1 **ShapeRotator: an R package for standardised rigid rotations of articulated Three-Dimensional**

2 **structures with application for geometric morphometrics**

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20 **SHORT RUNNING TITLE**

21 Rigid rotation of 3D structures

22   **Summary**

23   1.   The quantification of complex morphological patterns typically involves comprehensive shape

24   and size analyses, usually obtained by gathering morphological data from all the structures

25   that capture the phenotypic diversity in an organism or object. Articulated structures are a

26   critical component of overall phenotypic diversity, but data gathered from these structures is

27   difficult to incorporate in to modern analyses because of the complexities associated with

28   jointly quantifying 3D shape in multiple structures.

29   2.   While there are existing methods for analysing shape variation in articulated structures in

30   Two-Dimensional (2D) space, these methods do not work in 3D, a rapidly growing area of

31   capability and research.

32   3.   Here we describe a simple geometric rigid rotation approach that removes the effect of

33   random translation and rotations, enabling the morphological analysis of 3D articulated

34   structures. Our method is based on Cartesian coordinates in 3D space so it can be applied to

35   any morphometric problem that also uses 3D coordinates (e.g. spherical harmonics). We

36   demonstrate the method by applying it to a landmark-based data set for analysing shape

37   variation using geometric morphometrics.

38   4.   We have developed an R package (ShapeRotator) so that the method can be easily

39   implemented in the commonly used software programs *geomorph* and *MorphoJ*. This method

40   will be a valuable tool for 3D morphological analyses in articulated structures by allowing an

41   exhaustive examination of shape and size diversity.

42

43   **Key words:** morphology – articulation – motion correction – multi-modular morphology

Background

44

45   Data on shape and size variation is essential in many fields, including evolutionary biology

46 and ecology, engineering, medical science, and anthropology (Loncaric 1998; McIntyre & Mossey

47 2003; Slice 2006). For most of these studies, one of the most widely used tools for analysing

48 morphological variation within or between a group of organisms or objects are based on Cartesian

49 coordinates of landmarks (Bookstein 1997).

50   Of the wide array of methods using Cartesian coordinates, geometric morphometrics (GM) is the

51 most common, especially when analysing shape and size variation and covariation (Mitteroecker &

52 Gunz 2009; Adams *et al.* 2013). The first two steps of this GM procedure consist of a landmark

53 approach that: (1) gathers (two- or three-dimensional) coordinates of anatomically defined and

54 homologous loci, followed by (2) a generalised Procrustes analysis (GPA) that superimposes

55 configurations of each set of landmarks in all specimens, by removing all effects of size, translation

56 and rotation, in order to only obtain shape information (Klingenberg 2008; Adams *et al.* 2013).

57 Geometric morphometrics, therefore, allows accurate quantitative analyses of shape and size, in either

58 Two-Dimensional (2D) or Three-Dimensional (3D) space.

59   3D morphological analyses are the most accurate, as objects and organisms exist in 3D space. The

60 recent growth in x-ray micro CT scanning and surface scanning has seen a rapid increase in the

61 application of 3D geometric morphometric techniques, but progress has been hampered by the lack of a

62 simple method to incorporate data from complex articulated structures.

63   In evolutionary biology, identifying morphological differences among different groups or taxa is

64 crucial in order to understand evolutionary processes and their relationship to the environment (Losos

65 1990; Ricklefs & Miles 1994; Pagel 1999). This can be difficult, especially if traits have co-evolved, or

66 if morphological diversification has been hindered by phylogenetic legacy or trade-offs imposed by the

67 organism's functional habitat (Ghalambor *et al.* 2007). Complex body shape patterns require more

68 detailed analyses of shape, obtained by collecting data from several structures that capture the whole

69 gamut of morphological variation in an organism. One example of this is the extraction and assembly

70 of data from articulated structures, such as skeletons, for 3D analyses with geometric morphometric

71 techniques. This is especially important in functional morphological studies, as they usually involve

72 analysing more than one structure due to mechanical correlations or morphological integration. For

73 example, jointly analysing skull and mandible could be crucial to disentangle the relationship between

74   diet and head shape evolution (Cornette *et al.* 2013). Similarly, collectively evaluating different

75   modules in the limbs, especially when correlated to locomotion, or considering several structures

76   across the whole body, could improve our understanding of the effect of environmental conditions on

77   morphological evolution (Vidal-Garcia & Keogh, unpublished).

78   Unfortunately, non-rigid structures, such as articulated structures, will inevitably suffer the effects

79   of natural or free rotation or translation events and be different in each individual and structure

80   (Adams, 1999). These events could obstruct the correct quantification of shape variation by adding

81   rotation artifacts to GM analyses (Adams *et al.* 2004). Thus, orientation of these structures needs to be

82   corrected and standardised prior to performing shape analyses. Methods for shape analysis of landmark

83   data in articulated structures already have been described but the solution to this problem has been

84   implemented only in two-dimensional (2D) space (Adams, 1999).

85   Here we present the R package ShapeRotator: a simple geometric rigid rotation approach to study

86   3-Dimensional (3D) shape of articulated structures, or independent structures, within an organism. We

87   describe a method that removes shape variation due to the effect of translation between independent

88   structures and rotation generated by movement in an articulation, among others. Thus, our approach

89   translates and rotates articulated (or even independent) structures in order to obtain a comparable shape

90   data set once all effects of random movement and rotations have been removed (Fig. 1a).

91   We apply this method to a landmark-based data set for analysing shape variation using geometric

92   morphometrics, and provide the example data set used in ShapeRotator (to be available in CRAN) to

93   execute this rigid rotation. This rigid rotation then allows geometric morphometric analyses to be

94   performed in the two best well-known 3D GM analytical software packages: *geomorph* (Adams &

95   Otárola-Castillo 2013), and *MorphoJ* (Klingenberg 2011). This method also will allow exporting the

96   rotated coordinates for posterior analyses in other software platforms, even outside of the field of

97   geometric morphometrics. Since the basis of this method lies upon rigidly spinning any structure

98   defined by 3D coordinates, it could be used in any other shape analyses that use coordinate data, such

99   as continuous surface meshes used in spherical harmonics (Shen *et al.* 2009). Our method is a

100   convenient addition to the rapidly evolving tool kit of geometric morphometrics because it allows a

101   more comprehensive exploration of morphological diversity through the gathering of shape data from

102   complex 3D structures.

103

104 **Methodology**

105   We begin with a set of points $\widetilde{P} = \{\tilde{p}_0, \ldots, \tilde{p}_M\} \subset \mathbb{R}^3$ which represents a 3D object, and are

106   ordered so that $\tilde{p}_0$ represents the base point and $\tilde{p}_M$ represents the end point, by which we mean that

107   this object has an axis starting from $\tilde{p}_0$ and ending at $\tilde{p}_M$. Our goal is to rotate these points via a rigid

108   motion so that the axis on which these two points sit is either on the X, Y or Z-axis in $\mathbb{R}^3$. Rotation of

109   vectors in $\mathbb{R}^3$ is a well-known and easily resolved problem, and various formalisms exist in geometry.

110   Thus, we translate our set of points $\widetilde{P}$ so that $\tilde{p}_0$ maps to the origin $(0, 0, 0)$. This is a simple

111   transformation T defined by:

112   (1) $$p_i = T\tilde{p}_i = \tilde{p}_i - \tilde{p}_0$$

113   Note that the axis $X = \text{span}\{(1,0,0)\}$, $Y = \text{span}\{(0,1,0)\}$, $Z = \text{span}\{(0,0,1)\}$, where

114   each of the generating vectors are unit. Let us fix our desired axis to which we rotate the object to be

115 $A = \text{span}\{a\}$ where $a = (1,0,0)$, or $a = (0,1,0)$, or $a = (0,0,1)$. Since we have translated points

116 $\{p_i\}$ and vectors correspond to positions, we are simply looking to rotate the vector p_M to A, and each

117   other vector as a rigid motion with respect to this rotation. There are a number of ways to do this, but

118   the simplest way is to consider the plane spanned by p_M and A, and then to rotate by the angle between

119 p_M and A within this plane (Fig. 1b). Such a rotation is done via rotating on the axis to the plane, which

120   is determined by a normal vector to this plane.

121   Let us describe this set-up slightly more generally. For two vectors $u, v \in \mathbb{R}^3$, the axis to the plane

122   spanned by these two vectors is determined by a unit normal to the plane (there are two choices due to

123   orientation), which we denote by $N(u, v)$:

124   (2) $$N(u, v) = \frac{u \times v}{|u \times v|}$$

125   where $\times$ is the *cross product*. The angle between these vectors is then given by $\angle(u, v)$:

126   (3) $$\angle(u, v) = \arccos\left(\frac{u \cdot v}{|u||v|}\right)$$

127   where $\cdot$ is the *dot (scalar) product* between vectors. The rotation matrix about an axis $w \in \mathbb{R}^3$, where

128 $w = (w_1, w_2, w_3)$ is a unit vector, of angle θ radians is given by the well known matrix:

129   (4) $R'(w, \theta) =$

130
$$\begin{pmatrix} \cos\theta + w_1^2(1 - \cos\theta) & w_1 w_2(1 - \cos\theta) - w_3 \sin\theta & w_1 w_3(1 - \cos\theta) + w_2 \sin\theta \\ w_2 w_1(1 - \cos\theta) + w_3 \sin\theta & \cos\theta + w_2^2(1 - \cos\theta) & w_2 w_3(1 - \cos\theta) - w_1 \sin\theta \\ w_3 w_1(1 - \cos\theta) - w_2 \sin\theta & w_3 w_2(1 - \cos\theta) + w_1 \sin\theta & \cos\theta + w_3^2(1 - \cos\theta) \end{pmatrix}$$

131

132   Thus, to obtain a rotation matrix which is the rigid motion rotating the vector u to

133   v in the plane spanned by u and v, we obtain the expression:

134   (5) $R(u,v) \; = \; R'\big(N(u,v), \angle(u,v)\big)$

135   Getting back to our original problem, we set $v \; = \; p_M$ and $u \; = \; a$, and then we have the rotated points:

136   (6) $r_i \; = \; R(p_M, a)p_i \; = \; R'\big(N(p_M, a), \angle(p_M, a,)\big)p_i$

137   where $R(p_M, a)p_i$ is the action of the matrix $R(p_M, a)$ on the vector p_i.

138   It may be necessary to introduce a further constraint in the rotation. For instance, suppose $a \; = \; (0,1,0)$

139   and there is a point p_I, now rotated to r_I via the method we describe, which should lie in the Y-axis.

140   That is, we need to further rotate r_I to a point $r_I' \; = \; (*,*,0)$. To do this, we simply rotate in the axis a,

141   by an angle $\theta_Y(r_I) \; = \; \arctan((r_I)_3/(r_I)_1)$, where $r_I \; = \; ((r_I)_1, (r_I)_2, (r_I)_3)$. That is,

142   (7) $r_i' \; = \; R'\big(a, \theta_Y(r_I)\big)r_i$

143

144   **Implementation**

145   **Overview of the ShapeRotator package**

146   Here we illustrate the functions available within the ShapeRotator package and the basic steps

147   required in order to successfully implement the rotation on a data set of 3D coordinates. ShapeRotator

148   allows the rigid rotation of sets of both landmarks and semi-landmarks used in geometric

149   morphometric analyses, enabling morphometric analyses of complex objects, articulated structures, or

150   multiple parts within an object or specimen. The main steps required are: (1) importing the data and

151   fixating the rotation axes, (2) translating the whole data set of coordinates or points so that the main

152   selected point $\tilde{p}_0 = (0,0,0)$, and (3) rotating the two structures to the desired angle (as outlined on Fig.

153   2). This tutorial uses the example data set, which is included in this package.

154

155   **Importing a data set**

156   In the example data set we use two geometric morphometric data sets containing both

157   landmarks and semi-landmarks for two neighbouring and articulated bones (humerus and radioulna)

158   from a group of several species of frogs (details in Appendix S1), in tps format. We first import the

159   data sets using the R package *geomorph* (Adams & Otárola-Castillo 2013):

160   library(ShapeRotator)

161   library(geomorph)

162   radioulna <- readland.tps("radioulna.tps", specID = "ID", readcurves = F)

163   humerus <- readland.tps("humerus.tps", specID = "ID", readcurves = F)

164

165   These two GM data sets (radioulna and humerus) will be rotated on different rotation axes in

166 order to conform the aimed angle between them. This process is not exclusive to two neighbouring

167 structures, and thus, it could be performed for as many independent subunits as desired by choosing the

168 different angles among different rotation axes and all the translation processes. For more help on

169 importing the GM data sets please see Adams *et al.* (2014), and the associated help files. Please note

170 that this method also works for semi-landmarks as long as they have been equally-distance positioned

171 prior to the translation and the rigid rotation.

172

173 **Translating**

174   During this step each structure will be translated to the point of origin so that $\tilde{p}_0 = (0, 0, 0)$,

175 thus the distance from the coordinates of landmark_a (A_x, A_y, A_z) is substracted from all the

176 landmarks in all specimens, e.g. $(N_x - A_x, N_y - A_y, N_z - A_z)$ for landmark N. This translation is

177 made with the function *translate()*, as it follows:

178   translated_radioulna <- translate (radioulna[RU_landmark_a, , 1], radioulna)

179   translated_humerus <- translate (humerus[H_landmark_a, , 1], humerus)

180

181 **Fixing the rotation axis**

182   In order to fix a rotation axis in a structure we first need to select in our data set two suitable

183 landmarks for each structure which the axis will go through: landmarks A and B (for the first

184 structure), and landmarks D and E (for the other structure). In the radioulna example data set, landmark

185 A is the landmark in the 1st position and landmark B is in the 10th position. Similarly, for the humerus

186 data set, landmark D would be the landmark on the 52th position, and landmark E would be in the 19th

187 position. Finally, we also need to select an extra landmark that shares the same value for at least one of

188 its coordinates (two coordinates, ideally) with landmark b. This is needed for the simple reason that

189 there is not information about the orientation of the structure with only two landmarks per structure, so

190 even though the rigid rotation will work properly, it could position this structure in the wrong

191 ('mirroring') orientation. Thus, this orientation issue is corrected through landmark C. In this example,

192   landmark C is the 17th landmark, while landmark F is the 107th landmark in the humerus data set. We

193   need to know which landmarks will be selected in both structures prior to the rotation process.

194

195

196   **Rotating**

197   In the rotation step, we will use the function rotation() in order to rigidly rotate the two

198   structures to the desired angle, as it follows:

199   joined_dataset <- rotation(data.1 = translated_radioulna, data.2 = translated_humerus, land.a =

200   10, land.b=1, land.c=17, land.d=52, land.e=19, land.f=107, angle = 90)

201

202   The input datasets data.1 and data.2 correspond to the two translated datasets (in this case

203   translated_radioulna and translated_humerus. We then use the selected landmarks as explained in the

204   previous section. Finally, we include the angle (in degrees) that we would like to use to position the

205   two structures to one another. One of the options of the function rotation() is to select the desired angle

206   between the two structures so that we can perform the rigid rotation of each structure positioning them

207   in the selected angle in relation to each other. n order to do so we use the internal function

208   *vector.angle()*, by providing the desired angle in degrees (from 0° to 360°. The function *vector.angle()*

209   will return a vector that forms that angle with the vector (1, 0, 0). In the example data set in

210   ShapeRotator we rotate the coordinates from the two bones so that they form an angle of 90° degrees

211   within each other:

212   New_vector <- vector.angle(90)

213   So that New_vector = c(0, 1, 0). Thus we could check the vector that the function rotator() will

214   use, based on the input angle. The output from the function rotator() is a 3D array with the two joined

215   data sets (data.1 and data.2). Please note that the two datasets are joined based on their dimnames.

216   Thus, the order of the specimens in each dataset is not important, as long as all the cases match

217   perfectly between the two datasets in the same specimen. If there are extra specimens for one of the

218   datasets or the names do not match properly, rotator() will not include them in the output rotated joined

219   dataset.

220

221   **Exporting**

222   After the rotation process we could either use the joined GM array in further analyses or we

223   could also export it and save it in order to use it in another software, such as MorphoJ (Klingenberg

224   2011). In this step we will be using the function writeland.tps() in the R package *geomorph* (Adams &

225   Otárola-Castillo 2013) in order to save a tps file from the joined GM array:

226   writeland.tps(A="joined_arm", file = " joined_arm.tps", scale = NULL)

227

Other applications

229   Our method is an important addition to the tool kit of the geometric morphometrics field. It will

230   facilitate the analyses of compound 3D morphological datasets in geometric morphometrics analyses

231   but will also be useful outside of this field as it can be applied to any method that uses 3D coordinates.

232   The examples of applications are numerous in different fields of study, such as biology, anthropology,

233   palaeontology, medical sciences, archaeology, and engineering. For example, in evolutionary biology,

234   ShapeRotator would allow analyses of multiple or articulated hard structures (such as different

235   segments of an exoskeleton, different articulated bones, or neighbouring plant structures, among

236   others), different structures from the same object or organism (e.g. different and not adjacent body

237   parts), or pieces from damaged specimens. In medicine and veterinary science it could be used to

238   examine shape and size variation in different organisms' growth due to different nutritional treatments

239   or to examine how different structures respond to injuries or surgery. It would be useful in

240   palaeontology or archaeology when trying to quantify shape of different objects or organisms that

241   might have been preserved in disarticulated pieces.

242

Acknowledgements

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282

283 **FIGURES**

284
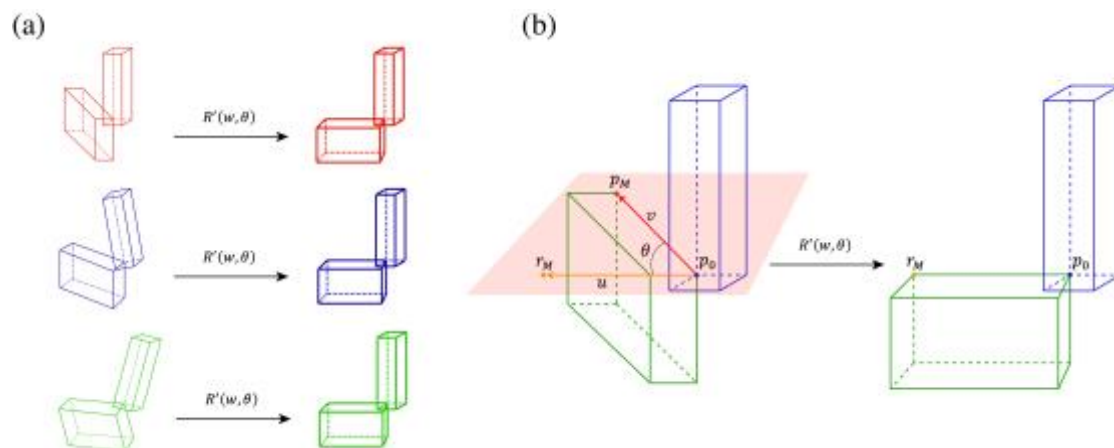
285 **Fig. 1.** (a) Application of the 3D rigid rotation method in three different scenarios, by rotating

286 articulated structures to a standardised position relative to each other. (b) Rotation method exemplified

287 by depicting the plane spanned by the already translated point p_M and A. Please note that p_0 depicts

288 the origin point (0, 0, 0). The rotated resulting point r_M, vectors u and v, and angle θ are also depicted.

289
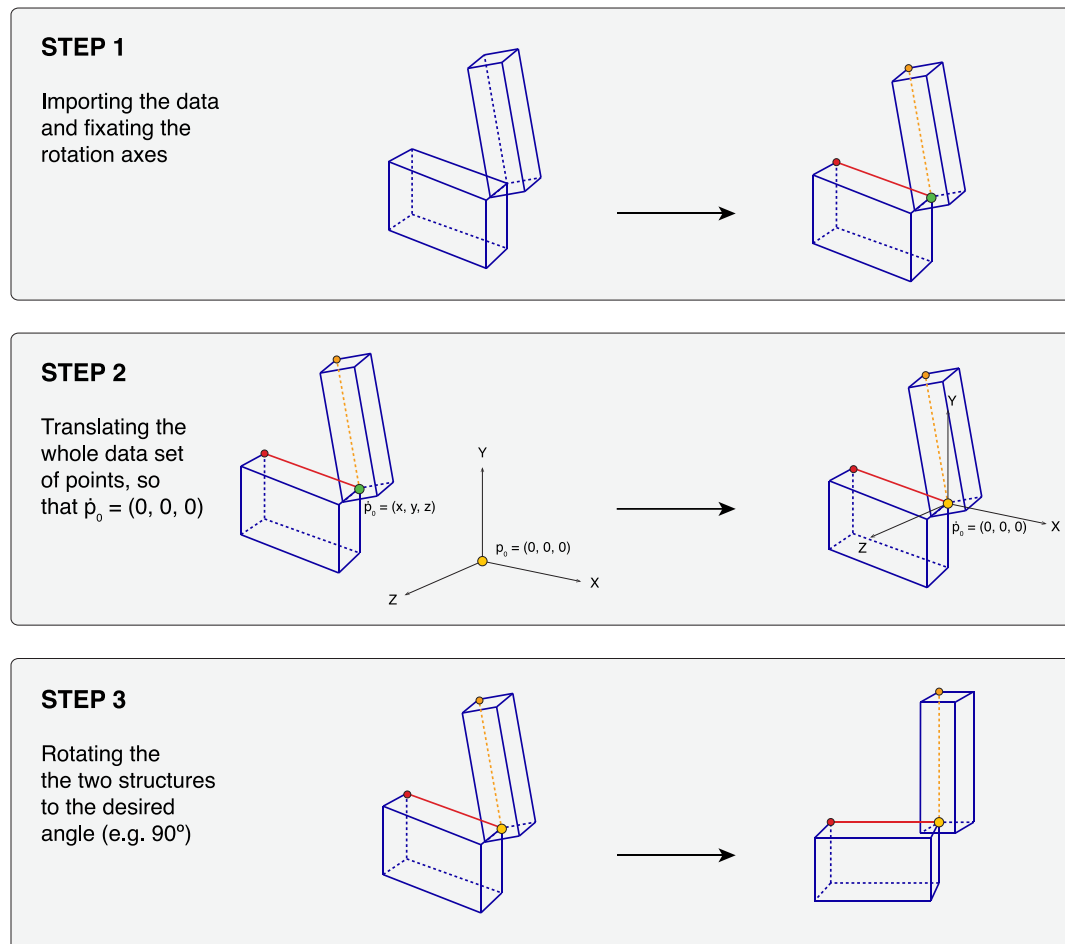
Fig. 2. Overview of the steps required in ShapeRotator, in order to rigidly rotate two articulated subunits. Step 1: importing the data and fixating the rotation axes; Step 2: translating the whole data set of coordinates or points so that the main selected point $\tilde{p}_0 = (0, 0, 0)$, with the function *translate()*; and Step 3: rotating the two structures to the desired angle (e.g. 90 degrees), with the function *rotator()*.