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Group-wise Shape Correspondence of Variable and Complex Objects

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Abstract

We present a group-wise shape correspondence method for analyzing variable and complex objects in a population study. The proposed method begins with the standard spherical harmonics (SPHARM) point distribution models (PDM) with their spherical mappings. In case of complex and variable objects, the equal area spherical mapping based SPHARM correspondence is imperfect. For such objects, we present here a novel group-wise correspondence. As an example dataset, we use 12 second mandibular molars representing 6 living or fossil euarchontan species. To improve initial correspondence of the SPHARM-PDM representation, we first apply a rigid transformation on each subject using five well-known landmarks (molar cusps). We further enhance the correspondence by optimizing landmarks (local) and multidimensional geometric property (global) over each subject with spherical harmonic representation. The resulting average shape model better captures sharp landmark representation in quantitative evaluation as well as a nice separation of different species compared with that of the SPHARM-PDM method.

1. Introduction

Shape analysis has been significantly highlighted in the medical imaging field for better understanding of population nature. In evolutionary histories, it is key to understand morphological structures. A molar shape in many mammalian species has been used to suggest ecological or phylogenetic affinities.¹ Yet a challenge arises from that complicated shape with high inter-subject variability, which requires a proper average model for reliable shape analysis. In general, consistent shape correspondence is a prerequisite of the average model computation.

Several studies proposed surface correspondence handled in its original space to avoid distortion of the original surface representation. In the particle-based registration,² particles move over the surfaces to form shape correspondence. The spectral-based registration³ utilizes intrinsic features extracted in the spectral domain rather than in the Euclidean space. One of the advantages is no mapping (transformation) distortion introduced during

registration in these non-parametric methods. However, it is non-trivial to establish continuous correspondence without interpolation of the discrete deformation field as discussed in.⁴

The most prevalent way of the surface representation is surface parametrization. In general, this requires a space mapping function that includes planar, hyperbolic or spherical parametrizations. Of various mappings, spherical parametrizations are most popularly used due to their convenience, reduced distortions, and computational efficiency.⁴ Moreover, in several pipelines, they incorporated geometric features (e.g., location information, curvature, etc.) as additional constraints for minimizing spherical mapping distortion.

In this paper, we extend the group-wise shape correspondence.⁴ Since we focus on variable structures possessing different shape patterns to the cortex, we propose a general version of that method designed originally for the cortical surfaces in terms of incorporation of multidimensional geometric properties for global alignment. It is noteworthy that the proposed method aims not at specific subjects but at general shape models, as we provide a general framework for addressing a shape correspondence problem.

Our main contributions are summarized as follows: a) the extension to the previous group-wise correspondence method for general shapes with incorporation of multidimensional geometric features, b) additional term for surface triangle regularization, and c) average shape model with more reliable population variability than the SPHARM-PDM method.⁵

2. Materials

The shapes analysed in this study consist of 12 second mandibular molars from 6 living or fossil euarchontan species: *Donrussellia* (subject 1, 2), *Pronothodectes* (subject 3, 4, 11, 12), *Saxonella* (subject 5), *Ptilocercus* (subject 6, 7), *Altanius* (subject 8, 9), and *Elphidotarsius* (subject 10). These molars are a subset of the sample utilized by,⁶ and a detailed explanation of sample preparation can be found in.¹ In brief, molds of actual toothrows were molded using a polyvinylsiloxane material (PresidentJet Plus) and cast in epoxy (EpoTek 301). The second mandibular molar was trimmed from the tooth row and scanned with the Scanco μ CT-40 machine at Stony Brook University's Center for Biotechnology. Three-dimensional surfaces of each tooth were segmented from the resulting DICOM or TIFF stacks using Amira 5.1 or Avizo 6.0. We manually annotated five distinct landmarks (molar cusps) on each surface model. Fig. 1 shows a complete set of the molars.

3. Method

3.1 SPHARM-PDM Surface Reconstruction

As already discussed in,⁷ the SPHARM-PDM represents objects of spherical topology. A spherical parametrization is computed via optimizing an equal area mapping of the 3D voxel mesh onto the unit sphere and minimizing angular distortions. A set of coefficients, which weighs spherical harmonic basis functions, are fitted to the 3D voxel mesh. In addition, SPHARM-PDM guarantees a one-to-one mapping between the reconstructed surface model and the unit sphere, which will play a key role for spherical parametrization and inverse

spherical mapping in the group-wise shape correspondence. Figure 2 illustrates an example initial mapping of landmarks onto the sphere via SPHARM-PDM.

3.2 Landmark-based Rigid Transformation

Given a set of landmarks, we globally minimize the landmark distance errors on the sphere in terms of rigid alignment. To find proper spherical rotations, we compute an optimal mean spherical position of landmarks for each subject and define a rotation axis $\hat{\mathbf{Z}}$ from the center of the sphere to the mean. On a unit sphere, formally, this is formulated by the following minimization:

$$\hat{\mathbf{Z}} = \arg \min_{\mathbf{Z}} \sum_{i=1}^L \arccos^2(\mathbf{X}_i \cdot \mathbf{Z}), \quad (1)$$

where L is the number of landmarks, and $\mathbf{X}_i$ is the i th landmark. This is an optimization problem known as Fréchet mean. Once $\hat{\mathbf{Z}}$ is determined, we consider Euler angles, i.e., pitch (elevation) θ , yaw (azimuth) ϕ , and roll (axis= $\hat{\mathbf{Z}}$) ψ . The rotation of $\hat{\mathbf{Z}}$ is given as a function of (θ, ϕ) :

$$\dot{\mathbf{Z}}(\theta, \phi) = [\cos(\theta_{\hat{\mathbf{Z}}} + \theta) \cos(\phi_{\hat{\mathbf{Z}}} + \phi), \cos(\theta_{\hat{\mathbf{Z}}} + \theta) \sin(\phi_{\hat{\mathbf{Z}}} + \phi), \sin(\theta_{\hat{\mathbf{Z}}} + \theta)]^T, \quad (2)$$

where $\theta_{\hat{\mathbf{Z}}}$ and $\phi_{\hat{\mathbf{Z}}}$ are elevation and azimuth of $\hat{\mathbf{Z}}$, respectively. We define a rotation axis and its rotation angle as follows:

$$\ddot{\mathbf{Z}}(\theta, \phi) = \frac{\hat{\mathbf{Z}} \times \dot{\mathbf{Z}}(\theta, \phi)}{\|\hat{\mathbf{Z}} \times \dot{\mathbf{Z}}(\theta, \phi)\|_2} \text{ and } \ddot{\psi} = \arccos(\hat{\mathbf{Z}} \cdot \dot{\mathbf{Z}}(\theta, \phi)). \quad (3)$$

Thus the location of any landmark on the sphere is determined by the Rodrigues' rotation formula as a function of (θ, ϕ, ψ) :

$$\hat{\mathbf{X}}(\theta, \phi, \psi) = \dot{\mathbf{X}} \cos \psi + (\dot{\mathbf{X}} \times \dot{\mathbf{Z}}(\theta, \phi)) \sin \psi + \dot{\mathbf{Z}}(\theta, \phi) \cdot (\dot{\mathbf{Z}}(\theta, \phi) \dot{\mathbf{X}})(1 - \cos \psi), \quad (4)$$

where

$$\dot{\mathbf{X}}(\theta, \phi) = \mathbf{X} \cos \ddot{\psi} + (\mathbf{X} \times \ddot{\mathbf{Z}}(\theta, \phi)) \sin \ddot{\psi} + \ddot{\mathbf{Z}}(\theta, \phi)(\ddot{\mathbf{Z}}(\theta, \phi) \cdot \mathbf{X})(1 - \cos \ddot{\psi}). \quad (5)$$

Finally we minimize the landmark distance errors for all corresponding landmarks to find an optimal set of the rotations:

$$\arg \min_{\{\theta, \phi, \psi\}} \sum_{i=1}^L \sum_{j=1}^N \arccos^2(\widehat{\mathbf{X}}_i^j(\theta_j, \phi_j, \psi_j) \cdot \bar{\mathbf{X}}_i), \quad (6)$$

where N is the number of subjects and $\bar{\mathbf{X}}_i$ is the Frechet mean of i th corresponding landmarks. In the experiment we used the NEWUOA optimizer⁸ for finding two rotational angles. In Fig. 2 landmarks are roughly aligned after rigid transformation. We use such rigid transformation for initialization of the proposed group-wise shape correspondence method.

3.3 Group-wise Shape Correspondence

Our method is based heavily on the group-wise pipeline in.⁴ As the target models are not of cortical shapes however we extend the idea of the method and provide additional optimization term for surface triangle regularization. Please refer to the original paper for details on the displacement encoding and the speed-up optimization.

3.3.1 Problem Definition—For N given triangulated surfaces mapped onto the unit sphere, each of which has the same number n of the common corresponding vertices, we let V^i be the i th surface, $i = 1, \dots, N$. The goal is to estimate continuous mapping functions of cortical correspondence $M_i: \mathbb{S}^2 \rightarrow \mathbb{S}^2$, which map surfaces into a common reference sphere such that

$$M_1(v^1) = M_2(v^2) = \dots = M_N(v^N), \quad (7)$$

where v^i are the corresponding locations on the i th subject surface. To formulate the correspondence problem, let $\mathbf{x}(M_j)$ be a column vector of the corresponding points of subject j deformed by M_j , i.e., $\mathbf{x}(M_j) = [M_j(v_1^j), \dots, M_j(v_n^j)]^T$. We assume that $\mathbf{x}(M_j)$ are instances drawn from a probability density function of $\mathbf{X}$. The amount of the information in the random sampling is given by the entropy $H[\mathbf{X}]$. This implies that by minimizing such an entropy, mapped/deformed corresponding points are driven closer to each other. Our minimization problem is thus formulated as follows.

$$\{\widehat{M}_1, \dots, \widehat{M}_N\} = \operatorname{argmin}_{\{M_1, \dots, M_N\}} H[\mathbf{x}]. \quad (8)$$

3.3.2 Entropy of Landmark Errors—A key step for entropy computation is the density estimation of corresponding landmarks. However, appropriate density estimation on the sphere can be computationally demanding, as the mean computation is non-trivial. We assume that the initial alignment well centralizes corresponding landmarks (see Fig. 2 for instance), which allows a mapping from the spherical space to the Euclidean space $\mathbb{S}^2 \rightarrow \mathbb{S}^3$. For each iteration of optimization, we compute the average over corresponding landmarks in

$\mathbb{R}^3$, which is projected back onto $\mathbb{S}^2$. Those landmarks are then projected onto the tangential plane at that approximated mean to enable Euclidean statistics.

3.3.3 Entropy of Multidimensional Geometric Property—Since only five landmarks are partially distributed over the sphere, we employ additional entropy computation over geometric properties (e.g. shape index, curvedness, etc.) densely sampled across the surface. We extend the idea of⁴ to incorporate a multidimensional geometric property map rather than using a single scalar map. Let $\mathbf{s}(\cdot)$ denote a multiple tuple of the property map at a given point and $\mathbf{v}^j$ be the point in the j th subject such that $u = M_j(\mathbf{v}^j)$, where u is a given point on the sphere. Given M_j , let $\mathbf{v}^j$ be a corresponding vertex to u . It holds $\mathbf{s}(M_1(\mathbf{v}^1)) \cong \dots \cong \mathbf{s}(M_n(\mathbf{v}^n))$ if shape correspondence is well established. By uniform icosahedron subdivision-based spherical sampling of u , geometric property agreement is straightforwardly plugged into the entropy minimization problem. To equally control property maps, we transform each property into a standard score during optimization.

3.3.4 Entropy Minimization—We model $\mathbf{x}(M_j)$ as an instance of $\mathbf{X}$ such that

$$\mathbf{x}(M_j) = \left[p_{\bar{\mathbf{v}}_1}(M_j(\mathbf{v}_1^j)), \dots, p_{\bar{\mathbf{v}}_n}(M_j(\mathbf{v}_n^j)), \mathcal{S}(\{M_j(\mathbf{v}^j)\}) \right]^T, \quad (9)$$

where $p(\cdot)$ denotes the projection of a vertex onto the tangential plane at the approximated mean over the corresponding landmarks, and $\mathcal{S}(\cdot)$ is multidimensional geometric properties. For the density estimation, we assume a multivariate Gaussian distribution with covariance Σ and therefore, the entropy is obtained by

$$H[\mathbf{X}] \approx \frac{1}{2} \ln |\Sigma| = \frac{1}{2} \sum \ln \lambda, \quad (10)$$

where λ are the eigenvalues of Σ . By letting $\bar{\mathbf{x}}$ be the sample mean and $\mathbf{z} = [\mathbf{x}(M_1) - \bar{\mathbf{x}}, \dots, \mathbf{x}(M_N) - \bar{\mathbf{x}}]$, the sample covariance is given by $\frac{1}{N-1} \mathbf{z} \mathbf{z}^T$. In general, the dimension of $\mathbf{X}$ is much larger than N , we instead compute eigenvalues of $\frac{1}{N-1} \mathbf{z}^T \mathbf{z}$ in the dual space for computational efficiency. We used the NEWUOA optimizer⁸ in the experiment.

3.3.5 Surface Triangle Regularization—For highly complex and variable shapes, surface triangle flipping is often observed during optimization as there is no such regularization in (10) that potentially allows overestimation of the resulting deformation fields. To address such an issue, we introduce additional term F to count the number of flipping triangles with respect to surface normals of the deformed spheres. Since no triangle flipping is desired during optimization, our final entropy is therefore given by

$$H[\mathbf{X}] = \begin{cases} \frac{1}{2} \sum \ln \lambda & F = 0, \\ \infty & \text{otherwise.} \end{cases} \quad (11)$$

3.4 Average Shape Model Reconstruction

An advantage of spherical harmonics representation is continuous, smooth reconstruction of signals on the sphere. This allows surface models to determine their corresponding points at any given points. To take advantage of such a spherical harmonic property, we generate sampling points over a unit sphere with icosahedron subdivision and find their corresponding points from the deformation field defined by the proposed spherical harmonic representation. For each sampling point, we compute the average location (x -, y -, and z -coordinates) of the corresponding points to generate a molar average model after Procrustes alignment based on the proposed shape correspondence. Fig. 3 illustrates the average models created by different shape correspondence methods.

4. Results

4.1 Evaluation of Average Shape Models

We used two geometric properties: curvedness and shape index proposed in.⁹ Those two properties are of complementary geometric characteristics, in that regions not covered by curvedness are well represented by shape index and vice versa. For the weighing balance between landmarks and geometric properties, we observed that equally weighted optimization achieves the best representation of the population average. In Fig. 3, the average model generated by the proposed method nicely captures five molar cusps and enhanced sharpness of ridge/valley of the average model. That average model also well represents variance of each area especially in the most anterior cusp that has a high variability across species.

To quantitatively evaluate the average shape models (their shape correspondences), we used generalization (the ability to describe instances outside of the training set) and specificity (the ability to represent only valid instances of the object) as described in.¹⁰ Fig. 4 illustrates generalization and specificity of the average models. In both cases, we observed that the reconstruction errors of the proposed method are smaller than those of other methods.

4.2 Principal Component Analysis on Molar Shapes

As an application to shape classification, we performed principal component analysis on the molars using different average models reconstructed by three correspondences (SPHARM-PDM, rigid transformation, and proposed method). Compared with the initial correspondence, we observed that both rigid transformation and the proposed method can nicely separate the most anterior cusp that has the largest intra-variation. It can be easily determined whether the location of the most anterior cusp is left or right according to that separation. In Fig. 5, the most anterior cusps of subject 1, 4, 7, and 11 are located to the same side (also see Fig. 1) along the first principal direction. There was no significant

difference of the first principal direction between rigid transformation and the proposed method, yet for several species (*Donrussellia*, *Ptilocercus*, and *Pronothodectes*), they were better classified along the the second principal direction in the proposed method.

5. Conclusion

We presented a group-wise shape correspondence method designed for general surface models. We proposed an extended version of the previous group-wise correspondence that incorporates multidimensional geometric properties, which is not limited to a specific population. Also, we addressed surface triangle regularity by introducing additional regularization term during the optimization. We have shown in the experiment that shape correspondence established by the proposed method achieves tight and reliable alignment and that the average model nicely captures inter-subject variability in visual and quantitative assessments. Since the proposed method provides a general pipeline of shape correspondence, we expect that the method can be easily adapted to any shape analysis study due to its flexibility. In the future, we will improve our method by automatically weighing each property component according to its importance. We will also perform our method on a large population study.

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Figure 1.

A complete set of 12 molar shapes with their colored shape correspondence established by the proposed method.

Figure 2.

Landmark distribution of 12 subjects on the sphere. Each color indicates the corresponding landmarks. (a) initial landmarks of the SPHARM-PDM surfaces, (b) aligned landmarks after rigid transformation on the sphere, and (c) final landmark alignment via the proposed method.

Figure 3.

Average model reconstruction of 12 subjects with different shape correspondence: (a) initial SPHARM-PDM, (b) rigid transformation on the sphere, and (c) the proposed group-wise shape correspondence. The colors indicate location variance at each vertex.

Figure 4. Shape correspondence evaluation: generalization and specificity. The proposed method achieves better performance in terms of the instance reconstruction error.

Figure 5. Molar shape space defined by different correspondence. Each species is labeled by a distinct color.