Algorithms to automatically quantify the geometric simliarity of anatomical surfaces

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March 2018

Outline

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Motivation

- Understand physical and biological phenomena (e.g. speciation, evolutionary adaption, etc.) by quantifying the similarity or dissimilarity of objects affected by the phenomena.
- In standard morphologists' practice, 10 to 100 points will be identified as landmarks. By comparing these landmarks, similarity and dissimilarity between patterns of shapes can be determined.
- The difficulty in acquiring personal knowledge of morphological evidence limits our understanding of the evolutionary significance of morphological diversity.
- Want an automatic tool to decide similarity or dissimilarity between objects, and hence, provides more insights on the phenomenon.

Outline

General Idea

- Given two shapes $\mathcal{S}, \mathcal{S}'$ (with boundaries but not holes), conformally map them onto D^2 by applying Riemann's *uniformization theorem*.
- Conformal geometry permits the reduction of the study of surfaces embedded in 3D space to 2D problems
- By finding a coupling between the conformal factors, or by finding a correspondence between the disks that respects the conformal factors, one may be able to define new distances that measures similarity and dissimilarity.

Outline

Conformal map

Definition

A map $\varphi : \mathcal{S} \to \mathcal{S}'$ between two (smooth) surfaces is *conformal* if for any two smooth curves Γ_1, Γ_2 on $\mathcal{S}$, the angle between their images Γ_1', Γ_2' is the same as that between Γ_1, Γ_2 at the corresponding intersection point.

Definition

Two Riemannian metrics g and h on a smooth manifold $\mathcal{M}$ are called *conformally equivalent* if $g = fh$ for some positive function f on $\mathcal{M}$. The function f is called the *conformal factor*.

Remark:

1. the conformal factor indicates the area distortion factor produced by the operation of conformal mapping.
2. the conformal factor defines a probability measure.

Disk-preserving Möbius transofrmation

If γ is a conformal mapping from $\mathcal{S}$ to $\mathcal{S}'$, and φ, φ' are confromal maps to the disk D^2 of $\mathcal{S}, \mathcal{S}'$, then the family of all possible conformal mappings from $\mathcal{S}$ to $\mathcal{S}'$ is given by $\gamma = \varphi'^{-1} \circ m \circ \varphi$, where m ranges over all the conformal bijective self-mappings of the unit disk D^2.

Definition

Such m is called a *disk-preserving Möbius transformation*. And the collection of such m is denoted by $\mathcal{M}$.

Hyperbolic measure

Let $d\eta(x, y)$ be the hyperbolic measure on the disk D^2, i.e.

$$d\eta(x, y) = [1 - (x^2 + y^2)]^{-2} dxdy$$

.

Let $f(x, y)$ be a conformal factor. And let
$\mathbf{f}(x, y) = [1 - (x^2 + y^2)]^2 f(x, y)$.
Then we have $\mathbf{f} d\eta = f dxdy$.

Push-forward and Transport Effort

Definition

Let μ be a probabilty measure, and τ be a differentiable bijection from D^2 to itself, the mass distribution $\mu' = \tau_* \mu$ defined by $\mu(u) = \mu'(\tau(u))J_\tau(u)$ where J_τ is the Jacobian of τ is the *transportation* (or *push-forward*) of μ by τ.

Remark: $\tau_* \mu = \mu \circ \tau^{-1}$.
Note that for any (well-behaved) function F on D^2,
$\int_{D^2} F(u)\mu'(u)du = \int_{D^2} F(\tau(u))\mu(u)du$.

Definition

The *total transport effort* $\varepsilon_\tau = \int_{D^2} d(u, \tau(u))\mu(u)du$ where $d(u, v)$ is the distance between u, v in D^2.

Optimal Transport

By infimizing ε_τ over all measurable bijections τ from D^2 to itself, we solve the Monge problem.

Alternatively, since the bijections are hard to search, consider the Kantorovitch problem, i.e. for all continuous functions F, G on D^2, let π be a coupling with marginals μ, ν satisfying that $\int_{D^2 \times D^2} F(u) d\pi(u,v) = \int_{D^2} F(u)\mu(u) du$ and $\int_{D^2 \times D^2} G(v) d\pi(u,v) = \int_{D^2} G(v)\nu(v) dv$, we find the Wasserstein distance by finding infimum of

$$E_\pi = \int_{D^2 \times D^2} d(u,v) d\pi(u,v)$$

over all couplings π.

Outline

Conformal Wasserstein distances (cW)

Instead of comparing two surfaces $\mathcal{S}, \mathcal{S}'$, one can compare two conformal factors $\mathbf{f}, \mathbf{f'}$ obtained by conformally flattening $\mathcal{S}, \mathcal{S}'$.
Let m be a disk-preserving Möbius transformation, then $\mathbf{f}$ and $m_*\mathbf{f} = \mathbf{f} \circ m^{-1}$ are both conformal factors for $\mathcal{S}$.
Then we define the conformal Wasserstein distance to be

$$\mathcal{D}_{cW}(\mathcal{S}, \mathcal{S}') = \inf_{m \in \mathcal{M}} \left[\inf_{\pi \in \prod(m_*\mathbf{f}, \mathbf{f'})} \int_{D^2 \times D^2} \tilde{d}(z, z') d\pi(z, z') \right]$$

, where $\tilde{d}(\cdot, \cdot)$ is the hyperbolic distance on D^2.
Remark:

1. $\mathcal{D}_{cW}$ is a metric.
2. However, computing $\mathcal{D}_{cW}$ involves solving a Kantorovich problem for every m.

Outline

Conformal Wasserstein neighborhood dissimlarity distance (cWn)

Instead, we quantify how *dissimilar* the "landscapes" are with a *measure of neighborhood dissimilarity*.
Let $N(0,R)$ be a neighborhood at 0, i.e., $N(0,R) = \{z; |z| < R\}$.
For any $m \in \mathcal{M}$ s.t. $z = m(0)$, $N(z,R)$ is the image of $N(0,R)$ under m.
Then we define the dissimilarity between $\mathbf{f}$ at z and $\mathbf{f'}$ at z' by

$$\mathbf{d}^R_{\mathbf{f},\mathbf{f'}}(z,z') = \inf_{m\in\mathcal{M}, m(z)=z'} \left[\int_{N(z,R)} |\mathbf{f}(w) - \mathbf{f'}(m(w))| d\eta(w) \right]$$

Conformal Wasserstein neighborhood dissimlarity distance (cWn) cont.

We defined the dissimilarity between $\mathbf{f}$ at z and $\mathbf{f'}$ at z' by

$$\mathbf{d}^R_{\mathbf{f},\mathbf{f'}}(z,z') = \inf_{m\in\mathcal{M}, m(z)=z'} \left[\int_{N(z,R)} |\mathbf{f}(w) - \mathbf{f}(m(w))| d\eta(w) \right]$$

The conformal Wasserstein neighborhood dissimilarity distance between $\mathbf{f}$ and $\mathbf{f'}$ is

$$\mathcal{D}^R_{cWn}(\mathcal{S},\mathcal{S}') = \inf_{\pi\in\prod(\mathbf{f},\mathbf{f'})} \int_{D^2\times D^2} \boldsymbol{d}^R_{\mathbf{f},\mathbf{f'}}(z,z') d\pi(z,z')$$

Remark

- Both cW and cWn are blind to isometric embedding of a surface in 3D
- Introduce a new extrinsic distance

Outline

Procrustes distance between surfaces

The standard Procrustes distance is between discrete sets of points $\mathbf{X} = (X_n)_{n=1,\cdots,N} \subset \mathcal{S}$ and $\mathbf{Y} = (Y_n)_{n=1,\cdots,N} \subset \mathcal{S}'$ by

$$d_p(\mathbf{X}, \mathbf{Y}) = \min_{R \text{ rigid motions}} \left[\left(\sum_{n=1}^{N} |R(X_n) - Y_n|^2 \right)^{1/2} \right]$$

where $|\cdot|$ is the standard Euclidean norm.
Often $\mathbf{X}$ and $\mathbf{Y}$ are sets of landmarks on two surfaces.
Remark:

1. $d_p(\mathbf{X}, \mathbf{Y})$ depends on choices of the sets of landmarks.
2. small number of N landmarks disregards a wealth of geometric data
3. identifying and recording X_n, Y_n requires time and expertise.

Continuous procrustes distance between surfaces (cP)

Instead, we consider a family of continuous maps $a : \mathcal{S} \to \mathcal{S}'$ and use optimization to find the "best" a.
We require a to be *area-preserving*.
We denote the set of all area-preserving diffeomorphisms by $\mathcal{A}(\mathcal{S}, \mathcal{S}')$. And let

$$\mathbf{d}(\mathcal{S}, \mathcal{S}', a)^2 = \min_{R \text{ rigid motions}} \int_{\mathcal{S}} |R(x) - a(x)|^2 dA_{\mathcal{S}}$$

.
Then we define the *continuous Procrustes distance between S and S'* by

$$\mathbf{D}_p(\mathcal{S}, \mathcal{S}') = \inf_{a \in \mathcal{A}(\mathcal{S}, \mathcal{S}')} \mathbf{d}(\mathcal{S}, \mathcal{S}', a).$$

Continuous procrustes distance between surfaces (cP) cont.

Remarks:

1. There exists closed from formulas for minimizing over rigid motions.
2. But it is hard to infimize over $\mathcal{A}(\mathcal{S}, \mathcal{S}')$
3. For reasonable surfaces (e.g. surfaces with uniformly bounded curvatures), transformations *a* close to optimal are close to conformal.
4. Thus it suffices to only explore a smaller space of maps obtained by small deformations of conformal maps.

Continuous procrustes distance between surfaces (cP) cont.

We modify the search as follows:
Let $m \in \mathcal{M}$, then m is a conformal map. Let ϱ be a smooth map that roughly aligns high density peaks and χ be a special deformation s.t. $\chi \circ \varrho \circ m$ is area-preserving (up to approximation error).
For each choice of peaks p, p' in the conformal factors of $\mathcal{S}, \mathcal{S}'$

1. runs through the 1-parameter family of m that maps p to p'
2. constructs a map ϱ that aligns the other peaks, as best possible
3. conpute $\mathbf{d}(\mathcal{S}, \mathcal{S}', \varrho \circ m)$.

Repeat for all choices of p, p'. Choose $\varrho \circ m$ s.t. it minimizes $\mathbf{d}$ and deform it to be area-preserving.
Then the map $a = \chi \circ \varrho \circ m$ is the approximate to correspondance map and $\mathbf{d}(\mathcal{S}, \mathcal{S}', a)$ is the approximate to $\mathbf{D}_p(\mathcal{S}, \mathcal{S}')$.

Outline

Data and run time

There are three independent data sets:

1. 116 second mandibular molars (teeth) of prosimian primates and non-primate close relatives
2. 57 proximal first metatarsals (bones behind big toe) of prosimian primates, New and Old World monkeys
3. 45 distal radii (bone in forearm) of apes and humans

For each shape, geometric morphometricians collected landmarks s.t. the points are biologically and evolutionarily meaningful. Then one can compute the Procrustes distances with the landmarks, producing Observer-Determined Landmarks Procrustes (ODLP) distances.
Running times for a pair of surfaces:

1. cP: $\sim$ 20 sec.
2. cWn: $\sim$ 5 min.

Outline

Mantel correlation analysis

To assess the relationship between distance matrices, they used a Mantel correlation analysis:
First correlate the entries in the two square arrays, and then compute the fraction among all possible relabelings of the row/columns for one of them, that leads to a larger correlation coefficient

Table 1. Results of Mantel correlation analysis for cP and cWN versus ODLP distances

	Obs. 1/cP		Obs. 2/cP		Obs. 1/cWn		Obs. 2/cWn	
Dataset	*r*	*P*	*r*	*P*	*r*	*P*	*r*	*P*
Teeth	0.690	0.0001	not applicable		0.373	0.0001	not applicable	
First metatarsal	0.640	0.0001	0.620	0.0001	0.365	0.0001	0.392	0.0001
Radius	0.240	0.0001	not applicable		0.075	0.166	not applicable	

Conclusion: cP outperforms cWn.

Distance matrix

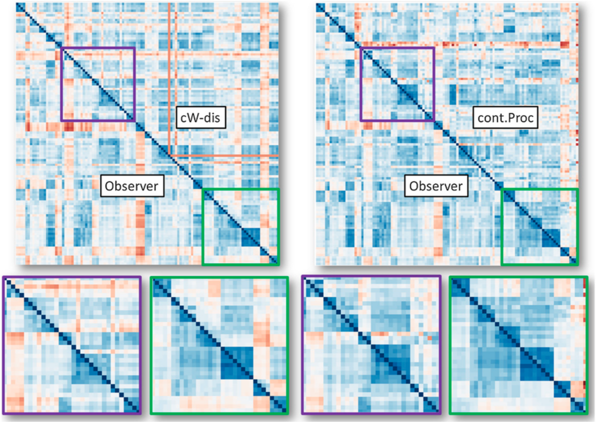


Fig. 1. For small distances, the structures of the matrices with cP, cWn distances and distances based on observer landmarks (ODLP) are very similar, with cP (on the right) the most similar to ODLP. The dataset illustrated here is dataset (A).

Conclusion: cP outperforms cWn.

Leave one out

- Each specimen (treated as unknown) is assigned to the taxonomic groups of its nearest neighbor among the reminder of the specimens in the data set (treated as known).

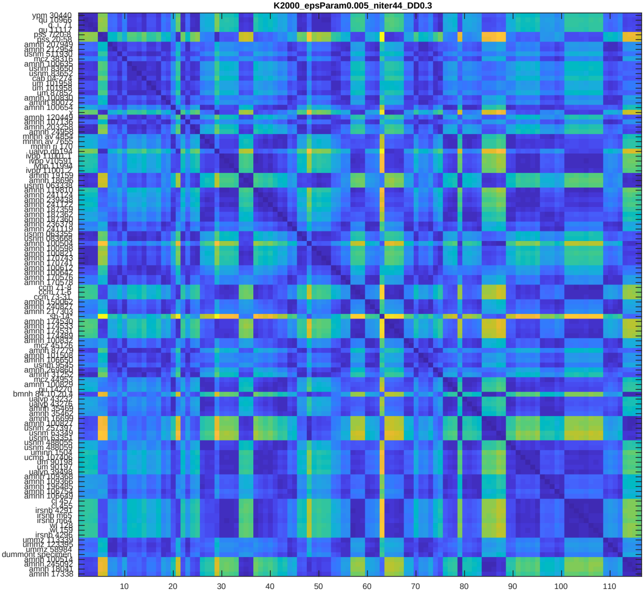
Outline

Procedure

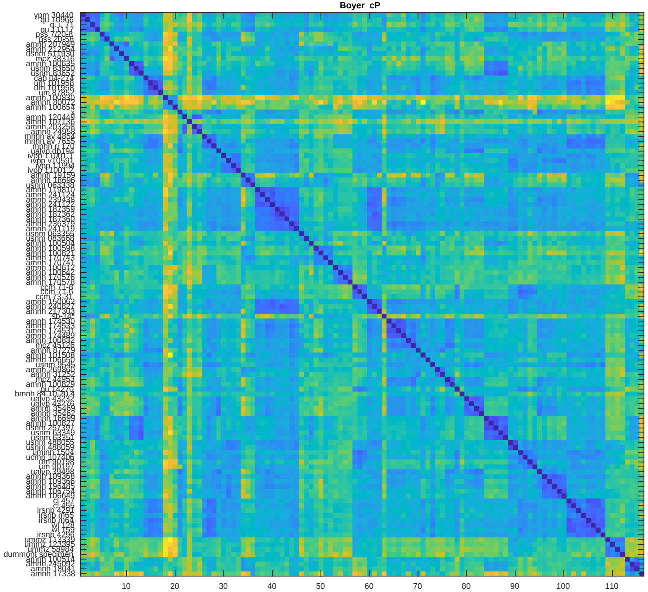
- Sample uniformly from surfaces and compute local distribution
- Define cost of transport based on local distribution matrix
- Use Sinkhorn's algorithm to find a coupling that minimizes the transportation cost
- obtain the third lower bound to the Wasserstein distance

Outline

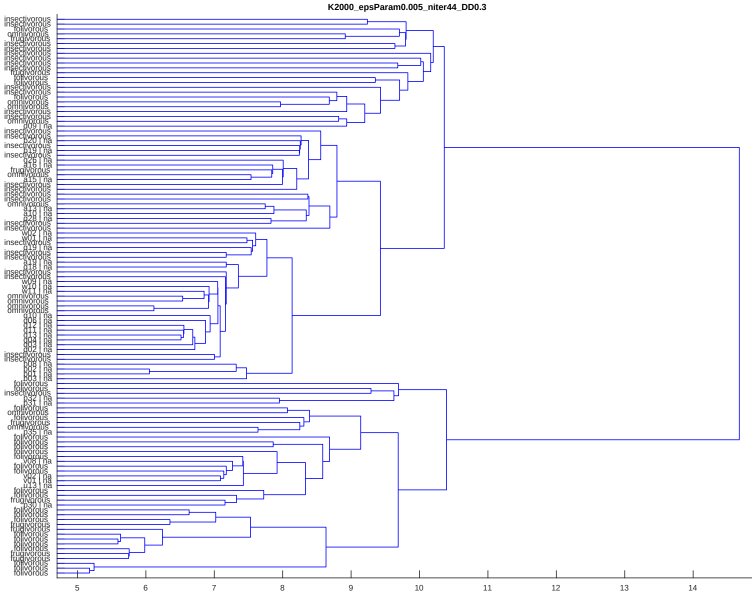
Distance matirx



Distance matirx of Boyer et al. using cP



Single Linkage Dendrogram



Single Linkage Dendrogram for Boyer et al. using cP