Biologically relevant distances between morphological surfaces representing teeth and bones.

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Workshop on Geometry and Shape Analysis in Biology.
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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
First: project on “complexity” of teeth
Then: find automatic way to compute Procrustes distances between surfaces — without landmarks
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

$p_1, p_2, \cdots, p_k$

second mandibular molar of a Philippine flying lemur
Geometric Morphometrics

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

- Use **spatial** coordinates of the landmarks as features

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

second mandibular molar of a Philippine flying lemur
**Geometric Morphometrics**

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

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

- 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
Geometric Morphometrics: Limitation of Landmarks

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![Image of a model with landmarks marked in various colors](image)
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Landmarked Teeth \[ \rightarrow \]

\[
d^2_{Procrustes} (S_1, S_2) = \min_{R \text{ rigid tr.}} \sum_{j=1}^{J} \| R(x_j) - y_j \|^2
\]
First: project on “complexity” of teeth

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Landmarked Teeth $\rightarrow$

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

Find way to compute a distance that does as well, for biological purposes, as Procrustes distance, based on expert-placed landmarks, automatically?
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\[ d^2_{Procrustes}(S_1, S_2) = \min_{R \text{ rigid tr.}} \sum_{j=1}^{J} \| R(x_j) - y_j \|^2 \]

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
We defined 2 different distances

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

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

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

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Continuous Procrustes Distance (cPD)

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

where $\mathcal{A}(S_1, S_2)$ is the set of area-preserving diffeomorphisms between $S_1$ and $S_2$, and $\mathbb{E}_3$ is the Euclidean group on $\mathbb{R}^3$. 
Continuous Procrustes Distance (cPD)

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

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

Correspondence-Based Shape Distances

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

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

\[ d_{ij} \cdot S_i \cdot S_j = D^{-1}W \] defines a random walk on the graph

\[ P = D^{-1}W \] defines a random walk on the graph
Diffusion Maps: “knitting together” local geometry

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

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

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

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

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

cPD

DD
Even better can be obtained!

HBDD

DD
to get DiffusionDistance: used local distances
  knitted together
  \rightarrow spectral parametrization
  \rightarrow distance.
to get **Diffusion Distance** : used local distances knitted together → spectral parametrization → distance.

mappings were used only to obtain numerical values for local distances.
to get Diffusion Distance: used local distances
  knitted together
  \implies \text{spectral parametrization}
  \implies \text{distance}

 mappings were used only to obtain numerical values for local distances.

 but they can do much more for us!

 in fact: we have a fiber bundle.
 ( because of the mappings )
Diffusion Distance: used local distances

knitted together

→ spectral parametrization

→ distance

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but they can do much more for us!

in fact: we have a fiber bundle.

( because of the mappings )
Connection.

\[\downarrow\]

family of mappings between fibers
Connection.

↓

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

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\[ S_0, S_1, S_2, S_3 \]

\[ M \]
**Horizontal Random Walk on a Fibre Bundle**

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Towards *Horizontal* Diffusion Maps

Diffusion Maps

\[ D^{-1}W u_k = \lambda_k u_k, \quad 1 \leq k \leq N \]

\[
D^{-1} \begin{pmatrix} \ldots & \ldots & e^{-d_{ij}^2/\epsilon} & \ldots \\ \vdots & \vdots & \vdots & \vdots \\ \ldots & \ldots & \ldots & \ldots \\ \end{pmatrix} \begin{pmatrix} \ldots \\ u_k(j) \\ \ldots \\ \end{pmatrix} = \lambda_k \begin{pmatrix} \ldots \\ u_k(j) \\ \ldots \\ \end{pmatrix}
\]
Towards *Horizontal* Diffusion Maps

**Horizontal Diffusion Maps**

\[ \mathcal{D}^{-1} \mathcal{W} u_k = \lambda_k u_k, \quad 1 \leq k \leq \kappa \]

\[ \mathcal{D}^{-1} \begin{pmatrix} \vdots & \vdots & e^{-\frac{d_{ij}^2}{\epsilon}} \rho_{ij}^{\delta} & \vdots \end{pmatrix} \begin{pmatrix} \vdots \\ \vdots \\ u_k[j] \\ \vdots \end{pmatrix} = \lambda_k \begin{pmatrix} \vdots \\ \vdots \\ u_k[j] \\ \vdots \end{pmatrix} \]
Correspondences Between Triangular Meshes

\[
\begin{bmatrix}
A_1 & A_2 & A_3 \\
B_1 & B_2 & B_3
\end{bmatrix}
\]
Correspondences Between Triangular Meshes

\[
\begin{bmatrix}
\cdots & B_1 & B_2 & B_3 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
A_1 & \cdots & 0 & 0 & 1 & \cdots \\
A_2 & \cdots & 1 & 0 & 0 & \cdots \\
A_3 & \cdots & 0 & 1 & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\end{bmatrix}
\]
Correspondences Between Triangular Meshes

\[
\begin{pmatrix}
\vdots & B_1 & B_2 & B_3 & \vdots \\
\vdots & 0 & 0 & 1 & \vdots \\
A_1 & \vdots & 1 & 0 & 0 & \vdots \\
A_2 & \vdots & 0 & 1 & 0 & \vdots \\
A_3 & \vdots & \vdots & \vdots & \vdots \\
\end{pmatrix}
\]
Correspondences Between Triangular Meshes

\[ f_{12}(A_3) \]

\[
\begin{pmatrix}
\vdots \\
\cdots 0 0 1 \\
\cdots 1 0 0 \\
\cdots 0 ? 0 \\
\vdots \\
\end{pmatrix}
\]

\[ s_1 \quad s_2 \]
Correspondences Between Triangular Meshes

\[
\rho_{12}(r, s) = \exp\left(-\frac{\|f_{12}(A_r) - B_s\|^2}{\delta}\right)
\]

\[
\begin{pmatrix}
\cdots & B_1 & B_2 & B_3 & \cdots \\
\cdots & \vdots & \vdots & \vdots & \vdots \\
A_1 & 0 & 0 & 1 & \cdots \\
A_2 & \cdots & 1 & 0 & 0 & \cdots \\
A_3 & \cdots & \cdots & \cdots & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
0.91 & 0.95 & 0.88 & \cdots & \cdots \\
\end{pmatrix}
\]
Towards *Horizontal* Diffusion Maps

Horizontal Diffusion Maps

\[ \mathcal{D}^{-1} \mathcal{W} u_k = \lambda_k u_k, \quad 1 \leq k \leq \kappa \]

\[
\begin{bmatrix}
\cdots & 
\cdots & 
\ddots & 
\cdots & 
\end{bmatrix}
\begin{bmatrix}
\cdots \\
e^{-d_{ij}^2/\epsilon} \rho_{ij}^\delta \\
\ddots \\
\cdots \\
\end{bmatrix}
\begin{bmatrix}
\cdots \n\\u_k[j] \n\\\cdots 
\end{bmatrix} = \lambda_k \begin{bmatrix}
\cdots \\
u_k[j] \n\\\cdots 
\end{bmatrix}
\]
Towards *Horizontal* Diffusion Maps

**Horizontal Diffusion Maps**

\[ D^{-1} \mathcal{W} u_k = \lambda_k u_k, \quad 1 \leq k \leq \kappa \]
Towards *Horizontal* Diffusion Maps

**Horizontal Diffusion Maps**

\[
\mathcal{D}^{-1} \mathcal{W} u_k = \lambda_k u_k, \quad 1 \leq k \leq \kappa
\]

Horizontal Diffusion Maps: For fixed \(1 \leq m \leq \kappa\), \(t \geq 0\), represent \(S_j\) as a \(\kappa_j \times m\) matrix

\[
\left( \lambda_1^{t/2} u_1[j], \ldots, \lambda_m^{t/2} u_m[j] \right)
\]
**Diffusion Maps vs. Horizontal Diffusion Maps**

**Diffusion Maps:** For fixed $1 \leq m \leq \kappa$, $t \geq 0$, represent $S_j$ as an $m$-dimensional vector

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

**Horizontal Diffusion Maps:** For fixed $1 \leq m \leq \kappa$, $t \geq 0$, represent $S_j$ as a $\kappa_j \times m$ matrix

$$
\left( \lambda_1^{t/2} u_{1[j]}, \cdots, \lambda_m^{t/2} u_{m[j]} \right)
$$
spectral coordinates for points in fiber bundle:

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

\( S_j \) on \( S_j \)
spectral coordinates for points in fiber bundle:

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

\(\downarrow\) "project" to geometry
on base manifold
spectral coordinates for points in fiber bundle:

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

\[\text{"project" to geometry on base manifold}\]

hor. dist \((S_i, S_j)\)

\[= \text{dist. between corresponding point clouds in } K\text{-dim space.}\]

\[= \left[ \sum_{p, q} \lambda_{k}(p, q) \left| u_{k}(i, p) - u_{k}(j, q) \right|^2 \right]^{1/2} \]
Even better can be obtained!

HBDD

DD
1. Global Registration
1. Global Registration
1. Global Registration
1. Global Registration
1. Global Registration
1. Global Registration
1. Global Registration
2. Automatic Landmarking: *Spectral Clustering*
2. Automatic Landmarking: *Spectral Clustering*
Ongoing and future directions.

- the "true" connection should be flat (biological reasons)

  ← incorporate this? as constraint?
  via projection?

  minimum spanning tree → not good
  Rob Raven: 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?
connection is reasonable for bones/teeth of closely related species.

primate molars

crab eater seal molars