1],]),
            c(X[di[,1],which[2],]),
            c(X[di[,2],which[1],]),
            c(X[di[,2],which[2],]),col=col)
}
plotCSC <- function(X,delta,...,di=NULL,which=1:d,</pre>
                      xlim=range(X),ylim=range(X),pch=1:k,
                      add=FALSE,col=par("col"),sim=1.0) {
```

```
if(length(dim(X)) == 2)
    dim(X) \leftarrow c(dim(X), 1)
  n \leftarrow dim(X)[3]
  d \leftarrow dim(X)[2]
  k \leftarrow dim(X)[1]
  par(pty="s")
  if( add )
    points(matrix(c(aperm(X,c(1,3,2))[,,which,drop=FALSE]),ncol=2),
            pch=gsi.getmod(pch,rep(1:k,n)),...,col=col)
    plot(matrix(c(aperm(X,c(1,3,2))[,,which,drop=FALSE]),ncol=2),
            pch=gsi.getmod(pch,rep(1:k,n)),...,xlim=xlim,ylim=ylim,col=col)
  if( ! is.null(di))
    segmentsC(c(X[di[,1],which[1],]),
            c(X[di[,1],which[2],]),
            c(X[di[,2],which[1],]),
            c(X[di[,2],which[2],]),delta=c(clo(delta,total=length(delta))),
            sim=sim)
}
segmentsC <- function(x0,y0,x1,y1,...,delta,sim=1.1) {</pre>
  xr < (x1-x0)/2
  yr <- (y1-y0)/2
  xm < -(x0+x1)/2
  ym < - (y0+y1)/2
  segments(xm-delta*xr,ym-delta*yr,xm+delta*xr,ym+delta*yr,
            ..., col=ifelse(abs(log(delta))>log(sim),
            ifelse(delta>1,"red","blue"),"black"))
}
eBe.new <- function(d,x,...,idx=cbind(...)) {</pre>
  erg <- rep(0,prod(d))
  erg[1+ c((idx-1) %*% cumprod(c(1,d[-length(d)])))] <- x
  dim(erg) <- d
  erg
}
eBe <- function(x,...,idx=cbind(...)) {</pre>
  d \leftarrow dim(X)
  X[1+c((idx-1) %*% cumprod(c(1,d[-length(d)])))]
}
"eBe<-" <- function(x,...,idx=cbind(...),value) {</pre>
  d \leftarrow dim(X)
  X[1+c((idx-1) %*% cumprod(c(1,d[-length(d)])))]<-value
  Χ
}
ginv <- function(M,eps=1E-8) {</pre>
  s \leftarrow svd(M)
  s$v %*% gsi.diagGenerate(ifelse(abs(s$d)>eps*s$d[1],1/s$d,0)) %*% t(s$u)
}
```

```
adjustDists <- function(X,dists,di,alpha=1,eps=1E-8,maxiter=100,verbouse=FALSE,premul=TRUE) {
  dists <- unclass(dists)</pre>
  if( length(dim(dists)) == 2 )
    return( structure(c(apply(dists,1,
            function(x) adjustDists(X,x,di,alpha=alpha,eps=eps,
                                     maxiter=maxiter, verbouse=verbouse,
                                     premul=TRUE))),dim=c(dim(X),nrow(dists))))
  n \leftarrow max(di)
  m <- length(dists)</pre>
  if( premul ) {
    h <- rmult(X[di[,2],]-X[di[,1],])
    d \leftarrow norm(h)
    X <- X * mean(dists)/mean(d)</pre>
  for( i in 1:maxiter ) {
    h <- rmult(X[di[,2],]-X[di[,1],])
    D <- normalize(h)</pre>
    d \leftarrow norm(h)
    A <- do.call("cbind", lapply(1:ncol(X),
                  function(i) eBe.new(c(m,n),D[,i],1:m,di[,2])-
                               eBe.new(c(m,n),D[,i],1:m,di[,1])))
    W <- diag(1/unclass(dists))</pre>
    verb <- ginv(W %*% A) %*% (W %*% (unclass(dists)-d))</pre>
    if( verbouse ) cat(norm(dists-d),"\n")
    X <- X + structure(alpha*verb,dim=dim(X))</pre>
    if( norm(verb) < eps* mean(dists) )</pre>
      break
    if( i==maxiter )
      warning("Maximum number of iterations reached")
  Х
}
triangleplots <- function(X,dits,...,tri=TRUE,main=NULL) {</pre>
  if(length(dim(dits))>1 ) {
    apply(dits,1,function(d) {triangleplots(X,d,...,tri=tri,main=main)})
    return(NULL);
    plot(acomp(X,parts=dits),...)
    if( !is.null(main) ) title(main=main)
    if(tri) lines(rcomp(cbind(c(1,1,0),c(0,1,1),c(1,0,1))))
par(mfrow=c(3,3))
triangleplots(adists,dits)
# triangleplots(adists,dits,center=T,tri=FALSE)
triangleplots(adists,dits,center=T,scale=TRUE,tri=FALSE,main="centered+scaled")
# figure Cluster Analysis
gordist <- acomp(rbind(todists(gorf.dat,fulldi),todists(gorm.dat,fulldi)))</pre>
row.names(gordist) <- c(paste(rep("F",30),1:30,sep=""),</pre>
                          paste(rep("M",29),1:29,sep=""))
hc <- hclust(dist(gordist),method="complete")</pre>
```

```
plot(hc)
dev.copy2eps(file="GorDendro.eps",horizontal=FALSE) # Fig
# figures dedro,p10,p11
fulldists <- acomp(todists(gorf.dat,di=fulldi))</pre>
meanfullcfg <- adjustDists(tt[,,1],mean(fulldists),premul=TRUE,di=fulldi)</pre>
x11(width=8,height=4)
par(mfrow=c(1,2))
plot(hc<-hclust(as.dist(variation(fulldists))))</pre>
plotCS(meanfullcfg,di=fulldi,col=cutree(hc,4),lwd=2,
       main="4 clusters",xlab="x",ylab="y");
plotCS(meanfullcfg,di=cbind(1,6),col=4,add=TRUE,lwd=2)
dev.copy2eps(file="qclust.eps",horizontal=FALSE)
dev.off()
# Figure Comparison of variation
gor.dat <- c(gorf.dat,gorm.dat)</pre>
dim(gor.dat) <- c(8,2,59)
gor.bmsp <- bookstein2d(gor.dat)$mshape</pre>
gor.book <- bookstein2d(gor.dat)$bshpv</pre>
par(cex=2)
par(mfrow=c(1,1))
plotCS(gor.book,xlab="x",ylab="y")
dev.copy2eps(file="Gorilla.eps",horizontal=FALSE)
par(mfrow=c(2,2))
di2 <- matrix(c(1,6, 1,5, 1,7, 6,7, 5,7, 4,5, 5,8, 7,8,
               4,8, 3,4, 4,2, 3,2, 2,8),byrow=T,ncol=2)
di3 \leftarrow matrix(c(1,6, 6,7, 7,8, 8,2, 2,3, 3,4, 4,5, 5,1, 1,7,
               1,8, 1,2, 1,3, 1,4 ),byrow=T,ncol=2)
di4 \leftarrow matrix(c(1,6, 6,7, 7,8, 8,2, 2,3, 3,4, 4,5, 5,1, 4,1,
               4,6, 4,7, 4,8, 4,2 ),byrow=T,ncol=2)
plotCS(gor.bmsp,di=di,xlab="x",ylab="y")
plotCS(gor.bmsp,di=di2,xlab="x",ylab="y")
plotCS(gor.bmsp,di=di3,xlab="x",ylab="y")
plotCS(gor.bmsp,di=di4,xlab="x",ylab="y")
dev.copy2eps(file="GorConnect.eps",horizontal=FALSE)
x11(width=8,height=4)
par(mfrow=c(1,2))
par(cex=1)
```

```
plotCS(adjustDists(gor.book[,,1],acomp(todists(gor.book,di=fulldi)),
          di=fulldi,premul=TRUE),xlab="x",ylab="y",main="Adjusted coordinates")
plotCS(adjustDists(gor.book[,,1],mean(acomp(todists(gor.book,
          di=fulldi))),di=fulldi,premul=TRUE),xlab="x",ylab="y",add=T,col="red")
par(cex=1)
plotCS(gor.book,xlab="x",ylab="y",main="Bookstein coordinates")
plotCS(gor.bmsp,xlab="x",ylab="y",col="red",add=TRUE)
dev.copy2eps(file="Gorilla1.eps",horizontal=FALSE)
dev.off()
# figure Principle component Analysis
par(mfrow=c(2,2))
adists <- acomp(todists(gor.book,di=di))</pre>
row.names(adists) <- c(paste(rep("F",30),1:30,sep=""),paste(rep("M",29),1:29,sep=""))
pr <- princomp(adists)</pre>
pr
plot(pr,main="screeplot")
plot(pr,type="biplot",main="biplot")
#plot(pr,type="loadings" )
barplot(pr$Loadings*2,main="compositional loadings")
k<-1;plotCSC(adjustDists(tt[,,1],mean(adists),di,premul=TRUE),
             di=di,delta=pr$sdev[k]*2*pr$Loadings[k,],
             sim=1.1,pch=paste(1:8),xlab="x",ylab="y",
             main="Effect of first component")
dev.copy2eps(file="GoriPrinc.eps",horizontal=FALSE)
```