Lovely Bones: a meeting of mathematical and biological minds

Ingrid Daubechies
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I.D. : mostly cheerleader.
It all started with a conversation with biologists....

More Precisely: biological morphologists

Study Teeth & Bones of extant & extinct animals still live today fossils
First: project on “complexity” of teeth

Then: find automatic way to compute Procrustes distances between surfaces — without landmarks

Landmarked Teeth $\rightarrow d^{2}_{Procrustes}(S_{1}, S_{2}) = \min_{R \text{ rigid tr.}} \sum_{j=1}^{\| R(x_{j}) - y_{j} \|_{2}}$

Find way to compute a distance that does as well, for biological purposes, as Procrustes distance, based on expert-placed landmarks, automatically?

examples: finely discretized triangulated surfaces
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Data Acquisition

Surface reconstructed from $\mu$CT-scanned voxel data
Geometric Morphometrics

- Manually put $k$ landmarks

second mandibular molar of a Philippine flying lemur
Geometric Morphometrics

- Manually put $k$ landmarks $p_1, p_2, \cdots, p_k$

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Geometric Morphometrics

• Manually put $k$ landmarks

\[ p_1, p_2, \cdots, p_k \]

• Use spatial coordinates of the landmarks as features

\[ p_j = (x_j, y_j, z_j), \ j = 1, \cdots, k \]

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Geometric Morphometrics

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- Use spatial coordinates of the landmarks as features $p_j = (x_j, y_j, z_j), \ j = 1, \cdots, k$

- Represent a shape in $\mathbb{R}^{3 \times k}$

second mandibular molar of a Philippine flying lemur
The *Shape Space* of $k$ landmarks in $\mathbb{R}^3$
Geometric Morphometrics: Limitation of Landmarks

- Landmark Placement: tedious and time-consuming
- Fixed Number of Landmarks: lack of flexibility
- Domain Knowledge: high degree of expertise needed, not easily accessible
- Subjectivity: debates exist even among experts
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Landmarked Teeth $\rightarrow$

$$d^2_{\text{Procrustes}} (S_1, S_2) = \min_{R \text{ rigid tr.}} \sum_{j=1}^{J} \| R (x_j) - y_j \|^2$$
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Landmarked Teeth →

\[ d_{\text{Procrustes}}^2 (S_1, S_2) = \min_{R \text{ rigid tr.}} \sum_{j=1}^{J} \| R(x_j) - y_j \|^2 \]

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examples: finely discretized triangulated surfaces
We defined 2 different distances

\[ d_{cWn} (S_1, S_2): \text{conformal flattening} \]
\[ \text{comparison of neighborhood geometry} \]
\[ \text{optimal mass transport} \]

\[ d_{cP} (S_1, S_2): \text{continuous Procrustes distance} \]
\[ \mathcal{D}(S_1, S_2) = \inf_{\Pi \in \Pi(\mu, \nu)} \int d_R^{\mu, \nu}(z, \omega) \ d\Pi(z, \omega) \]
conformal Wasserstein neighborhood distance

\[ D(S_1, S_2) = \inf_{\pi \in \Pi(\mu, \nu)} \int d_R^{\mu, \nu}(z, \omega) \ d\pi(z, \omega) \]
Continuous Procrustes Distance (cPD)

\[ D_{cP}(S_1, S_2) = \left( \int_{S_1} \| x - C(x) \|^2 \, d\text{vol}_{S_1}(x) \right)^{\frac{1}{2}}, \]

where \( C : S_1 \to S_2 \) is an area-preserving diffeomorphism.
Continuous Procrustes Distance (cPD)

\[ D_{cP}(S_1, S_2) = \left( \inf_{R \in E(3)} \int_{S_1} \| R(x) - C(x) \|^2 \, d\text{vol}_{S_1}(x) \right)^{\frac{1}{2}}, \]

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\]

where \( \mathcal{A}(S_1, S_2) \) is the set of area-preserving diffeomorphisms between \( S_1 \) and \( S_2 \), and \( E_3 \) is the Euclidean group on \( \mathbb{R}^3 \).
Continuous Procrustes Distance (cPD)

\[ d_{CP}(S_1, S_2) = \inf_{C \in \mathcal{C}} \inf_{R \in \mathbb{E}_3} \left( \int_{S_1} \| R(x) - C(x) \|^2 \, d\text{vol}_{S_1}(x) \right)^{1/2} \]
We defined 2 different distances

\[ d_{cWn}(S_1, S_2): \text{ conformal flattening} \]
\[ \text{comparison of neighborhood geometry} \]
\[ \text{optimal mass transport} \]

\[ d_{cP}(S_1, S_2): \text{continuous Procrustes distance} \]
Bypass Explicit Feature Extraction

\[ D(S_1, S_2) = \inf_{f \in A(S_1, S_2)} F(f; S_1, S_2) \]
Multi-Dimensional Scaling (MDS) for cPD Matrix
Diffusion Maps: “Knit together” local geometry to get “better” distances

Small distances are much more reliable!
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Diffusion Maps: “knitting together” local geometry

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- Solve eigen-problem

$$Pu_j = \lambda_j u_j, \ j = 1, 2, \ldots, m$$
Diffusion Maps: “knitting together” local geometry

- $P = D^{-1} W$ defines a random walk on the graph
- Solve eigen-problem

$$P u_j = \lambda_j u_j, \ j = 1, 2, \cdots, m$$

and represent each individual shape $S_j$ as an $m$-vector

$$\left(\lambda_1^{t/2} u_1(j), \cdots, \lambda_m^{t/2} u_m(j)\right)$$
Diffusion Distance (DD)

Fix $1 \leq m \leq N$, $t \geq 0$,

$$D_m^t(S_i, S_j) = \left( \sum_{k=1}^{m} \lambda_k^t (u_k(i) - u_k(j))^2 \right)^{\frac{1}{2}}$$
Diffusion Distance (DD)

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MDS for cPD & DD

![cPD](image1)

![DD](image2)
Even better can be obtained!

HBDD

DD
to get Diffusion Distance: used local distances
knitted together
→ spectral parametrization
→ distance.
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to get Diffusion Distance: used local distances knitted together
\implies \text{spectral parametrization}
\implies \text{distance}

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But they can do much more for us!

In fact: we have a fiber bundle.

(But because of the mappings)
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knitted together

→ spectral parametrization

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But they can do much more for us!

In fact: We have a fiber bundle.

(Because of the mappings)
Connection.

↓

family of mappings between fibers
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family of mappings between fibers

Tingran Gao: use these to define a much more detailed diffusion structure on the higher-dimensional object

→ "project" at a later stage to obtain "horizontal" part of diffusion.
Horizontal Random Walk on a Fibre Bundle

Fibre Bundle $\mathcal{E} = (E, M, F, \pi)$

- $E$: total manifold
- $M$: base manifold
- $\pi : E \rightarrow M$: smooth surjective map (bundle projection)
- $F$: fibre manifold
Horizontal Random Walk on a Fibre Bundle

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Horizontal Diffusion Maps: Embedding the Entire Bundle

\[ u_1 \quad u_2 \quad u_3 \quad u_4 \quad u_{\kappa-1} \quad u_{\kappa} \]

......
Horizontal Diffusion Maps: Embedding the Entire Bundle
Horizontal Diffusion Maps
Automatic Landmarking — Interpretability
Horizontal Diffusion Maps: Embedding the Base Manifold

\[ u_1 \quad u_2 \quad u_3 \quad u_4 \quad u_{K-1} \quad u_K \]

\[
\begin{array}{cccccc}
& & & & & \\
\text{..} & & & & & \\
& & & & & \\
\end{array}
\]
Horizontal Diffusion Maps: Embedding the Base Manifold

\[ u_1 \quad u_2 \quad u_3 \quad u_4 \quad u_{\kappa-1} \quad u_{\kappa} \]

\[ \begin{array}{cccccc}
\end{array} \]

\[ \mapsto \left( \left\langle u_i[1], u_j[1] \right\rangle \right)_{i,j=1}^{\kappa} \]

......
Horizontal Diffusion Maps: Embedding the Base Manifold

$$u_1^2 \quad u_2^2 \quad u_3^2 \quad u_4^2 \quad u_{\kappa-1}^2 \quad u_\kappa^2$$

$$\kappa \rightarrow \left( \langle u_i^2, u_j^2 \rangle \right)_{i,j=1}^\kappa$$
Horizontal Diffusion Maps: Embedding the Base Manifold

\[ u_1 \rightarrow u_2 \rightarrow u_3 \rightarrow u_4 \rightarrow u_{\kappa-1} \rightarrow u_{\kappa} \]

\[ \left( \langle u_i[3], u_j[3] \rangle \right)_{i,j=1}^{\kappa} \]
Horizontal Diffusion Maps: Embedding the Base Manifold

\[ \langle u_i, u_j \rangle_{\kappa, i,j = 1} \]
Species Clustering

Horizontal Base Diffusion Distance *(with Maps)*

Diffusion Distance *(without Maps)*
Species Clustering

Horizontal Base Diffusion Distance (with Maps)
spectral coordinates for points in fiber bundle:

$$(j, p) \rightarrow (u_k (j, p))_{k=1, \ldots, K}$$

\text{pt p on } S_d^j \text{ on } S_d^j
spectral coordinates for points in fiber bundle:

$$(j, p) \quad \xrightarrow{\text{pt } p \text{ on } S_j} \quad (u_{k_2}(j, p))_{k=1, \ldots, K}$$

\[\text{"project" to geometry on base manifold}\]
spectral coordinates for points in fiber bundle:

\[(j, p) \quad \rightarrow \quad \left( u_k(j, p) \right)_{k=1, \ldots, K} \]

\[\uparrow \text{“project” to geometry} \quad \text{on base manifold}\]

\[\text{hor. dist } (S_i, S_j) \quad = \quad \text{dist. between corresponding point clouds in } K\text{-dim space.}\]

\[= \left[ \sum_{p, q} \lambda_k(p, q) \left| u_k(i, p) - u_k(j, q) \right|^2 \right]^{1/2} \]
Ongoing and future directions.

- The "true" connection should be flat (biological reasons)
  - Incorporate this? as constraint? via projection?

  Minimum spanning tree → not good
  Rob Ravier: more robust way of propagating information over collection in a "flat" way.

- From landmarked collection
  - Can determine consistent maps biologically meaningful.
  ⇒ Examples of good maps
    Learn how to map surfaces?
    Learn how to landmark?
multi-resolution; coarse & fine-graining. The connection is reasonable for bones/teeth of closely related species.

primate molars

crabeater seal molars