Landmark-free geometric methods in biological shape analysis

Supplementary Material

Patrice Koehl[1*] **and Joel Hass**[2]

[1] **Department of Computer Science and Genome Center, University of California, Davis, CA 95616, USA**
[2]**Department of Mathematics, University of California Davis, Davis, CA 95616, USA**

[*]**To whom correspondence should be addressed; E-mail: koehl@cs.ucdavis.edu.**

Material & Methods

A general algorithm for computing the distance between two surfaces of genus zero

The algorithm described here is derived from our initial studies of conformal mapping of genus zero surfaces described in [1, 2], which provide comprehensive descriptions. We focus here on the general concepts and on the differences with the original algorithm.

Let F_1 and F_2 be two surfaces of genus zero, represented by the meshes $\mathcal{M}_1$ and $\mathcal{M}_2$, respectively. Both meshes are taken to be triangular, with $\mathcal{M}_i = (V_i, E_i, T_i), i = 1, 2$, where $\{V_i, E_i, T_i\}$ denote the vertices, edges and triangles, respectively. These two meshes are completely independent of each other, and are likely to have different combinatorics. We define the distance $d_{SD}(F_1, F_2)$ between the two surfaces as the sum of the distortions of the optimal conformal mapping f_{min} of the surface F_1 onto F_2 and of its inverse, f_{min}^{-1}, where distorsion relates to difference from isometry and is computed using Equation (2) in the main text of the manuscript.

To find the optimal mapping f_{min}, we rely on the idea that any conformal mapping f between F_1 and F_2 can be written as the composition of two discrete conformal mappings C_1 and C_2 that map F_1 and F_2 onto the sphere, and a Möbius transformation m from the sphere to itself. In optimizing the map produced from this composition, C_1 and C_2 are fixed, while m is variable and depends on six degrees of freedom, summarized in a parameter vector $\vec{h}$.

This optimization is implemented in the following algorithm.

Journal of the Royal Society Interface 1–4; doi: 10.1098/rspa.00000000
September 1, 2015

Algorithm 1 *Conformal mapping with minimal distortion between two discrete surfaces F_1 and F_2 of genus zero*

Initialization. (1) Scale the meshes $\mathcal{M}_1$, $\mathcal{M}_2$ representing F_1 and F_2 to have total area one. Set $E_{min} = +\infty$
(2) Find C_1 and C_2 that conformally map $\mathcal{M}_1$ and $\mathcal{M}_2$ onto the sphere.
for each j in $[1, 24]$ **do**
  (3) Initialize Möbius transformation $m_0 = m(j)$. Set $f_0 = C_2^{-1} \circ m_0 \circ C_1$.
  for $n = 0, \ldots$ until convergence **do**
    (4) Generate $f_n(\mathcal{M}_1)$ and $f_n^{-1}(\mathcal{M}_2)$
    (5) Compute $E_{SD}(f_n)$ and its gradient $\boldsymbol{\nabla} E_{SD}(f_n)$ with respect to $\vec{h}_n$.
    (6) Check for convergence: if $E_{SD}(f_n) <$TOL, break.
    (7) Update $\vec{h}_{n+1} = \vec{h}_n - \alpha_n \boldsymbol{\nabla} E_{SD}(f_n)$. Set $m_{n+1} = m(\vec{h}_{n+1})$
    (8) Update $f_{n+1} = C_2^{-1} \circ m_{n+1} \circ C_1$
  end for
  if $E_{SD}(f_n) < E_{min}$ **then**
    (9) Update $E_{min} = E_{SD}(f_n)$; $f_{min} = f_n$
  end if
end for
(10) **Output.** The distance between the two surfaces, $d_{SD}(F_1, F_2) = E_{min}$, and the optimal mapping f_{min}.

The scaling of the surface meshes in step (1) makes our comparison method insensitive to global changes of scale. While not necessary, this step allows us to measure scale invariant properties. It is appropriate when the global scale used to describe the vertex positions of the input surfaces is unknown.

Step (2) follows the approach proposed by Springborn and colleagues, which introduces a notion of discrete conformal equivalence [3]. In this method, the mesh $\mathcal{M}$ representing a genus zero surface F is first made topologically equivalent to a disk by removing a vertex v_0 and its star. The transformed mesh is projected conformally on a plane through an optimization procedure [3]. The planar mesh is then warped onto the sphere by stereographic projection. Vertex v_0 is reinstated on the North pole of the sphere and connected back to the mesh. Finally, we apply a Möbius normalization to ensure that the center of mass of all vertices is at the origin of the sphere. Full details on the implementation of this algorithm are provided in Ref. [1].

The loop with variable j corresponds to different initial conditions for optimzing the conformal mapping f. A random or a trivial initial guess (such as the identity transformation) is likely to lead to a local minimum. We have therefore developed a simple procedure to automatically generate better starting points. The idea is to use the best ellipsoid approximation to each surface to give the initial alignment. While this alignment is specified by setting the images of three points, we do not rely on user selected landmarks or on local geometric features to select these points. Instead, we simply compute for surface F_1 the three principal components of its vertices, identified to the three axes of the corresponding best fit ellipsoid. These three axes cut F_1 in three pairs of points, (A_1, A_1'), (B_1, B_1') and (C_1, C_1'). Using the same procedure on F_2, we get three corresponding pairs of points, (A_2, A_2'), (B_2, B_2') and (C_2, C_2'). There are twenty four choices of correspondences between these two sets of points that lead to an alignment of the axes of the two ellipsoids with proper orientation (we do not impose an ordering of the axes). Each of these correspondences j defines a unique Möbius transformation, $m(j)$. Each of these transformations is then used as an initial guess for the steepest descent procedure.

Step (4) uses the following method. A vertex v_i in $\mathcal{M}_1$ has image $v_i' = C_1(v_i)$ in the spherical mesh $C_1(\mathcal{M}_1)$. We locate the image $v_i'' = m(v_i')$ on the spherical mesh $C_2(\mathcal{M}_2)$, namely we identify the triangle t of $C_2(\mathcal{M}_2)$ that contains v_i'' and compute barycentric coordinates (α, β, γ) of v_i'' in t. Finally, we compute the position of $v_i''' = f(v_i)$ on the surface F_2 by propagating the barycentric coordinates (α, β, γ) onto the triangle t' in $\mathcal{M}_2$ that corresponds to t. Full details on the implementation of this method are provided in [1].

The value of TOL in step (6) is set to a small constant related to machine error. The damping parameter α_n in step (7) is obtained using a line search method.

Taking chirality into account

The algorithm described above is orientation dependent and therefore sensitive to chirality. For example, it will not identify the left and right hands of a person as being similar, as they cannot be superimposed onto each other. Thus our method can distinguish a shape from its reflection. When comparing anatomical surfaces such as bones from humans or primates, this is a definite feature, as it allows for separating bones from the left side of the body from bones from the right side of the body. In some cases however, samples have been pooled and need to be compared independently of their chirality. We propose the following method to handle such cases. Let $\mathcal{M}_1$ and $\mathcal{M}_2$ be the meshes representing two surfaces. We start by comparing $\mathcal{M}_1$ and $\mathcal{M}_2$ using the algorithm described above, and set E_1 the energy of the corresponding optimal mapping. We then apply a reflection on $\mathcal{M}_1$ (multiplying for example the z-coordinates of all vertices in $\mathcal{M}_1$ by -1 and inverting the orientation of all its triangles), to generate an inverted mesh $\mathcal{M}_1'$. We compare $\mathcal{M}_1'$ and $\mathcal{M}_2$, and set E_2 the energy of the corresponding optimal mapping. The distance between $\mathcal{M}_1$ and $\mathcal{M}_2$ is then set to $\min(E_1, E_2)$.

Preprocessing the meshes

To test our algorithm, we used three independent datasets, representing three different regions of the skeletal anatomy, of humans, other primates, and their close relatives. Those three datasets contain 61 proximal first metatarsals of prosimian primates, New and Old World monkeys (data set A), 45 distal radii of apes and humans (data set B), and 116 second mandibular molars of prosimian primates and non primate close relatives (data set C), respectively. They were originally assembled by Boyer and colleagues [4]. They are available on the web site of one of the co-authors of Ref. [4]:

(`http://www.wisdom.weizmann.ac.il/~ylipman/CPsurfcomp/`),

Digital models of all specimens were created using micro-CT and medical CT imaging devices (for details, see [4]). The raw digitized surfaces include noise, which we process using the following steps:

i) Detect and remove small, disconnected components (a few of the files contained isolated tetrahedra).

ii) Detect and remove topological oddities, such as more than two triangles attached to an edge. The resulting meshes are manifolds.

iii) Detect and clean up boundaries: remove “dangling" triangles, i.e. triangles with two boundary edges.

iv) Apply three iterations of simple Laplacian smoothing, using the software package MeshLab (`http://meshlab.sourceforge.net`).

v) Detect and fill all holes.

Step (v) is a requirement for our method, as it is currently designed for surfaces of genus zero, without boundary. To fill a hole, we detect all vertices and edges on the boundary, build the center of gravity G of these vertices, and add to the mesh all the triangles formed by connecting G to the edges of the boundary. The 61, 45, and 116 resulting smoothed triangular meshes for data sets A, B, and C, respectively, have similar sizes, with approximately 5,000 vertices and 10,000 triangles on average.

References

[1] P. Koehl and J. Hass. Automatic alignment of genus-zero surfaces. *IEEE Trans. on Pattern Anal. Mach. Intell.*, 36: 466–478, 2014. doi: 10.1109/TPAMI.2013.139.

[2] J. Hass and P. Koehl. How round is a protein? exploring protein structures for globularity using conformal mapping. *Front. Mol. Biosci.*, 1:26, 2014.

[3] B. Springborn, P. Schröder, and U. Pinkall. Conformal equivalence of triangle meshes. In *Proc. SIGGRAPH Asia*, pages 79–89, 2008.

[4] D.M. Boyer, Y. Lipman, E. StClair, J. Puente, B.A. Patel, T. Funkhouser, J. Jernvall, and I. Daubechies. Algorithms to automatically quantify the geometric similarity of anatomical surface. *Proc. Natl. Acad. Sci. (USA)*, 108:18221–18226, 2011.