

IMP:SemiLand6

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Introduction

This is a manual for the SemiLand6 program, which is an IMP program to allow use of semi-landmark data. Please read the file

SemiLand_becki.pdf (an example application of semi-landmarks) prior to reading this file, to get a sense of what semi-landmark methods are meant to do. You may also want to get a copy of MakeFan6, a tool to aid in digitizing points along curves.

READ THE UPDATE AT THE END OF THIS MANUAL. As of December 6, 2002, the bending energy based method is NOT STABLE, an alternative approach is available!

Semi-landmarks

The incorporation of information about curves into landmark based morphometrics has been pioneered by Bookstein and Green (Bookstein 1996, 1997, Bookstein et al. 2002, Green 1995, 1996). This method utilizes *semi-landmarks*, points allowed to slide along curves to minimize the bending energy of deformation from a mean form (see Bookstein 1991 for a discussion of bending energy). After the iterative formation of a mean reference form, the landmarks and semi-landmarks are used in a Procrustes Superimposition based analysis. We present here a purely conceptual description of the incorporation of curves into landmark based analyses, readers interested in the details of the math are directed to the works of Bookstein and Green.

It is important to note that this use of the bending energy constitutes a fundamental change in how that thin plate spline is used, relative to the decomposition of

deformations into Partial Warp plus Uniform component scores or to the use of the thin plate splines to extrapolate patterns of deformation when plotting a deformation grid. In both of these uses, biological homology is determined by the researcher's choice of landmarks. In using the thin plate spline to match or choose positions along a contour, the thin plate spline is being used in an attempt to establish biological homology of points along these contours. Clearly, for this operation to have any chance of success, the curves must be homologous, the method of semi-landmark alignment put forward by Green and Bookstein then attempts to extend this homology to specific points on the curves. While the thin-plate spline has proven to be a robust tool for the analysis of shape, it is important to stress the point that the use of the spline to align points along curves and establish biological homology of points is a substantial extension of the use of the thin plate spline, which cannot automatically be assumed to have the same reliable and robust nature as earlier uses of the spline.

The assumptions implied by the use of the thin plate spline do not alter the statistical results one obtains using tests based on Partial Warp plus Uniform Component scores. When carrying out a thin-plate spline decomposition to generate Partial Warp plus Uniform component scores, the eigenvectors of the bending energy matrix form a useful basis set of orthogonal axes for describing non-uniform deformations of the reference. The inclusion of the Uniform components (Bookstein 1996) completes the basis set of vectors necessary to describe all possible deformations of a reference form. It is important to realize that there a wide variety of alternative approaches to forming basis sets for deformations (Dryden and Mardia 1998), many other interpolation functions could be used in the same fashion to generate complete, orthogonal basis sets for

deformations, each of which would mathematically function equally as well as the Principal Warps and Uniform axes.

Likewise, the use of the thin plate spline to extrapolate the pattern of deformation from the observed deformations at landmarks to the regions of space on an organism between landmarks will not alter statistical findings. Descriptions of deformation grids must of course be formed bearing in mind that they were drawn using extrapolation methods based on the spline, rather than on direct observation of points in the region between landmarks.

In the use of the thin plate spline to align semi-landmarks along curves, the spline is being used to attempt to locate biologically homologous points along curves. So the assumptions of the thin plate spline are included in all subsequent statistical analyses of those points, unlike earlier, clearly established uses of the spline in geometric morphometrics.

Green (1996) defines *contours* as individually identifiable curves that are homologous between images or specimens. A contour may begin and end at identifiable landmarks (an *open* contour), or the contour might form a closed loop on the specimen (a *closed* contour). In working with landmarks, each landmark should be a biologically homologous point on the organism, mathematically, points have a dimension of zero. In working with curved homologous structures, the entire contour is a one-dimensional object made of an infinite number of points. The homology is represented by this entire infinite set of points along the contour.

Clearly, working with an infinite set of points is not practical, although these infinite sets would be homologous and preserve all the information known about the curves.

To work with curves, we need to reduce the number of points used to represent the curve from infinity down to a more manageable number, while preserving the homology of the points used and also preserving the useful information about the curves. What we need to do is pick a subset of the infinite number of points on the curve to represent the curve.

The points along the curve are not homologous in the same manner as landmark points are, but the curves represented by these points are homologous. The difficulty posed by this method is how to choose “equivalent” points along curves on specimens drawn from a variable population.

The approach put forward by Bookstein and Green is to measure the landmark locations and a uniformly spaced series of points along each curve (henceforward these points along curves will be referred to as *semi-landmarks*) for each specimen in a study.

The next step is to construct a *model*, which Green (1996) calls a central configuration (ideally, it should be roughly the mean of all measured landmark configurations) of all the landmarks plus a set of semi-landmarks spaced along each of the contours in the study. The model is formed in an iterative manner, initially all landmarks and contours are roughly aligned, and the model is formed by taking the mean of all landmark and semi-landmark locations. Then each semi-landmark of each specimen is allowed to slide along the tangent line to the curve at each point to minimize the bending energy required to transform the corresponding point on the model to the semi-landmark position of the specimen. This procedure is carried out for each specimen in the data set. The landmark and semi-landmark positions in a new model (or mean specimen) are then calculated and the process is iterated until there is no significant change in the model specimen.

The criteria used by sliding the semi-landmarks along a contour of the target specimen is that the bending energy required to deform the location of the corresponding semi-landmark on the model to match the location of the semi-landmark on the target should be minimized. This is a parsimonious criteria in that minimizing the bending energy implies that the contour on the model has changed as smoothly as possible to match the contour on the target. By sliding the semi-landmarks along the contour so as to minimize the bending energy, a set of semi-landmarks on the target form is located that represents the smoothest possible deformation of the corresponding semi-landmarks on the model form. Other criteria for sliding semi-landmarks along a contour are also possible, sliding could be carried out to minimize the euclidean distance between corresponding semi-landmarks or to place the semi-landmarks on the target contour along the normal to the contour on the model form (see Sampson et al. 1996). Bookstein (1997) argues that the bending energy criteria is the approach most consistent with the overall goals of landmark-based geometric morphometrics, particularly if thin-plate spline decompositions are to be used in the analysis.

The sets of coordinates of landmarks and semi-landmarks produced by this procedure do not lie within Kendall's Shape space, but in some other space, the details of which appear not to have been worked out to date. The approach to the statistics of semi-landmarks that appears to be the most reasonable is to rely on permutation, resampling and bootstrap approaches, rather than on analytic statistical tests which require an understanding of the nature of the mathematical space underlying landmark plus semi-landmark data.

Since the semi-landmarks are allowed to slide along a contour, each semi-landmark has only one degree of freedom, despite being represented by two coordinates. The single degree of freedom is the location of the semi-landmark along the curve. Landmarks in two dimensions each have 2 degrees of freedom, prior to the Procrustes superimposition which removes 4 degrees of freedom from the set of measured coordinates. The mismatch between the number of coordinates and the number of measured variables (coordinates) poses difficulties for many standard statistical packages.

Semi-landmarks and Helper Points

In order to accurately slide semi-landmarks along a contour to minimize the bending energy of deformation of a given specimen from the reference, it is desirable to have many closely spaced semi-landmarks along the curve. However, using many semi-landmarks along a curve and then combining these semi-landmarks with a limited set of landmarks means that each homologous landmark is represented by a single point with 2 degrees of freedom and the single homologous contour is represented by many semi-landmarks. This means that the effects of variance in the semi-landmark locations may overwhelm signals in the landmark locations, not because they are biologically more important, but simply because they are represented by a larger number of measurements.

There are some approaches to differentially weighting landmarks and semi-landmarks within a study (Green 1996,???), but the approach we present here is the use of helper points. Helper points are treated like semi-landmarks during the procedure of sliding semi-landmarks along the contour to minimize bending energy. Once the model form has been constructed, and the semi-landmarks along the contour have been positioned, the helper points are discarded prior to any statistical analysis of the shapes.

The software developed for use in this study (IMP:SemiLand6, Sheets 2002) allows for use of a protocol file which identifies landmarks, semi-landmarks, helper points and contours. This means that it is possible to produce a variety of alternative protocol files for a study, varying the number of semi-landmarks and helper points used to determine what effect these choices have on the outcome of the study.

Using SemiLand6

You will need a data set which has both landmarks and points along curves already digitized. The program IMP:MakeFan6 was designed to place alignment “fans” on your image to make it easy to consistently digitize points along a curve. Other programs may provide similar capabilities. Digitize your specimens and then convert the data file into TPS format, using CoordGen6 to convert from the TPS format to a format IMP can read.

Semi-Landmark Protocols

In any study which involves the use of semi-landmarks, a file called a *protocol* will be required to identify which points in the input data file are landmarks, semi-landmarks and helper points, and which points are members of which curves.

Additionally, it is necessary to identify whether each curve is open (with landmarks at each end) or closed (comprised of a closed loop of semi-landmarks and helper points).

You will have to use a word processor or text editor to create a protocol file to identify the landmarks, curves, semi-landmarks and helper points to the software. In fact,

you may want to try using several protocols to vary the ratio of helper points to semi-landmarks.

Coding information

Information about curves, landmarks, semi-landmarks and helper points, will be organized by curve. Each curve has a number. Curve 0 is the set of all landmarks that are not on a curve, so Curve 0 is not a “curve” at all, but a mathematical group of all landmarks in the study. Each open curve is identified by a positive integer value, starting with 1. Consecutive open curves are labeled 2,3,4...etc. Each closed curve is identified by a negative integer value, starting with -1 and decreasing, so consecutive curves are identified as -2,-3,-4. Do not skip integer values when writing a protocol, a protocol file with curves 1,2,4 will not work, they must be curves 1,2,3.

Likewise, points are coded with numbers, landmarks are coded as 0, semi-landmarks are coded as 1 and helper points are denoted as 2.

Each curve has a set of points that lie along it. They have a curve ordination number, that describes the location of the point relative to the starting point of the curve. The first point along the curve is 1, the second is 2 and so on.

Format of the protocol file

In the protocol file used to specify the curves, landmarks, semi-landmarks and helper points in use in a given study, each line of the file represents a single point appearing on a

curve (or on "Curve 0", the set of all landmarks). Curves are listed one after another, with Curve 0 coming first. The first entry on a line is the curve number, followed by the ordination of the point (landmark, semi-landmark or helper) along the curve, the number of the digitized point (from TPSDig), and finally by the identifying code (0,1,2) to specify the type of point in use.

A fragment of a protocol file might look like:

```
0 1 1 0
0 2 2 0
0 3 8 0
0 4 9 0
0 5 10 0
1 1 2 0
1 2 3 1
1 3 4 1
1 4 5 1
1 5 6 1
1 6 7 1
1 7 8 0
-1 1 11 1
-1 2 12 2
-1 3 13 1
-1 4 14 2
-1 5 15 1
-1 6 16 2
```

This example has 5 landmarks, one open curve and one closed curve.

I have included several examples files, proto1.txt and proto2.txt for use with the meraspid.txt example file, which shows how different protocols may be used in processing a single data set.

Running SemiLand6.

- 1.) Load the data file, using the load data button.
- 2.) Load the protocol using the load protocol button.

3.) The replot button can be used to redraw the display, using different display options.

4.) The output options may be accessed on the file menu. You can save files with all data (landmarks, semi-landmarks and helper points), only the landmarks and semi-landmarks specified in the protocol, or only the landmarks. These files can then be analyzed in other software packages.

IMPORTANT READ THIS

SemiLand6, notes on the 4th Beta Version

I am having difficulty getting a stable semilandmark alignment procedure to operate consistently using the thin plate spline based approach presented by Bookstein and Green. There are some definite failures of my current implementation of this approach, for example, the software returns different results in some cases depending on the direction one traverses a curve during the alignment procedure.

I've spent a lot of time on the problem and haven't been able to get it stabilized in a way that I am comfortable with. I hope to return to work on the problem, but life exerts many pressures on us all.

At the moment, there is a different semi-landmark alignment method implemented in semiland6. The approach is to slide the semi-landmarks along the curve to minimize the *Procrustes distance* between the subject and a reference. Not that this is a different criteria than presented by Bookstein and Green, who used minimization of *bending energy* as the criteria for positioning semi-landmarks along curves. It is not really clear to me which criteria is preferable or optimal. Minimizing bending energy is parsimonious in that it assumes the least possible localization of the deformation necessary to deform one curve into another. Minimization of Procrustes distance is parsimonious in that it assumes the smallest distance between the two shapes, given the placement of points on the reference curve.

So at this point, I have "locked out" the bending energy based method in SemiLand 6, so that the only alignment option is one based on minimization of Procrustes distance. Hopefully I will be able to get the bending energy based approach operating in a consistent way in the near future, so that both methods will be available in SemiLand6.

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