Two ‘schools’ of geometric morphometrics

(1) Landmarks via distances:
- Choose *landmarks* according to *biological* criteria:
  - Homology or analogy.
- Choose interlandmark *distances* according to *geometric* criteria:
  - Finite networks: triangulations, trusses, etc.
- Choose *analysis* according to *statistical or graph-theory* criteria:
  - Log-transformations and allometry.
  - Decomposition of variance (e.g., size/shape).
  - “Morphospace” analysis (ordination).
  - Hierarchical analysis of between-taxon ‘distances’ (cluster analysis).
  - Hierarchical analysis of character states (character trees).
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(2) Landmarks directly:
   - Choose landmarks according to biological criteria:
     • Homology or analogy.
   - Choose analysis according to statistical or geometric criteria:
     • Shape coordinates.
     • Procrustes rotations (e.g., LSTRA, RFTRA).
     • Biorthogonal grids (tensor fields).
     • Thin-plate splines (warps).
• Problem:
  – Have sets of landmark configurations.
    • One set per individual.
    • Same number of homologous points per set.
  – How can they be compared directly?
• One solution: superimposition.
  – ‘Mapping’ of configurations onto one another.
  – Corresponding (homologous) landmarks should be as close as possible to one another.
  – Independent of:
    • Orientation
    • Translation
    • Scale
Superimposition methods

(1) Bookstein shape coordinates for triangles:

(2) Procrustes superimpositions:

(a) LSTRA: least-squares theta-rho analysis.

(b) RFTRA: resistant-fit theta-rho analysis.

(c) Generalized Procrustes analysis (GLS, GPA).
Bookstein shape coordinates

= Two-point registration, edge-matching, baseline registration.

• Begin with two triangles with homologous vertices.
• Specify two vertices to form a baseline:
  – E.g., A and B.
• Translate, rotate and rescale triangles to align baselines.
  – Baseline normalized to length 1.
• Superimposed triangles:

• Third landmark (C, in this case) is a point in the new coordinate system (“shape space”).
• When two triangles are superimposed, difference in position of point C in the two forms describes the difference in shape between the two triangles.
• Choice of baseline alters shape coordinates and perceptions of shape differences among triangles:
• Formulation in matrix algebra:
  – Applied separately to all triangles:

\[
X = \begin{bmatrix}
  x_1 & y_1 \\
  x_2 & y_2 \\
  x_3 & y_3 \\
\end{bmatrix}
\]

Normalized coordinates:

\[
X_n = \frac{1}{x_2} X_r
\]

Translation and registration:

\[
X_t = X - 1t = \begin{bmatrix}
  x_1 & y_1 \\
  x_2 & y_2 \\
  x_3 & y_3 \\
\end{bmatrix} - \begin{bmatrix}
  1 \\
  1 \\
  1 \\
\end{bmatrix} \begin{bmatrix}
  x_1 \\
  x_2 \\
\end{bmatrix}
\]

Rotation: \[ e = [1 \ 0]' \]

\[
\theta = \cos^{-1} \left( \frac{x_2 \cdot e}{\sqrt{x_2 \cdot x_2} \cdot \sqrt{e \cdot e}} \right)
\]

\[
H = \begin{bmatrix}
  \cos \theta & \sin \theta \\
  -\sin \theta & \cos \theta \\
\end{bmatrix}
\]

\[
X_r = X_t H'
\]
• Shape space is a morphospace:
• Extends to multiple triangles:
  – Produces cluster of points representing vertices.
  \[= \text{Shape coordinates}.\]
• Choice of different baselines produces different but comparable portrayals of shape variation:
• Scatters representing groups of landmark coordinates can be analyzed using multivariate methods (e.g., MANOVA):

Sexual dimorphism in gorilla scapulas (Slice 2005)
• Triangles can be averaged by finding the centroids of scatters of landmarks:

Mean shape coordinates of landmarks of iron-age brooches
(Dryden 2001)
• Principal component analysis of iron-age brooches.
  – Variation in shape along PCs:
• Size variation:
  – Triangles ordered by some measure of overall size:
    • E.g., area or mean length of sides.
  – Size trajectories plotted within the shape space:
    • Represent allometry in the general sense.
    • No necessary predictions about nature of trajectory:
      – E.g., linear or non-linear.
• Example: series of triangles growing allometrically (via Huxley’s model):
• Ontogenetic change in *Serrasalmus gouldingi* between juvenile and adult specimens:
• Comparisons of ontogenetic change in two piranha species (solid and dotted lines):
• Deformations:
  – For triangles, there is a single homogeneous deformation described by principal axes:
    • Directions and magnitudes of maximum and minimum change.
  • ‘Dilatations’ from biorthogonal analysis.
• Summary: Bookstein shape coordinates:
  – Based on selected baseline between two specified landmarks.
    • Choice of baseline has minor effects on multivariate analyses.
  – Other landmarks carried along as baselines of triangles are normalized and aligned.
    • Explicit adjustment for size variation analogous to use of ratios.
    • Assumes isometric size variation.
  – Result is a ‘shape space’, = morphospace.
    • Forms can be averaged and predicted.
    • Size variation characterized \textit{a posteriori}.
  – Coordinates used directly in multivariate analyses.
    • PCA, DFA, MANOVA, etc.