This software implements the Generalized Procrustes Surface Superimposition (GPSA) and associated ordination and visualization methods described in Pomidor et al. (2016). The program is written in Java and should run on any platform with a native Java Runtime Environment (JRE – https://java.com). Source code accompanies the publication, and updated versions, if any, are available from <a href="http://morphlab.sc.fsu.edu">http://morphlab.sc.fsu.edu</a>

	Output prefix:	_gpsa_	
	Output suffix:		
	Se	elect prototype file (.ply)	
	S	elect surface (.ply) files	
	General	ized Procrustes Surface Analysis	
		Ordination	
	Shape/Form	Generator X 1.00	
	Vi	sualization Auto Sequence	
SA Versio	n: 20160308		

INSTALLATION: to install the program, simply download the .zip file and unzip into a convenient directory.

RUNNING THE PROGRAM: The directory created by unzipping the program offers several ways to run the program. Some are operating system specific. In the simplest case and assuming you have an appropriate Java runtime or development system installed, you can just double-click the gpsa.jar file. This is probably not the best approach since the program will run with the default maximum memory

allocation for your system which might be inadequate for some data sets. Instead, you can use for different operating systems...

Microsoft Windows: gpsa.bat Unix-like operating systems: gpsa.sh Apple Macintosh OS X: gpsa

Each of these allocate, by default, 4G of maximum memory for program use. This is the amount necessary to process the data sets used for and distributed in association with the paper. Note, this software was created solely for the initial development of the algorithm. While the program will process each of the rather large data sets associated with the paper, it needs to be restarted between processing the data sets of this size. Future versions are expected to optimize memory, core, and other resource utilitzation.

Also, **you must not move the above files from their original directories**. To create desktop links to quickly access the program, first make an Alias or Link to the appropriate program, then move that file to the desired location.

**DEFINITIONS:** 

- 1) ".ply" indicates a surface mesh file in the Polygon File Format (<u>https://en.wikipedia.org/wiki/PLY\_%28file\_format%29</u>).
- 2) "R" refers to the language/environment distributed by the R Core Team (2015).

### CONFIGURATION FILE:

The program also saves the last working directory into a configuration file in the user's home directory. This is a visible (I hate hidden config files) ascii file named gpsa.configuration.

### **PROGRAM OPERATION:**

**Translate, Rotate, Scale** – <- hidden at the moment and not functional as of this writing. All surfaces are translated, rotated, and scaled to minimum squared Procrustes surface metric distance.

**Output prefix** – text to be added to the beginning of each of the output filenames. **Output suffix** – text to be added to the beginning of each of the output filenames. Output filenames generated by the program are based on input filenames with the above pre/suffixes.

**Select prototype file (.ply)** – the user is presented with a file-selection window with which he/she can select the single surface file on which to base the superimposition. This can be an external prototype or one of the surfaces to be fit.

**Select surface (.ply) files** – the user is presented with a file-selection window with which he/she can select a number of files for superimposition.

**Generalized Procrustes Surface Analysis** – executes the GPSA. This can take some time depending upon the number and size (vertices) of the surfaces being fit. Timers are shown to indicate start and elapsed time.

**Ordination** – the ordination button, available after GPSA, performs the principle-coordinates-based ordination as described in the paper. Coordinates of each surface one each axis are saved to a file.

**Shape/Form Generator** – generates surface visualization of a specimen on the axis specified in the provided drop-down menu at the indicated score. By default, the score is set to the maximum positive projection of the data onto the selected axis.

**Visualization Auto Sequence** – this tool is designed to help the user generate a sequence of evenly spaced visualizations of surfaces along a given axis. The user is presented with a dialog with which he/she can set the beginning and ending scores to visualize and the number of steps between these two extremes to visualization. By default, Begin and End are set to the minumum and maximum projections of the data onto the specified axis.

### **PROGRAM OUTPUT:**

Given default output pre/suffixes, prototype file – proto.ply, and surface files – surf1.ply, surf2.ply, and surf3.ply, the program outputs the following files...

\_gpsa\_surf1.ply \_gpsa\_surf2.ply \_gpsa\_surf3.ply – the original surface files aligned to the prototype.

\_gpsa\_mean.ply – the average surface.

\_*gpsa\_heatmap.ply* – the average surface with vertices colored to reflect the magnitude of variation in the sample at each vertex.

<u>\_gpsa\_interspecimenPSMvalues.dat</u> – an ascii file containing the Procrustes surface metric distances between specimens as a square, symmetric matrix.

 $_gpsa\_homologized\_points.dat$  – a tet file containing a matrix of homologized vertex coordinates. Each row is a specimen and will contain the coordinates (columns) for all vertices. This file can be HUGE. For instance, fitting 20 scans resulting in a mean with 500k vertices would contain 20x500kx3 = 30 million numbers.

*\_gpsa\_ordination\_projections.RData* – R data file containing the coordinates of the specimens on the ordination axes.

\_gpsa\_ordination\_values.RData – the singular values associated with each of the ordination axes in R format.

 $_gpsa\_Axis1\_max.ply-$  if the Shape/Form button is used to visualize a surface, the filename will be patterned as: Output prefix + Axis + i + "\_" + val + ".ply", where i is the axis chosen with the drop-down menu and value is the selected value on that axis for the visualization. The default for this value is the score of the specimen with the maximum positive projection. The vertices of the resulting surfaces are color-coded from blue to red based on the root-sum-of-squared regression coefficient, which indicates the magnitude, but not direction, of displacement at each vertex.

# \_gpsa\_Axis1\_min.ply

## <steps>

\_gpsa\_Axis1\_max.ply – if the Visualization Auto Sequence generator is used, the user is presented with a dialog in which to enter the minimum and maximum starting values for scores on the selected axis (chosen in the drop-down menu in the main program window) and the number of steps for which to

generate visualizations. By default, 1 step is chosen, and the program generates surfaces only for the beginning and ending values. More steps produce surfaces equally spaced between these two values. By default, the Begin and End values are set to the minimum and maximum projections of the data on the chosen axis.

For more information, feel free to contact the FSU Morphometrics Lab: morphlab@fsu.edu.

### **REFERENCES**:

Pomidor, Benjamin J., Jana Makedonska, and Dennis E. Slice. "A Landmark-Free Method for Three-Dimensional Shape Analysis." PLOS ONE 11, no. 3 (March 8, 2016): e0150368. doi:10.1371/journal.pone.0150368.

R Core Team (2015). R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. URL https://www.R-project.org/.