GUIDELINES TO USE THE DATA AND R SCRIPTS

The present document contains a detailed description of the data and R scripts used in the article "3D geometric morphometrics of thorax-pelvis covariation and its application for predicting the thorax shape of the Kebara 2 Neandertal" (insert DOI here when published) to allow researchers to reproduce the research findings.

DATA

The data provided here are:

- "N60_coordinates.txt". 3D coordinates (z,y,z) of the landmarks digitized on 3D torso models of n = 60 H. sapiens.
- "Thorax_temp_mlk_stern.txt". 3D coordinates (z,y,z) of the landmarks digitized on a 3D thorax model that works as reference for the thin plate spline interpolations.
- "Thorax_temp.ply". 3D model (.ply) of the aforementioned thorax that works as reference for thin plate spline interpolations.
- "Pelvis_temp_mlk.txt". 3D coordinates (z,y,z) of the landmarks digitized on a 3D reference pelvis model for doing the thin plate spline interpolations.
- "Pelvis_temp.ply". 3D model (.ply) of the aforementioned pelvis that works as reference for thin plate spline interpolations.
- "Kebara2_thorax_reconstructions.txt". 3D coordinates (x,y,z) of the landmaks digitized on the 3D thorax reconstruction made by Gómez-Olivencia et al. (2018) (Recons_K2_GO) and on the 3D thorax reconstruction made by Sawyer and Maley (2005) (Recons_K2_SM).
- "Kebara_2_pelves_reconstructions.txt". 3D coordinates (x,y,z) of the landmaks digitized on the 3D pelvis reconstruction made by Rak and Arensburg (1987) (Recons_K2_RA) and on the 3D pelvis reconstruction made by Sawyer and Maley (2005) (Recons_K2_SM).
- "Groups_N27males.txt". Classifiers for drawing the ellipse in the PLS plot of Model A.

- "Groups N60sapiens.txt". Classifiers for drawing the ellipse in the PLS plot of Model B.
- "Groups_N33females.txt". Classifiers for drawing the ellipse in the PLS plot of Model C.
- "Actual_pred_thorax_N27.txt". 3D coordinates of n = 27 actual male thoraces + n = 27 predicted male thoraces.
- "Actual_pred_thorax_N60.txt". 3D coordinates of n = 60 actual H. sapiens thoraces + n = 60 predicted H. sapiens thoraces.
- "Actual_pred_thorax_N33.txt". 3D coordinates of n = 33 actual female thoraces + n = 33 predicted female thoraces.
- "FreqA_actual.txt". A list of Procrustes distances between every possible pair within a sample composed of n = 27 actual male thoraces (column C) reflecting the actual intraspecific variation of that sample.
- "FreqA_pred.txt". A list of Procrustes distances between each actual thorax and its prediction using Model A. The entire Procrustes distance matrix is available through Mendeley Data (Link to dataset: , Dataset DOI: 10.17632/v4x29hwb5n.1).
- "FreqB_actual.txt". A list of Procrustes distances between every possible pair within a sample composed of n = 60 actual H. sapiens thoraces (column C) reflecting the actual intraspecific variation of that sample.
- "FreqB_pred.txt". A list of Procrustes distances between each actual thorax and its prediction using Model B
- "FreqC_actual.txt". A list of Procrustes distances between every possible pair within a sample composed of n = 33 actual female thoraces (column C) reflecting the actual intraspecific variation of that sample.
- "FreqC_pred.txt". A list of Procrustes distances between each actual thorax and its prediction using Model C.

R SCRIPTS

The R scripts provided here are:

- Model A.R. Code to load data, re-slid semilandmarks against a mean configuration, calculate two-blocks partial least squares (PLS) analysis of n = 27 males with shape deformations along PLS vectors via thin plate spline interpolation, cross-validated and nonvalidated prediction error of Model A, best and worst human predictions based on Model A and Kebara 2 thorax predictions using the pelvis reconstruction made by Rak and Arensburg (1987) and by Sawyer and Maley (2005). Lastly, the resulting predictions are superimposed to the thorax reconstructions made by Sawyer and Maley (2005) (not uploaded to Git, see article for more details) and Gómez-Olivencia al. (2018)(available Figshare by in https://doi.org/10.6084/m9.figshare.7012256).
- Model_B.R. Code to load data, re-slid semilandmarks against a mean configuration, calculate two-blocks partial least squares (PLS) analysis of *n* = 60 *H. sapiens* with shape deformations along PLS vectors via thin plate spline interpolation, cross-validated and nonvalidated prediction error of Model B, best and worst human predictions based on Model B and Kebara 2 thorax predictions using the pelvis reconstructionS made by Rak and Arensburg (1987) and by Sawyer and Maley (2005). Lastly, the 3D models of the resulting predictions are superimposed to the thorax reconstructions made by Sawyer and Maley (2005) (not uploaded to Git, see article for more details) and by Gómez-Olivencia et al. (2018) (available in Figshare https://doi.org/10.6084/m9.figshare.7012256).
- Model_C.R. Code to load data, re-slid semilandmarks against a mean configuration, calculate two-blocks partial least squares (PLS) analysis of n = 33 females with shape deformations along PLS vectors via thin plate spline interpolation, cross-validated and nonvalidated prediction error of Model C, best and worst human predictions based on Model C and Kebara 2 thorax predictions using the pelvis reconstructions made by Rak and Arensburg (1987) and

by Sawyer and Maley (2005). Lastly, the 3D models of the resulting predictions are superimposed to the thorax reconstructions made by Sawyer and Maley (2005) (not uploaded to Git, see article for more details) and by Gómez-Olivencia et al. (2018) (available in Figshare https://doi.org/10.6084/m9.figshare.7012256).

• Other.R. Code to create the different plots for visualizations (see article for more details).