The Tps series of software

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Commentary

The tps series of software

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Abstract

The development and the present state of the "tps" series of software for use in geometric morphometrics on Windows-based computers are described. These programs have been used in hundreds of studies in mammals and other organisms.

Some history

Work on the tps series of programs was begun by me in late 1990. At that time the only software specifically designed for the new field of geometric morphometrics was that developed by Fred Bookstein and Bill Green for the mainframe computer running the MTS operating system at the University of Michigan. As that operating system was only available at about a dozen computing centers around the world, the need for new and easy to use software was quite apparent. This was quite striking at the NSF-sponsored workshop on morphometrics held at Stony Brook University in the summer of 1990. New methods were described by Bookstein but participants were not able to actually try them on their own data. At the same time, the microcomputer revolution had started and it was clear that the new software should be developed for these new devices. It was also clear that the new software should include highly interactive graphics because it is easier to understand shape differences visually than numerically.

The first programs developed in the series were the MS-DOS programs TPSPLINE and TPSRW. The TPSPLINE software smoothly transforms the positions of landmarks and an overlaying grid for one specimen so that its landmark positions would map exactly onto another set. The grid was then subjected to the same transformation. The thin-plate spline function was used to provide this maximally smooth transformation, Bookstein (1989). The transformed grid produces a graphic in the spirit of the D'Arcy Thompson transformation grids, Thompson (1917). However, these transformed grids represent the actual differences in the location of landmarks rather than intuitive sketches, Klingenberg (2013). The GRF software of Rohlf and Slice (1991) was available at the time of the morphometrics workshop at the University of Michigan, Rohlf and Bookstein (1990). It was not made part of the series because the generalized Procrustes computation was to be made part of most of the programs in the series.

The use of "tps" in the names of these and later software was because they made use of the thin-plate spline function. At the time the software was first written, the use of the thin-plate spline function and its decomposition by spatial scale into principal and partial warps seemed to be an essential component of the new statistical methods. Later, e.g., Rohlf (1999), it became clear that the computation of partial warp and uniform scores could be eliminated because a PCA of these scores differed from that of Procrustes coordinates (after their projection onto the multivariate space tangent to Kendall's shape space) by only a multiplication by an orthonormal matrix i.e., a rotation. This is important because test statistics for standard multivariate statistical methods are invariant to such transformations. For example, they yield the same plots of PCA scores. However, this relationship is only exact if the shape coordinates have been projected onto the space tangent to Kendall's shape space, see Rohlf (1999). Unfortunately, not all morphometric software performs this projection so that the PCA is performed in a space that is curved. The amount of curvature depends on the amount of shape variation, see Slice (2001). Of course with very similar shapes the curvature will be very small. The decomposition of shape differences at different spatial scales (as captured by the partial warps) is mathematically elegant but these individual components are unlikely to be directly interpretable biologically for reasons such as those presented in Rohlf (1998). However, Bookstein (2015) shows that they can be very important for the study of integration because they allow one to take variation at different spatial scales into account.

The TPSRW software, described in Rohlf (1993), performed an analysis of relative warps as defined by Bookstein (1989, 1991). The TPSPLINE and TPSRW programs were available by the time of the 1991 morphometrics workshop in Valsain, Spain, Marcus et al. (1993). By the time of the 1992 morphometrics workshop in Paris, France, the TPSREG software was also available. It performed a multivariate multiple regression of partial warp scores onto one or more independent variables. It is "multivariate" because there will always be more than one shape variable and "multiple" because the software allows more than one independent variable.

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The programs use the `.tps` file format designed for holding the 2D and 3D coordinates of landmark points and, optionally, the name of the image file corresponding to the landmarks for each specimen. It was later generalized to also hold coordinates of points along curves and entire outlines. The landmark coordinates can also be saved as matrices using the `.nts` (NTSYSpc) file format. Both formats are described in the help files included with each program. Numerical results such as matrices of principal warps and partial warp scores, relative warp scores, etc. can be saved using the `.nts` (NTSYSpc), `.m` (Matlab), and `.csv` file formats. These are all plain ASCII text files than can be viewed and modified for use with other software by using a text editor such as the Windows Notepad (although more powerful editors are more convenient when more extensive changes are needed). The decision to develop a series of specialized programs rather than one comprehensive program was made to enable at least some software for geometric morphometrics to be available as soon as possible.

Towards the end of the 1990s development was switched from MS-DOS to the Windows 3.1 operating system and by the time of the 1997 morphometrics workshop in Rome, Italy, the software had been rewritten and new software developed for use with MS-Windows 95. It was soon migrated to Windows NT. This change made the analysis of larger datasets possible as well as better graphics. This also meant that only minimal changes to the software would then be needed for compatibility with the new versions of Windows. The present suite of programs in this series were written in a standard way for Windows 7, 8, and 8.1 but should run on future versions of Windows as well as emulators on Linux (e.g., WINE, http://www.winehq.org/) and MacOS computers. It should be noted that the software all have help files that provide both technical information about what the programs do, notes on how to use each program, and usually examples. The programs are listed below in alphabetical order.

The present programs in the TPS series

TpsDig2. This software is used to capture the coordinates of landmarks for a wide variety of 2D image formats. The intended usage of the software is to start with a .tps file that contains lines with "LM=0" and "IMAGE=xxx" (where "xxx" is the name of an image file) for all the specimens in a study. This initial `.tps` file can be created automatically using one of the options in the tpsUtil program. One can then move through the images by pressing the red left and right arrow buttons. The images can also be transformed in order to enhance them so that the landmarks are easier to see. Coordinates of points along outlines and curves can also be captured. For high-contrast images, complete outlines can be captured automatically, Souto-Lima and Millien (2014) is an example using molars of voles. TpsDig2 is an update of TpsDig. The update was needed for compatibility with high resolution image files that are now used. The program can also be used to measure distances, angles, and areas.

TpsPLS. A program to perform a two-block partial least-squares analysis, 2BPLS, as described by Rohlf and Corti (2000). The software can be used to analyze and visualize patterns of covariation, if any, between a set of variables and a sample of shapes from the same set of specimens. An early example of this is given in Adams and Rohlf (2000). A recent example relating fractures of different teeth to mandible shape in carnivores is given in Meloro (2012). The software can also be used to study the covariation between the shapes of two structures for the same set of specimens. An example of this is given in Pizzo et al. (2009). Configurations of landmarks corresponding to various positions in the space of the singular warps can be displayed.

TpsRegr. This performs a multivariate multiple regression of shape (using warp and the uniform component scores as the dependent variables) regressed on one or more independent variables. The independent variables can be observed variables such as temperature or elevation or they can be dummy variables that code various experimental designs using the method usually called "fitting constant", e.g., Sokal and Rohlf (2012). This allows one to perform MANOVAs and ANCOVAs of shape variation. Choizzi et al. (2014) is a recent example for Soemmerring's Gazelle. Cardini and O'Higgins (2004) also used it

to test for differences in cranial shape in Marmots. Paired comparison designs are often useful. Visualizations are provided to show the effects of variation in each independent variable. The results are given in terms of both Procrustes statistics and conventional multivariate tests. Permutation test statistics are also provided. The permutations can be constrained to be either within or among blocks of specimens so as to conform to certain experimental designs. Configurations of landmarks predicted by the regression can be displayed. The shape changes associated with each independent variable can be explored by simply moving a slider back and forth. This software has been used in many studies. For example, Bastir and Rosas (2004) regressed mandible shape on size to study allometry in humans, Slater and Van Valkenburgh (2008) regressed cranial shape on tooth length for sabretooth cats. An estimated image corresponding to a predicted configuration of landmarks can be created using the TpsSuper software but that does not seem to have been done often. In addition to the usual interactive mode, the program can also be completely controlled using batch mode commands. This is very useful when the software is used in simulation studies.

TpsRelw. This is the most used program in the series. Examples are too numerous to list here. The program computes the average shape and then aligns all specimens to this average shape using a Generalized Procrustes analysis, Rohlf and Slice (1990). The average shape, aligned specimens, and centroid sizes can be saved to files. It then performs an analysis of relative warps, i.e., a principal components analysis of shape variation relative to spatial scale, Bookstein (1989, 1991) and Rohlf (1993). Its α parameter allows weights to be given to differences in landmarks at different spatial scales in the average shape estimated using generalized Procrustes analysis (often called the reference or the consensus configuration). However, α is now usually set to zero so that analysis is then simply a principal components analysis of shape variation (as captured by the set of partial warp scores) and no longer relative to spatial scale. It produces the same results as a PCA of the Procrustes shape coordinates if they are projected onto the tangent space. In the plot of the relative warp scores, shapes can be displayed corresponding to arbitrary positions in the ordination by moving a small red circle with the mouse. Plots for positions at the extremes along each axis are often published along with the ordination. Animations corresponding to arbitrary sequences of positions in space can also be constructed. Another important feature of this software is that it can slide semilandmarks along curves as described by Bookstein (1997). While this is the only software in the tps series that provides this operation, that is not a limitation to the use of this method because the resulting landmark and semilandmark configuration for each specimen can be output and used as input to the other programs in this series. The tpsUtil software can be used to create the file that defines the points that are to be used as semilandmarks rather than the usual fixed landmarks. Because the ordination plots do not provide many options for customization, the scores are often entered into other software. Unfortunately, such software often does not preserve the relative scales of the axes. The plots can be very misleading unless the axes are to the same scale. Figure 3 in Cardini et al. (2015) is a good example of the correct scaling. The ordination plot is elongated along the first axes because the first eigenvalue is so much larger than the second. It also shows shapes corresponding to different locations in the plot. The plot proposed by Bookstein (2015) can also be produced.

TpsSmall. This is a simple program designed to help a user assess whether the amount of shape variation in a dataset is small enough to justify the use of standard multivariate statistical methods in the tangent space. Fortunately, this is almost always true in studies of mammals. A possible exception due to the breadth of shapes included is given in Marcus et al. (2000), a study of variation in the skulls representing the orders of living mammals. The program plots a matrix of Procrustes distances element by element against a matrix of Euclidean distances in the tangent space and reports their uncentered regression slope and correlation. It also reports on the largest Procrustes distance relative to the largest possible Procrustes distance, $\frac{\pi}{2}$. The distance matrices can also be saved to a file for use in other software (such as to cluster

specimens based on their Procrustes distances). This software can also use 3-dimensional coordinates.

TpsSplin. This software does not perform any statistical analyses. It simply displays a grid overlaying one specimen transformed using the thin-plate spline so that the positions of its landmarks coincide with those of another specimen. It also allows this transformation to be decomposed by spatial scale. Plots can be displayed showing the overall transformation as well as for just the affine part, the non-affine part or the latter's decomposition into the contribution of individual partial warps. As mentioned above, these decompositions seemed more interesting when the software was first developed than they do now for the reasons given in Rohlf (1998). The software is still useful for displaying the shape differences between two specimens or two group means.

TpsSuper. This software has several options for the unwarping of images. An unwarped image is an image that has been transformed so that its landmarks match those of a specified target configuration of landmarks. The operation is called "unwarping" rather than "warping" because, instead of mapping each pixel in the original image to its position in the transformed image, each pixel in the transformed image is looked-up in the original image. This prevents gaps in the transformed image in regions that are expanded relative to the first image. See Bookstein (1991) for more discussion and an example. The target configuration is often an average of all the specimens but it can also be a configuration of landmarks predicted by regression using tpsRegr, a point in a PCA plot using tpsRelw, or an estimate of a node in a phylogenetic tree using TpsTree, see Rohlf (2002) for an example of the latter. It can also compute an average of a sample of images that have been unwarped to match a specified configuration. Examples are given in Gharaibeh et al. (2000) for mid-sagittal MRI images of human brains and in Bookstein et al. (2007) to show the effects of prenatal alcohol on the brains of children. While most geometric morphometric studies display statistical results as landmark configurations, the addition of unwarped images can be very helpful for biological interpretation. I believe that unwarped images should be used more often as they are more informative than just positions of landmarks and wireframes.

TpsTree. Given a phylogenetic tree or a dendrogram from a cluster analysis, the program provides visualizations of estimated configuration of landmarks corresponding to the nodes or to arbitrary locations along the branches. Estimates are computed using the squared-change parsimony model as described in Maddison (1991). In conjunction with the TpsSuper software, predicted images can be displayed for the nodes on the tree. Rohlf (2002) is an example. The software can also output a phylogenetic covariance matrix — useful in comparative studies that use the phylogenetic generalized least-squares method to analyze their data. See Rohlf (2001) for a discussion. A matrix of independent contrasts, Felsenstein (1985), can also be produced.

TpsTri. This software was designed to display various properties of shape spaces when there are just 3 landmarks. It does not provide any statistical analyses of shape variation. It can plot samples of shapes (user provided or from built-in simulations) on the various shape or form spaces that have been proposed for use in morphometrics. It can show, for example, why the reference shape should be at least close to the mean shape of a sample of shapes. It can also display some of the properties of the various shape spaces that have been proposed. This software was used to prepare the plots of shape spaces in Rohlf (2000a); Slice (2001), and in many other papers describing properties of some of shape spaces.

TpsUtil. This software resulted from a wide variety requests for special operations needed when carrying out a morphometric studies. Rather than providing many specialized utility programs, the operations were combined into a single program. It can, for example, change file formats, delete or reorder landmarks, delete or reorder specimens, split or combine files, and change file formats. The software can also compute areas, prepare input files for sliding of semilandmarks in tpsRelw. It includes an option to "unbend" the positions of landmarks in an attempt to undo distortions in preserved fish. A common use of tpsUtil is to build the initial `.tps` file that is used as input to the TpsDig2 software. I am still open to suggestions for additional operations.

Other, more specialized programs

The following programs were written because they were needed for particular papers I wrote. However, the programs were generalized somewhat so that they might also be of use to others — either to duplicate my simulations or to perform additional experiments.

TpsBias. This software was used for the computations and illustrations in Rohlf (2003). That study examined the patterns of error and bias for several methods for estimating of the mean shape for a sample. While that study only simulated isotropic variation at each landmark, the software can also be used to investigate more general models (different amounts of variation at each landmark and with correlated variation within and between landmarks). The results for these latter models have not yet been published but the conclusions are very similar — Procrustes methods have much better statistical properties (less bias and smaller mean square error) than other morphometric methods that have been proposed – even though these models violate the assumptions of the Procrustes-based methods. The program can also be completely controlled using batch mode commands for use in simulation studies.

TpsPower. This software was used for the computations and illustrations in Rohlf (2000b). It allows one to determine the probability of correctly deciding that two samples of shapes were drawn from populations with different mean shapes. The results are given for several test statistics. The original version of the software was constrained to the isotropic model but more general models can also be investigated. In addition to the usual interactive mode, the program can also be completely controlled using batch mode commands for when the software is used in simulation studies.

Future development?

It was originally expected that the programs would eventually be combined into a single comprehensive package. That development now seems less important because there are now several such general programs available. It is a sign of the growing maturity of the field. There are stand-alone programs such as MorphoJ (http://www.flywings.org.uk/morphoj_page.htm), Morpheus et al (http://morphlab.sc.fsu.edu/software.html), NTSYSpc (http://www.exetersoftware.com), IMP (http://www3.canisius.edu/~sheets/IMP%208.htm), or the EVAN Toolbox (for members of the European Virtual Anthropology Network). There are also collections of procedures for R such as the `geomorph` package (http://www.geomorph.net). It is tempting to generalize the tps series to allow for 3-dimensional coordinates but no firm decision has been made. ✍

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