Biologically relevant distances between morphological surfaces representing teeth and bones.

Ingrid Daubechies, Duke University.

Workshop on Geometry and Shape Analysis in Biology.

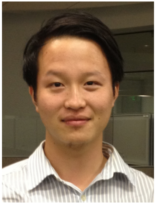
IMS Singapore June 2017

Collaborators

Rima Alaifari
ETH Zürich

Doug Boyer
Duke

Ingrid Daubechies
Duke



Tingran Gao
Duke

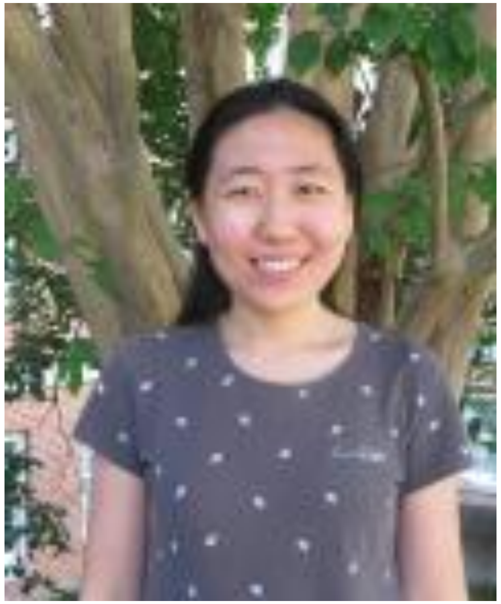
Yaron Lipman
Weizmann

Roi Poranne
ETH Zürich

Jesús Puente
J.P. Morgan

Robert Ravier
Duke

Shahar Kovalsky
Duke



Shan Shan
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Panchali Nag
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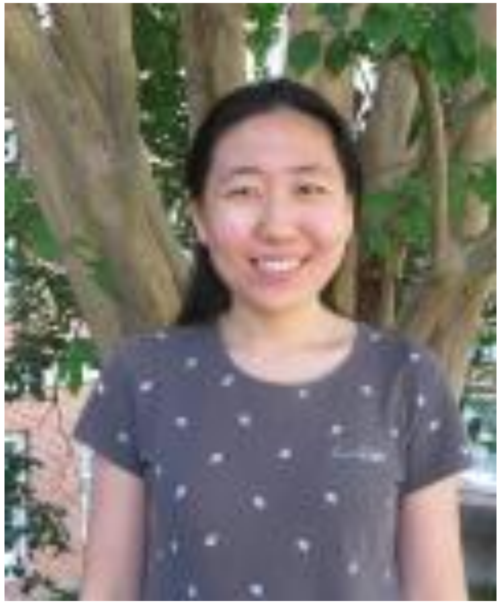

Shan Shan
Duke

Panchali Nag
Duke

I.D. : mostly cheerleader.

It all started with a conversation with biologists....

Doug Boyer

Jukka Jernvall

More Precisely: biological morphologists

↓

Study Teeth & Bones of

extant & extinct animals

still live today   fossils

First: project on "complexity" of teeth

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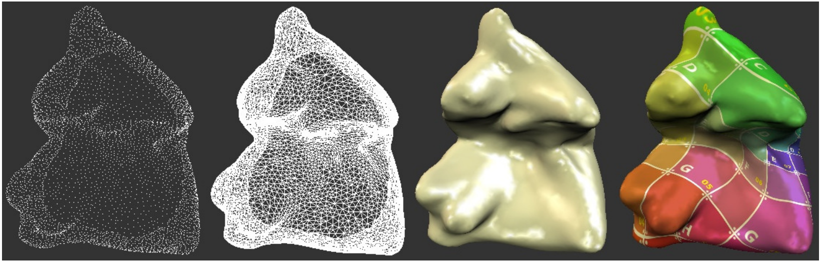
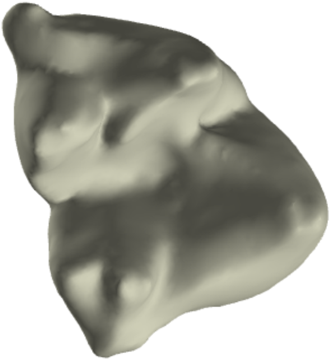
Then: find automatic way to compute Procrustes distances between surfaces — without landmarks

Data Acquisition



Surface reconstructed from μCT-scanned voxel data

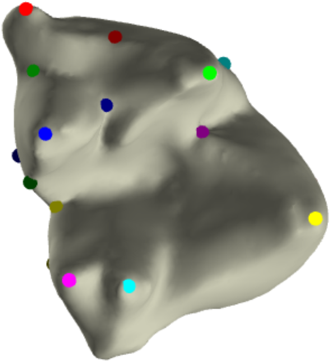
Geometric Morphometrics



second mandibular molar of a Philippine flying lemur

- Manually put k landmarks

Geometric Morphometrics



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$$p_1, p_2, \cdots, p_k$$

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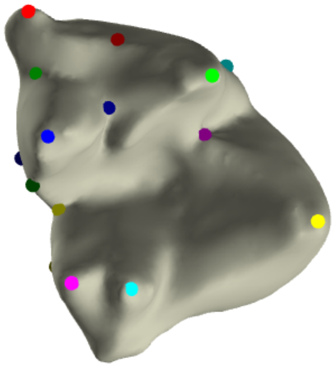

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- Use spatial coordinates of the landmarks as features

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

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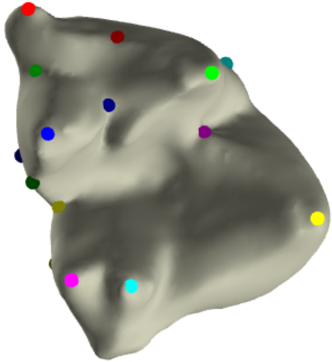

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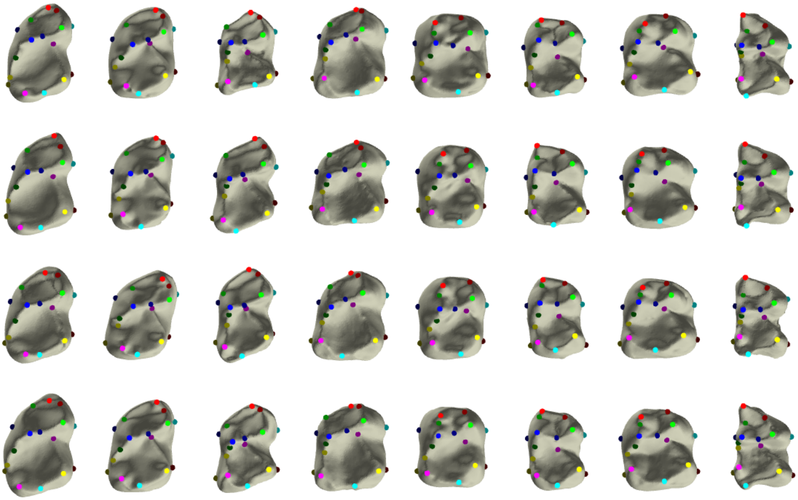
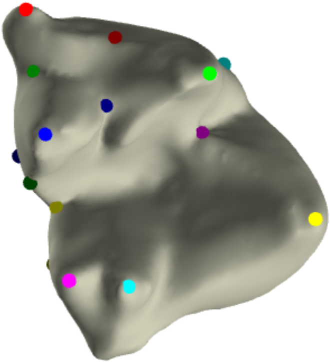
- Represent a shape in $\mathbb{R}^{3\times k}$

The *Shape Space* of k landmarks in $\mathbb{R}^3$



Geometric Morphometrics: Limitation of Landmarks



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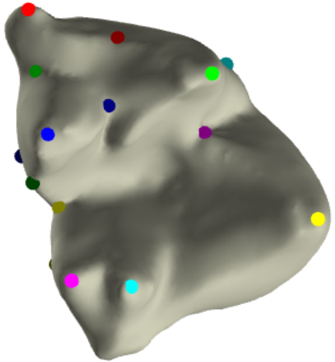

- Landmark Placement: tedious and time-consuming

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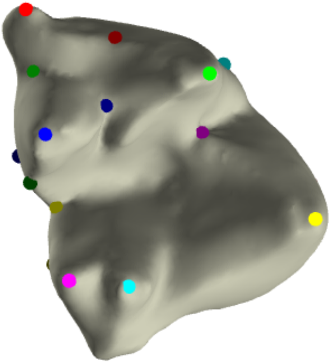

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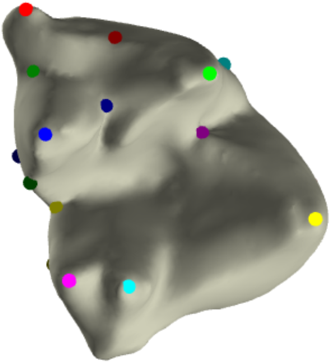

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- Domain Knowledge: high degree of expertise needed, not easily accessible

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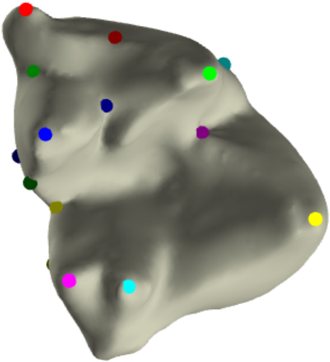

- Landmark Placement: tedious and time-consuming
- Fixed Number of Landmarks: lack of flexibility
- Domain Knowledge: high degree of expertise needed, not easily accessible
- Subjectivity: debates exist even among experts

First: project on "complexity" of teeth
Then: find automatic way to compute Procrustes distances between surfaces — without landmarks

Landmarked Teeth $\longrightarrow$

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

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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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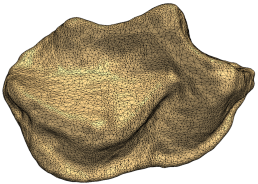
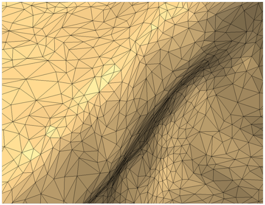
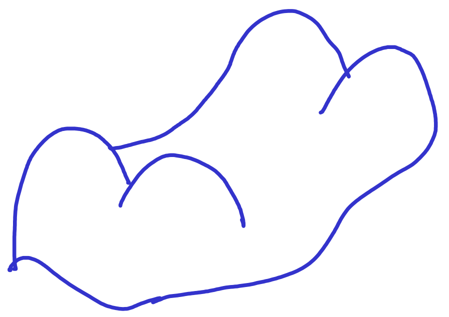
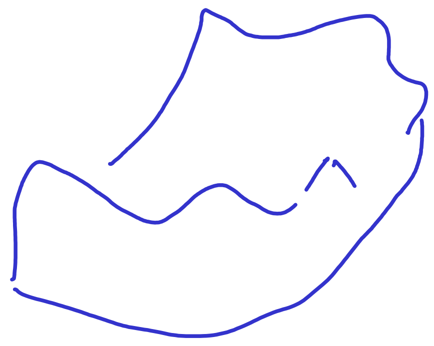
examples: finely discretized triangulated surfaces

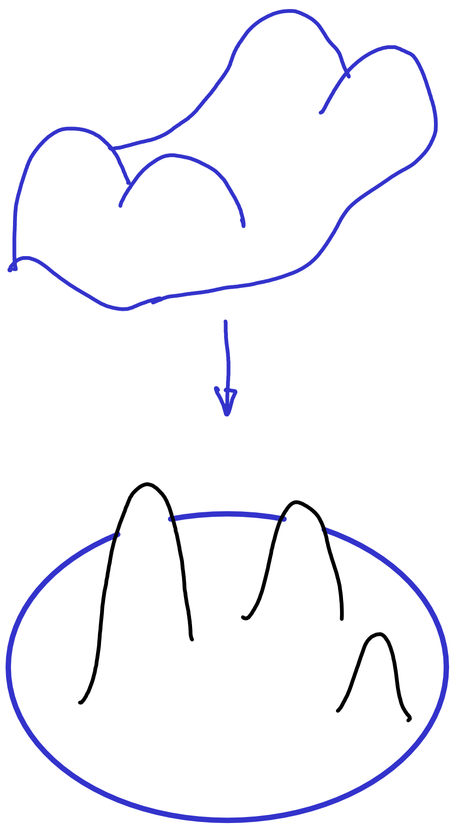


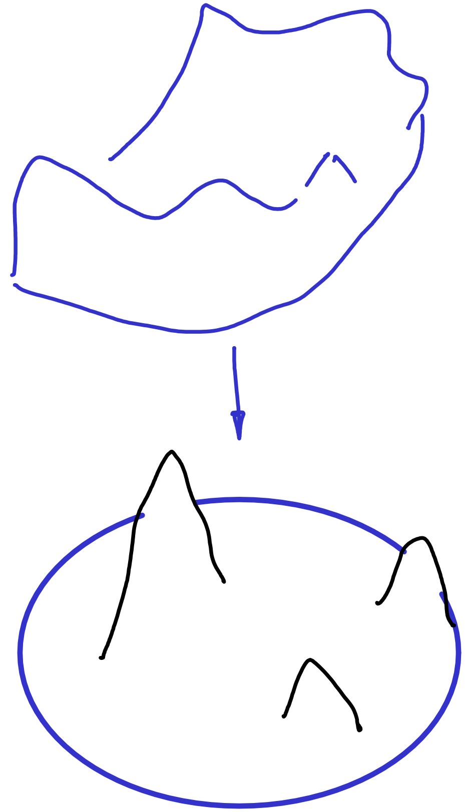


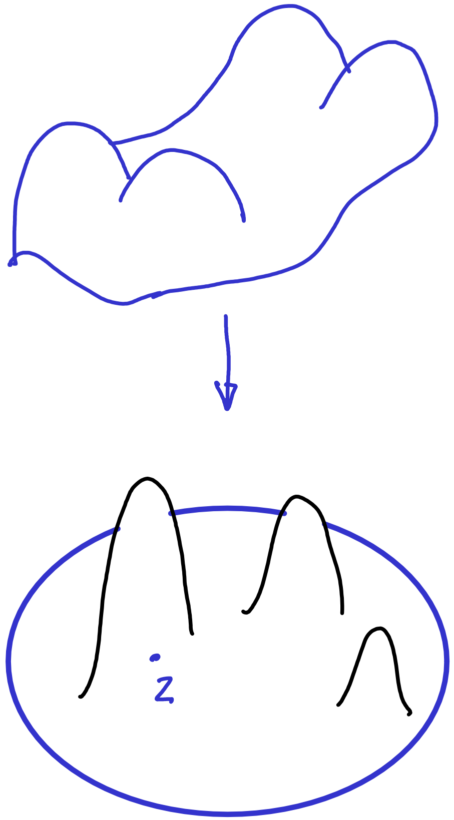
We defined 2 different distances

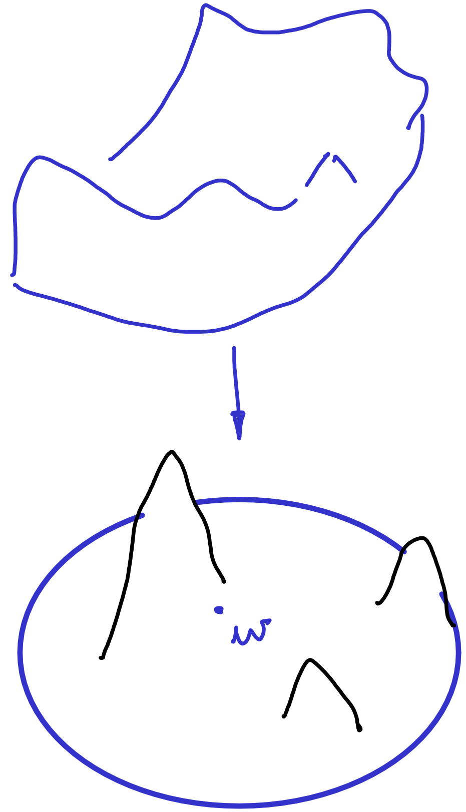
$d_{\mathrm{cWn}}(S_1, S_2)$:	conformal flattening
	comparison of neighborhood geometry
	optimal mass transport
$d_{\mathrm{cP}}(S_1, S_2)$:	continuous Procrustes distance

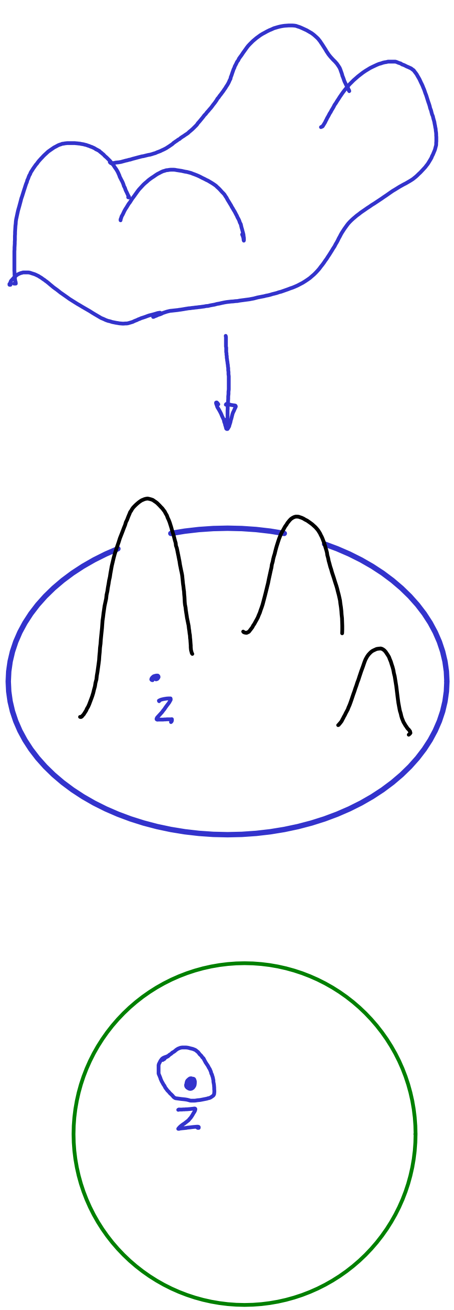





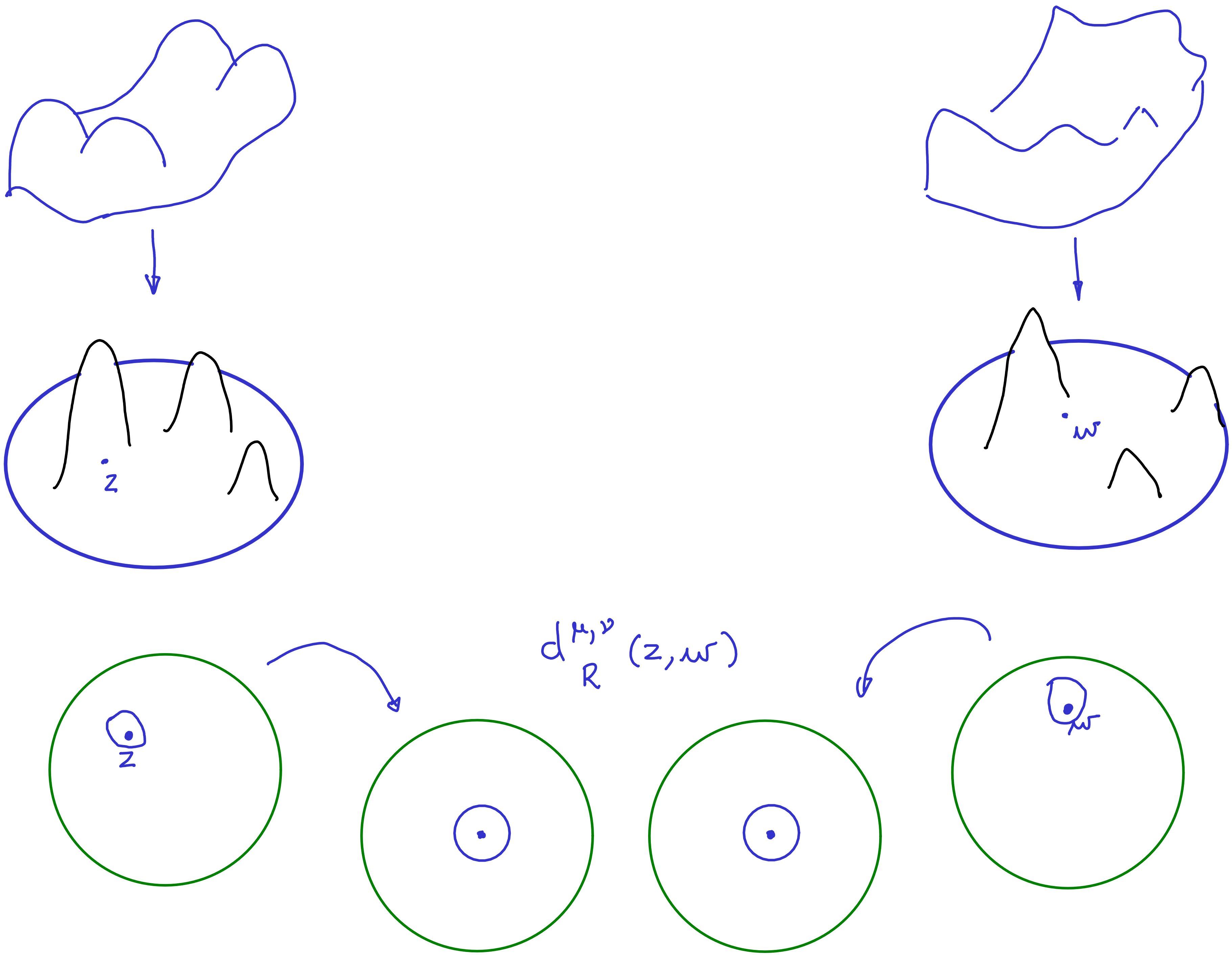



z

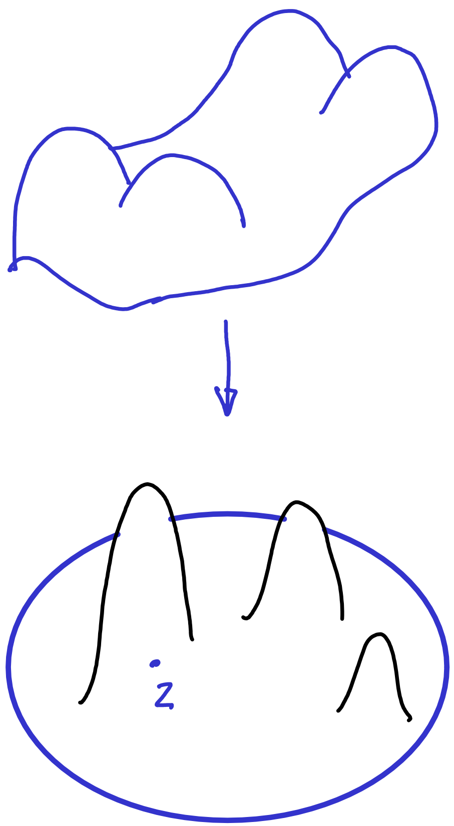

w


z
z

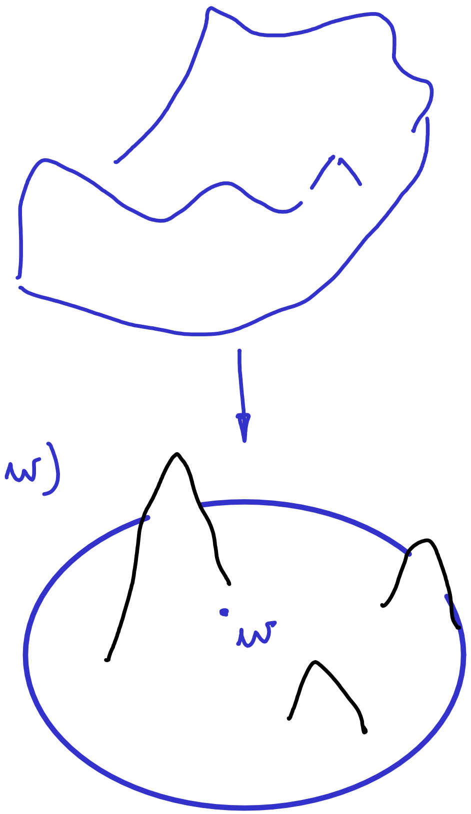

w
w



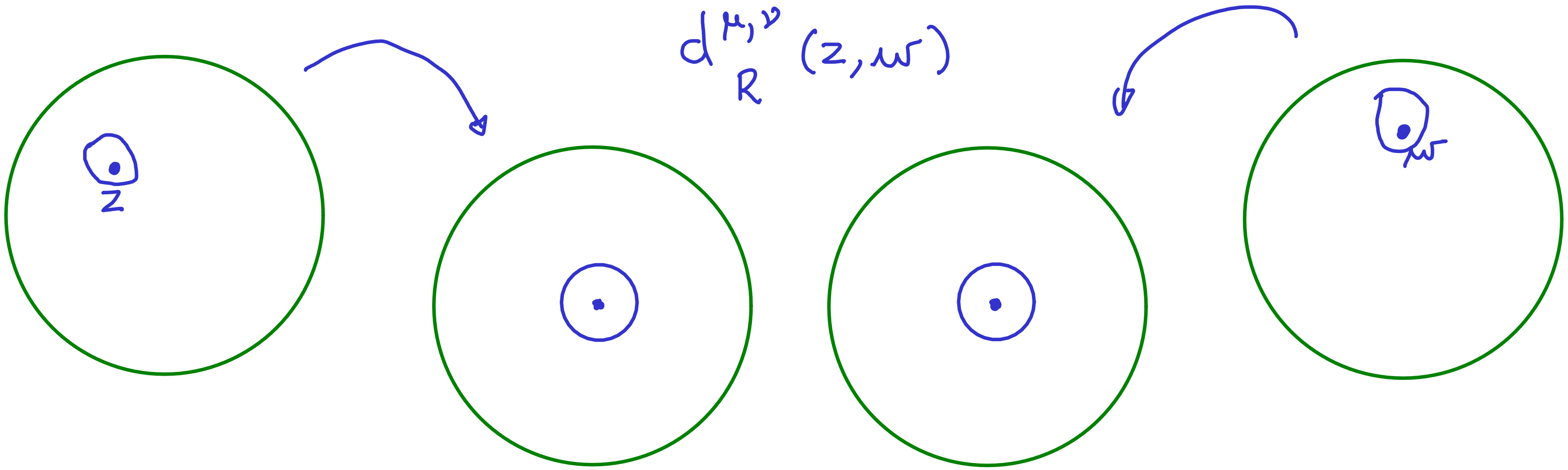
z
w
$d_R^{\mu,\nu}(z,w)$
z
w



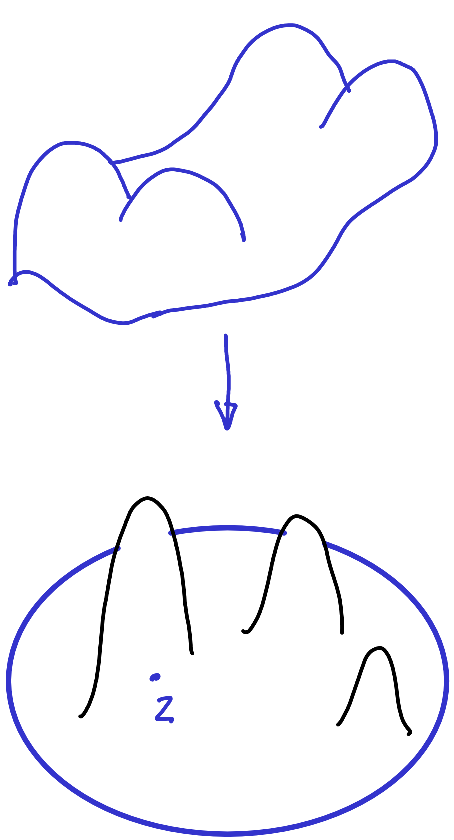
$$D(S_1, S_2) = \inf_{\pi \in \Pi(\mu, \nu)} \int d_R^{\mu,\nu}(z, w)\, d\pi(z, w)$$



$$d_R^{\mu,\nu}(z, w)$$



conformal Wasserstein neighborhood distance



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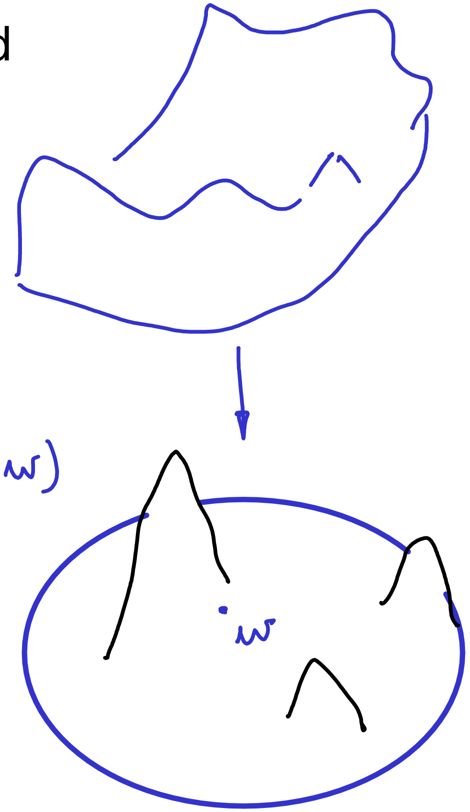

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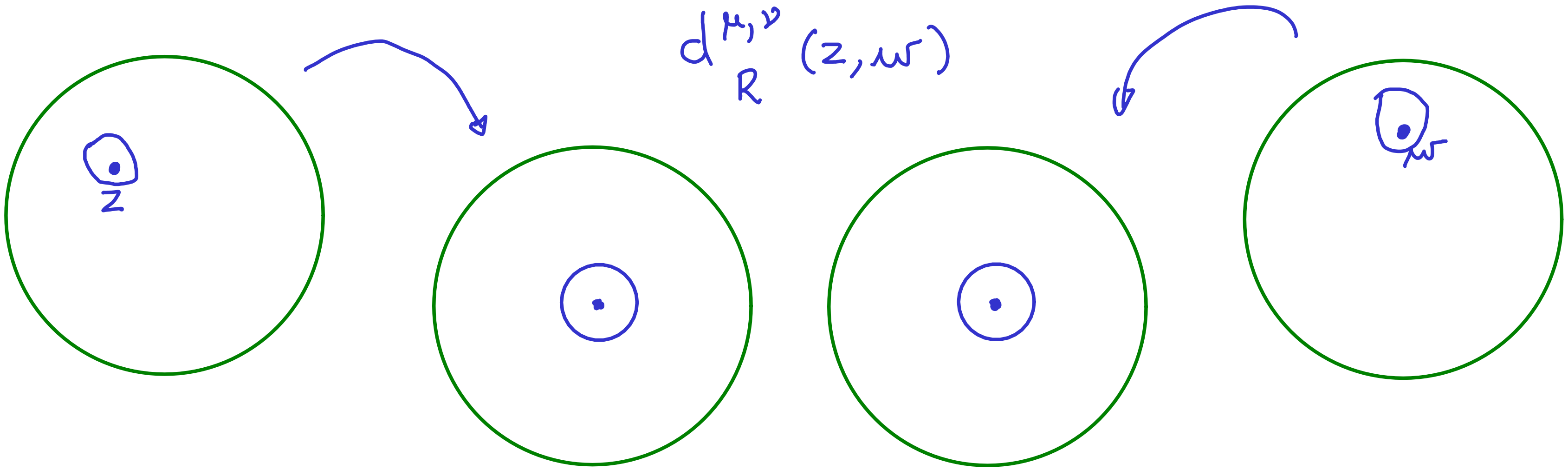
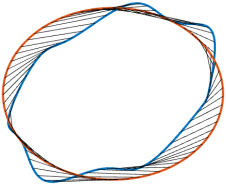


Continuous Procrustes Distance (cPD)

$$D_{\mathrm{cP}}\left(S_1, S_2\right) = \left(\int_{S_1} \| \quad x \quad - \mathcal{C}\left(x\right) \|^2 \, d\mathrm{vol}_{S_1}\left(x\right) \right)^{\frac{1}{2}},$$

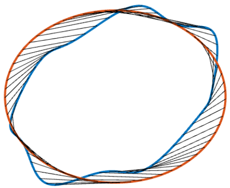
where $\mathcal{C} : S_1 \to S_2$ is an area-preserving diffeomorphism.

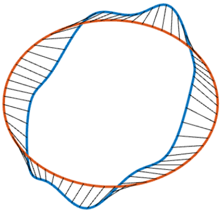


Continuous Procrustes Distance (cPD)

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

where $\mathcal{C} : S_1 \to S_2$ is an area-preserving diffeomorphism, and $\mathbb{E}_3$ is the Euclidean group on $\mathbb{R}^3$.





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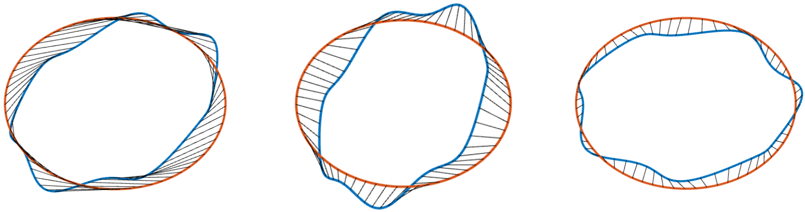
where $\mathcal{A}\left(S_1,S_2\right)$ is the set of area-preserving diffeomorphisms between S_1 and S_2, and $\mathbb{E}_3$ is the Euclidean group on $\mathbb{R}^3$.



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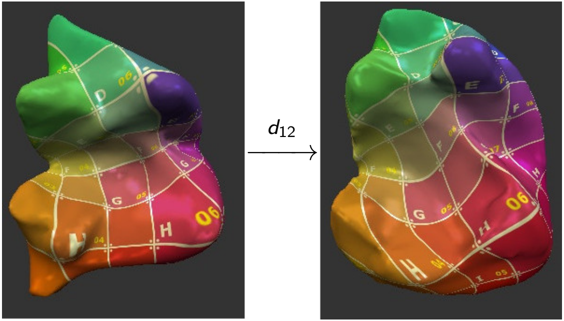

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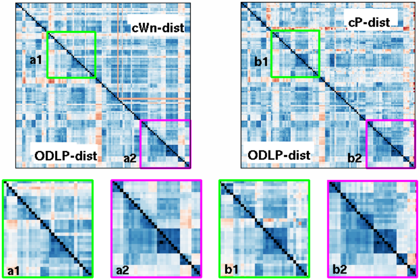
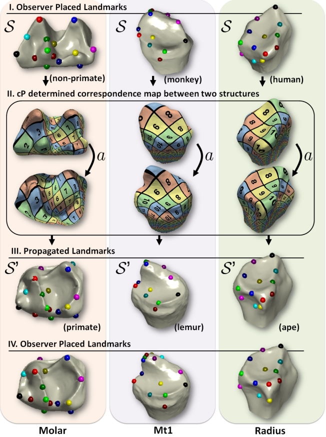
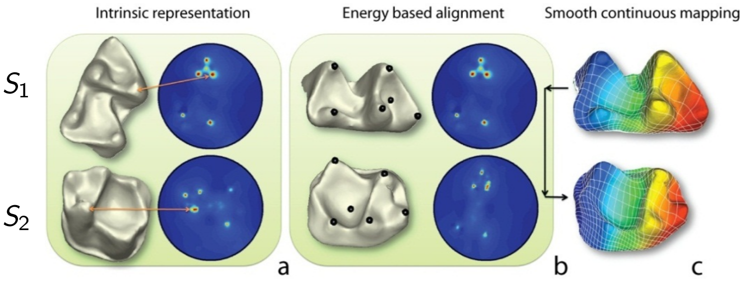
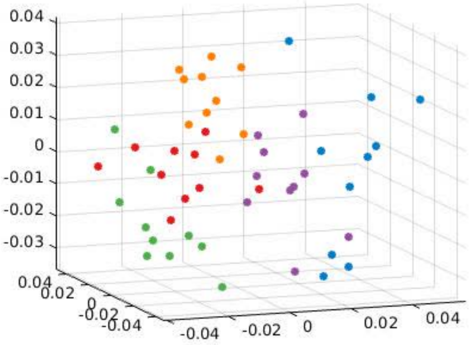




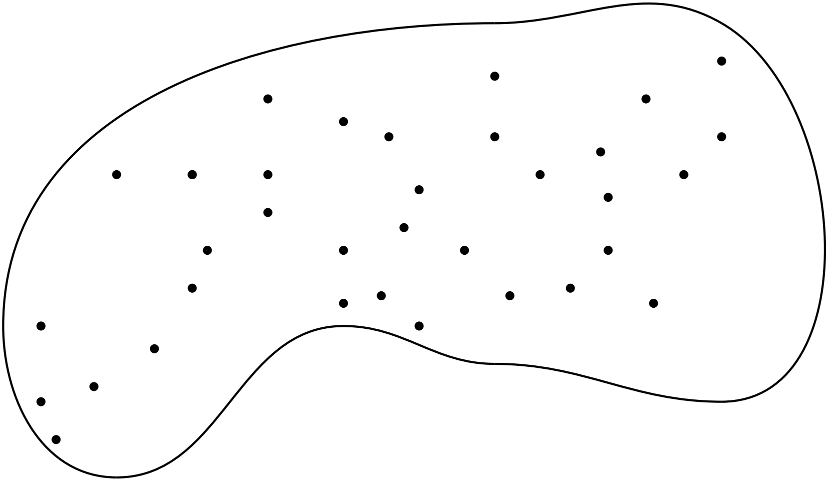
Bypass Explicit Feature Extraction



Multi-Dimensional Scaling (MDS) for cPD Matrix

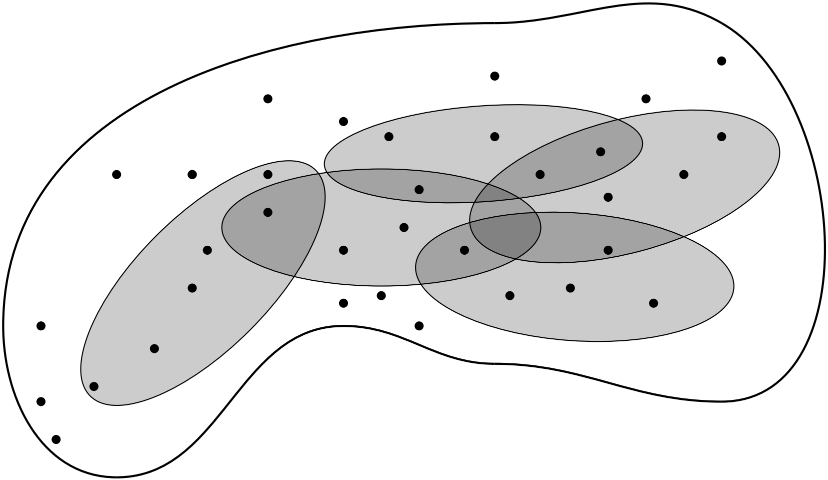


Diffusion Maps: "Knit together" local geometry to get "better" distances



Small distances are much more reliable!

Diffusion Maps: "knitting together" local geometry



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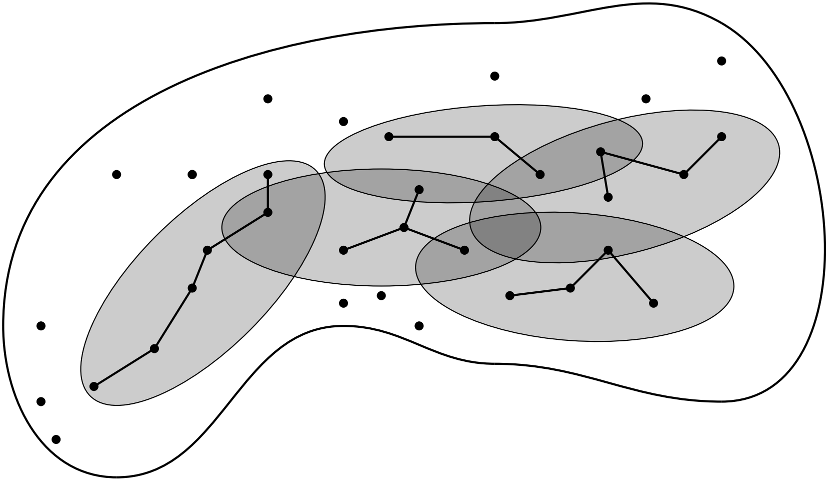

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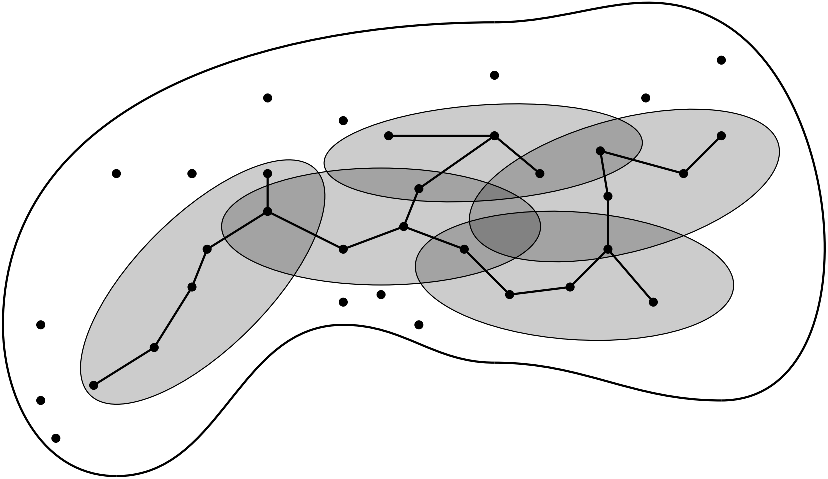

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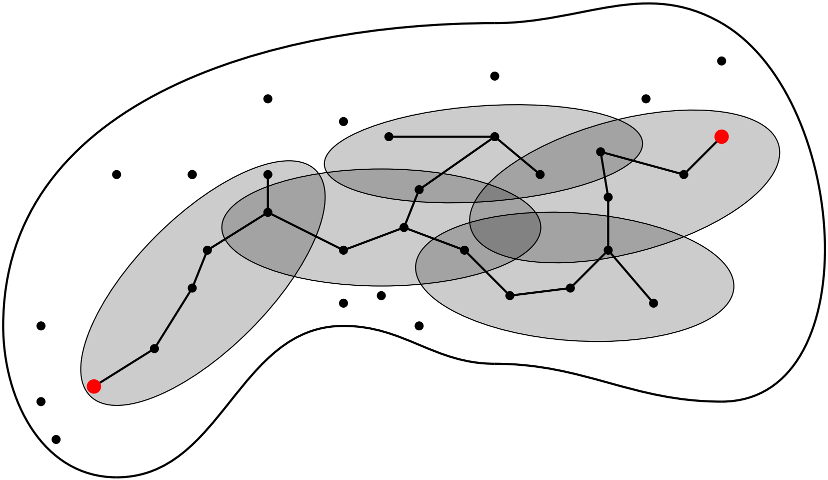

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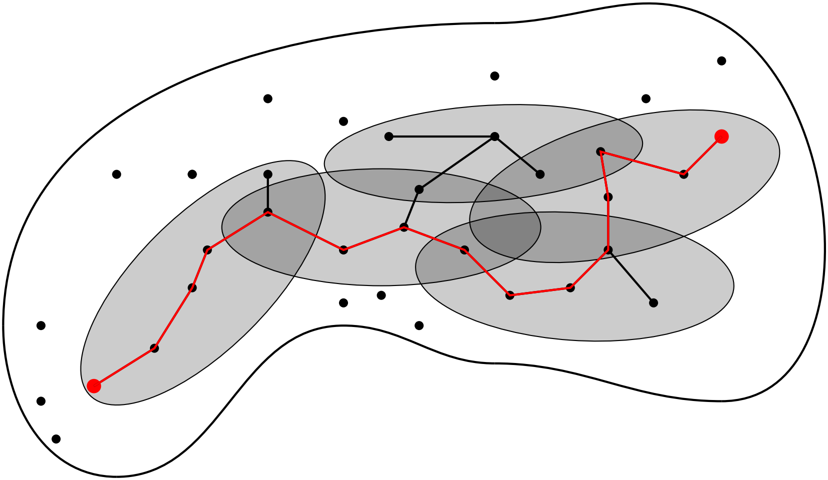

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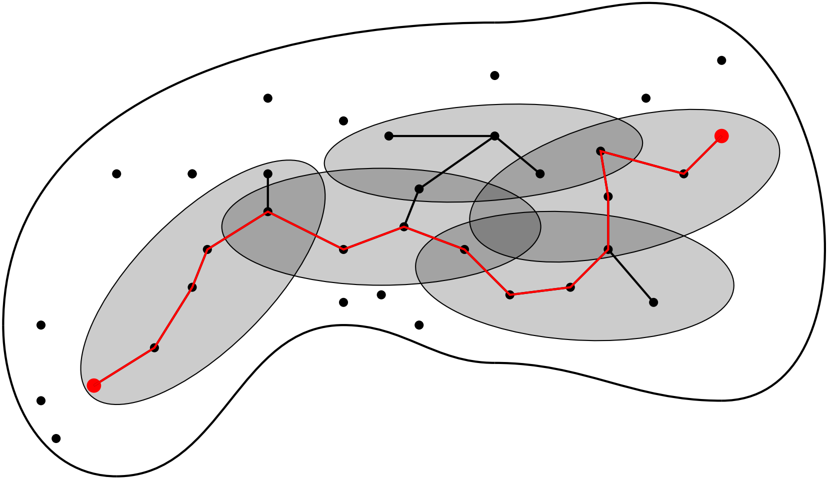

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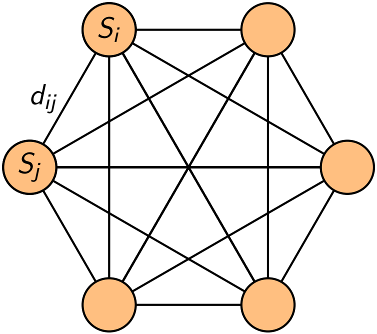

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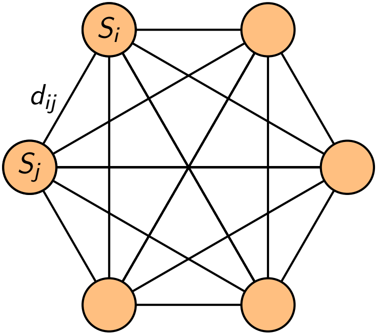

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$$Pu_j = \lambda_j u_j, \; j = 1, 2, \cdots, m$$

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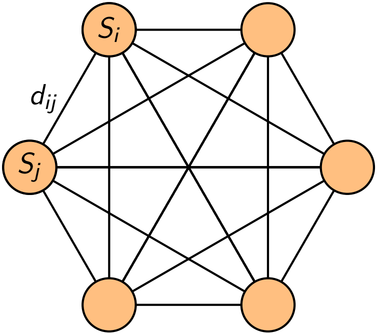

- $P = D^{-1}W$ defines a random walk on the graph
- Solve eigen-problem

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

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

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

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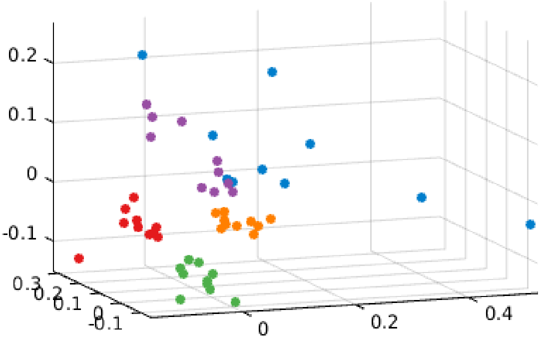
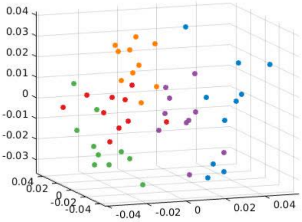
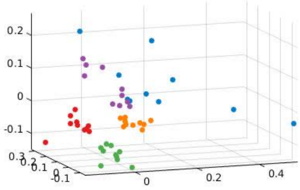


MDS for cPD & DD

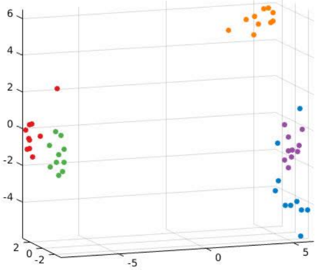


cPD

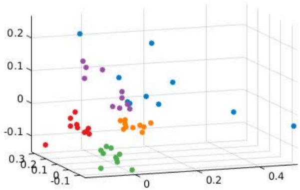


DD

Even better can be obtained!



HBDD



DD

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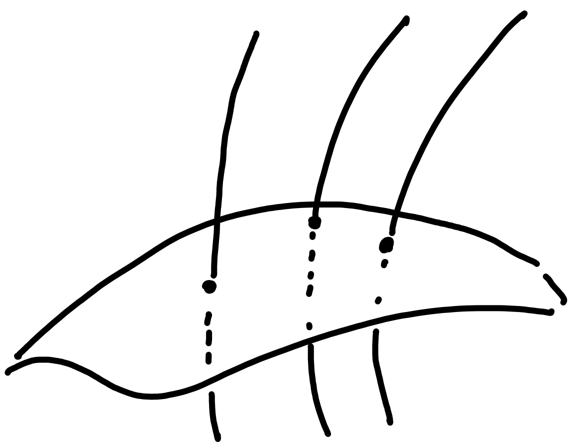
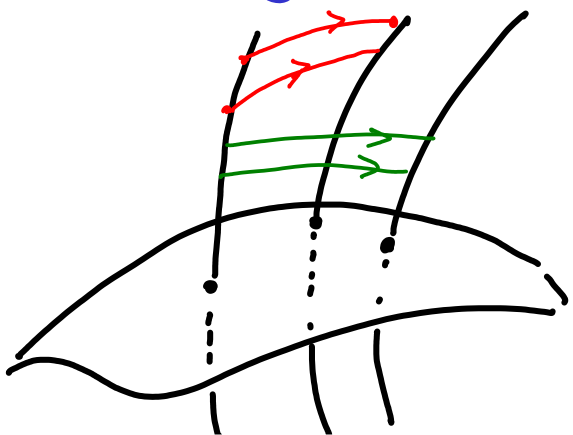
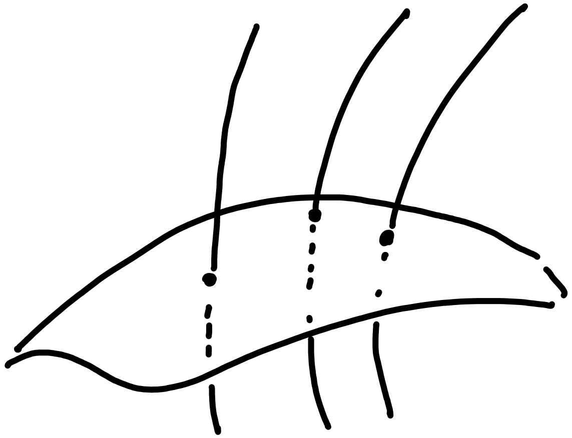
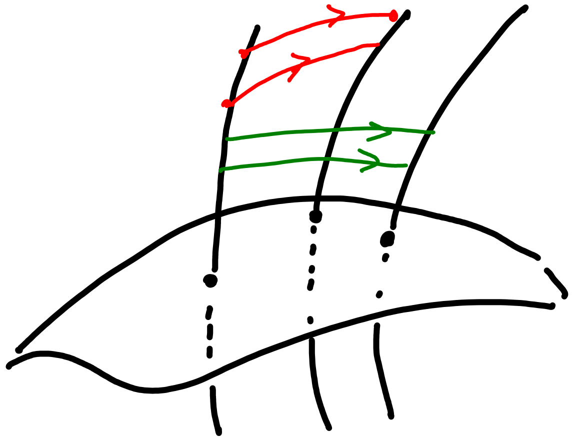




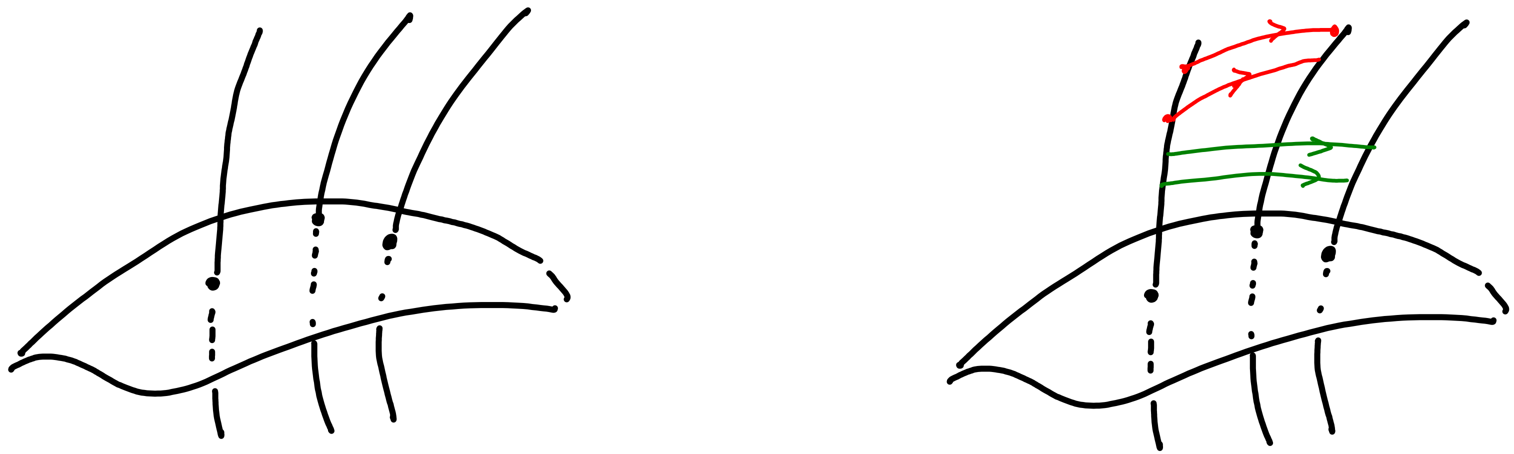




Connection.

↓

family of mappings between fibers



Connection.

$\downarrow$

family of mappings between fibers

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

$\longrightarrow$ "project" at a later stage to obtain "horizontal" part of diffusion.

Horizontal Random Walk on a *Fibre Bundle*

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

- E: *total* manifold
- M: *base* manifold
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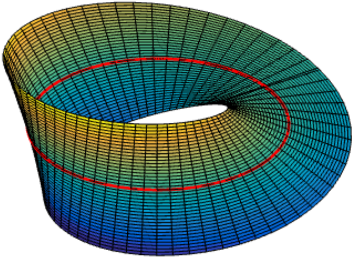

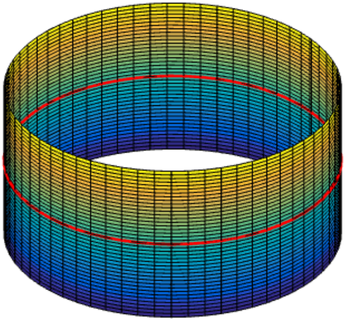

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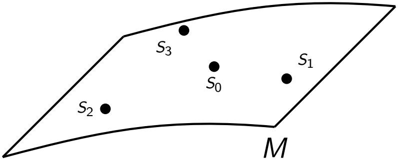

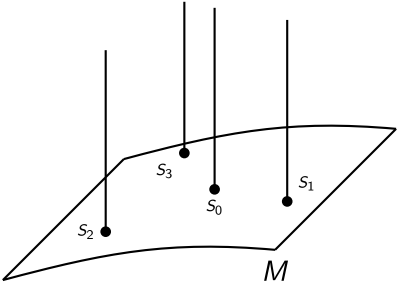

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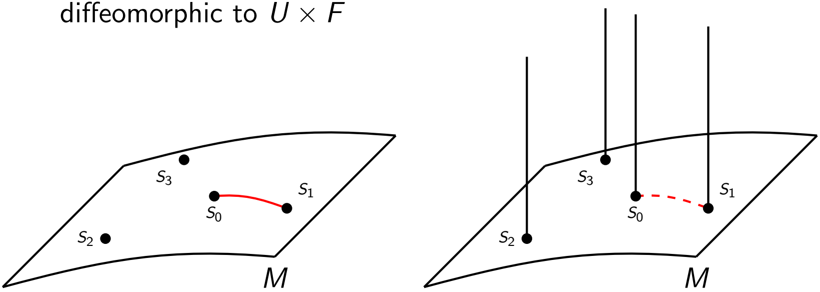

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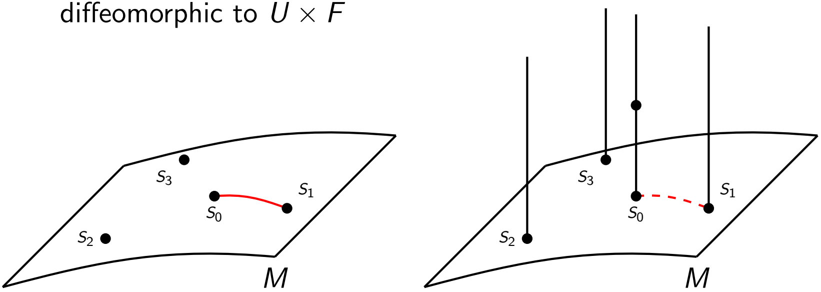

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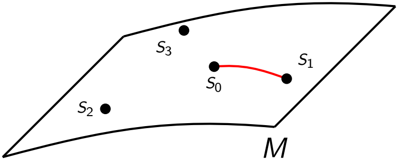

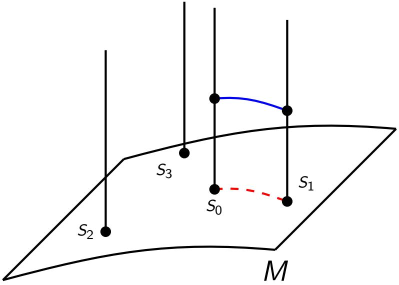

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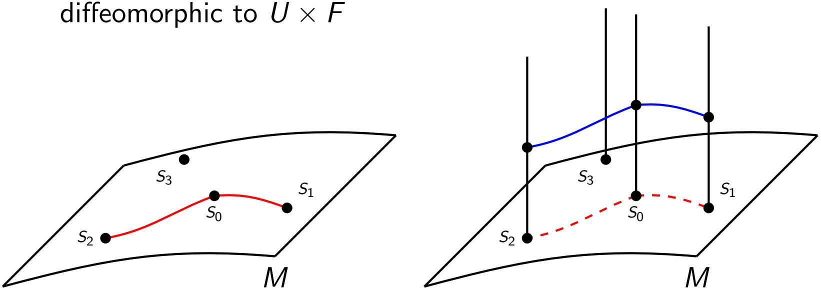

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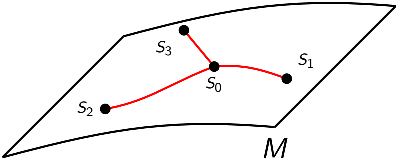
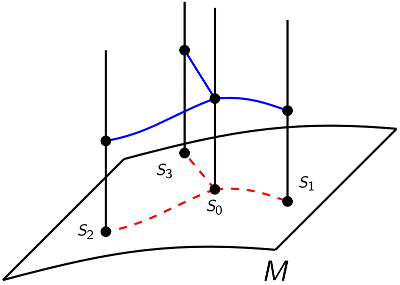




Towards *Horizontal* Diffusion Maps

Diffusion Maps

$$D^{-1}Wu_k = \lambda_k u_k, \quad 1 \leq k \leq N$$

$$D^{-1}\begin{pmatrix} & & & \vdots & \\ & & & \vdots & \\ \cdots & \cdots & & e^{-d_{ij}^2/\epsilon} & \cdots \\ & & & \vdots & \end{pmatrix}\begin{pmatrix} \vdots \\ \vdots \\ u_k(j) \\ \vdots \end{pmatrix} = \lambda_k \begin{pmatrix} \vdots \\ \vdots \\ u_k(j) \\ \vdots \end{pmatrix}$$

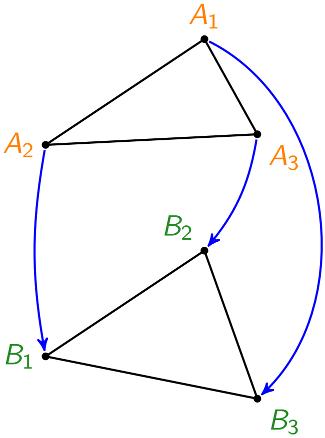
Towards *Horizontal* Diffusion Maps

Horizontal Diffusion Maps

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

$$\mathcal{D}^{-1}\begin{pmatrix} & & \vdots & \\ & & \vdots & \\ \cdots & \cdots & e^{-d_{ij}^2/\epsilon}\rho_{ij}^{\delta} & \cdots \\ & & \vdots & \end{pmatrix}\begin{pmatrix} \vdots \\ \vdots \\ u_{k[j]} \\ \vdots \end{pmatrix} = \lambda_k \begin{pmatrix} \vdots \\ \vdots \\ u_{k[j]} \\ \vdots \end{pmatrix}$$

Correspondences Between Triangular Meshes



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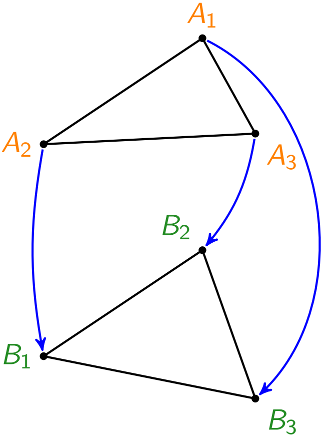

$$
\begin{array}{cc}
 & \xrightarrow{\hspace{6em} S_2 \hspace{6em}} \\
 & \begin{array}{ccccc} \cdots & B_1 & B_2 & B_3 & \cdots \end{array} \\
S_1 \Bigg\downarrow \begin{array}{c} \vdots \\ A_1 \\ A_2 \\ A_3 \\ \vdots \end{array} &
\begin{pmatrix}
 & \vdots & \vdots & \vdots & \\
\cdots & 0 & 0 & 1 & \cdots \\
\cdots & 1 & 0 & 0 & \cdots \\
\cdots & 0 & 1 & 0 & \cdots \\
 & \vdots & \vdots & \vdots &
\end{pmatrix}
\end{array}
$$

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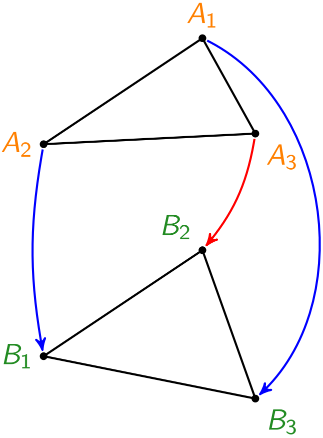

$$
S_2 \longrightarrow
$$

$$
S_1 \downarrow \quad
\begin{array}{c}
\\ \vdots \\ A_1 \\ A_2 \\ A_3 \\ \vdots
\end{array}
\begin{array}{c}
\begin{array}{ccccc}
\cdots & B_1 & B_2 & B_3 & \cdots
\end{array} \\
\begin{pmatrix}
 & \vdots & \vdots & \vdots & \\
\cdots & 0 & 0 & 1 & \cdots \\
\cdots & 1 & 0 & 0 & \cdots \\
\cdots & 0 & \boxed{1} & 0 & \cdots \\
 & \vdots & \vdots & \vdots &
\end{pmatrix}
\end{array}
$$

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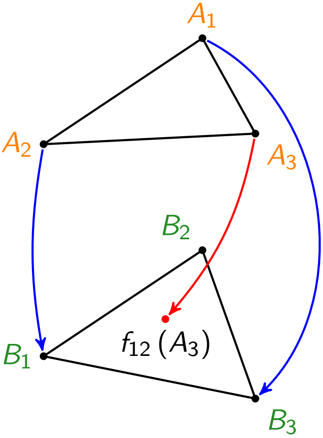

$$\begin{array}{c c c} & & \overrightarrow{\qquad\qquad S_2 \qquad\qquad} \\ & & \begin{array}{ccccc} \cdots & B_1 & B_2 & B_3 & \cdots \end{array} \\ S_1 \big\downarrow & \begin{array}{c} \vdots \\ A_1 \\ A_2 \\ A_3 \\ \vdots \end{array} & \begin{pmatrix} & \vdots & \vdots & \vdots & \\ \cdots & 0 & 0 & 1 & \cdots \\ \cdots & 1 & 0 & 0 & \cdots \\ \cdots & 0 & \boxed{?} & 0 & \cdots \\ & \vdots & \vdots & \vdots & \end{pmatrix} \end{array}$$

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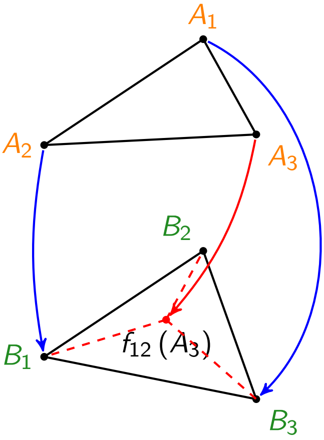

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$$\rho_{12}^{\delta}(r, s) = \exp\left(-\frac{\left\|f_{12}(A_r) - B_s\right\|^2}{\delta}\right)$$

Towards *Horizontal* Diffusion Maps

Horizontal Diffusion Maps

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

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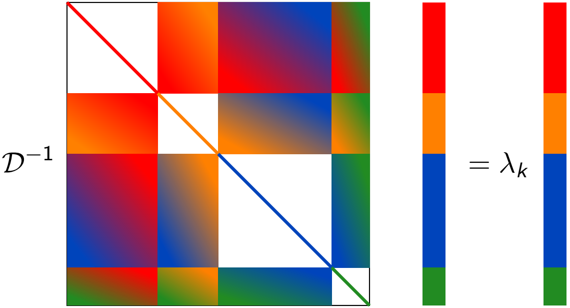

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Horizontal Diffusion Maps: For fixed $1 \leq m \leq \kappa$, $t \geq 0$, represent S_j as a $\kappa_j \times m$ *matrix*

$$\left(\lambda_1^{t/2}u_{1[j]}, \cdots, \lambda_m^{t/2}u_{m[j]}\right)$$

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*

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

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:

$$(j, p) \longrightarrow \Big(u_k(j, p) \Big)_{k=1,\dots K}$$

S_j

pt p on S_j

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S_j

pt p on S_j

$\big\downarrow$ "project" to geometry on base manifold

Spectral coordinates for points in fiber bundle:

$$(j,p) \longrightarrow \left(u_k(j,p) \right)_{k=1,\dots K}$$

j ↔ S_j; p ← pt p on S_j

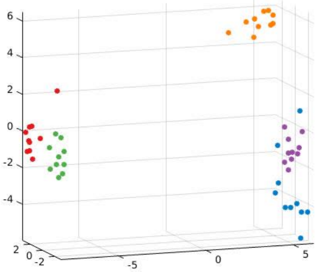
↓ "project" to geometry on base manifold

hor. dist (S_i, S_j)

= dist. between corresponding point clouds in K-dim space.

$$= \left[\sum_{p,q} \lambda_k^{\varepsilon,\delta}(p,q) \left| u_k(i,p) - u_k(j,q) \right|^2 \right]^{1/2}$$

Even better can be obtained!



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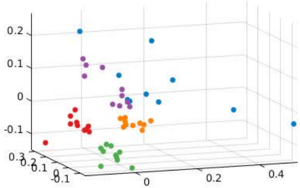
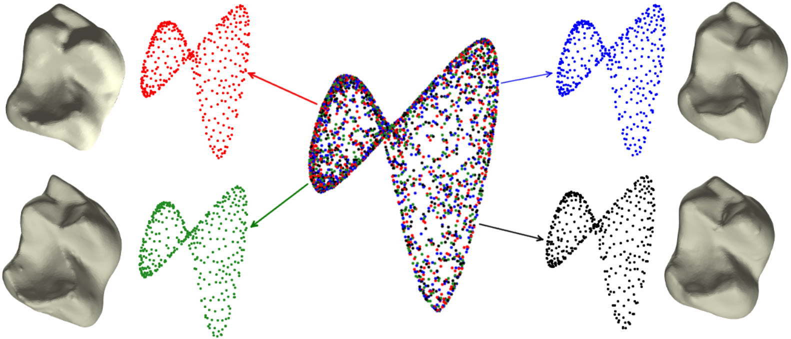


DD

1. Global Registration



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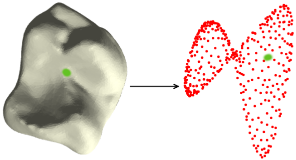

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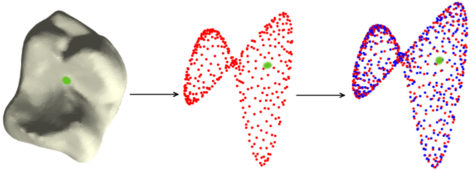

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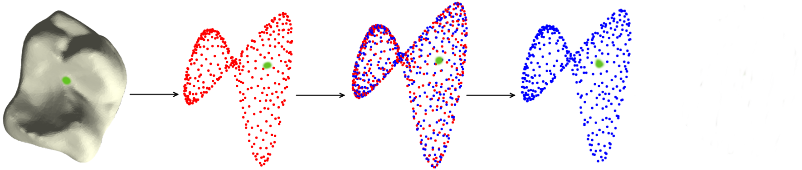

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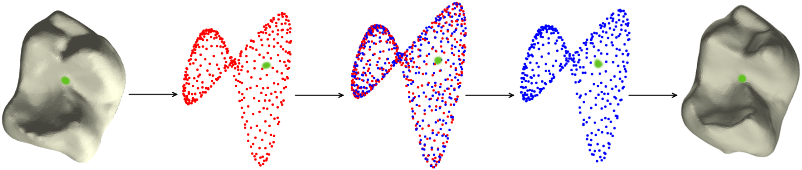

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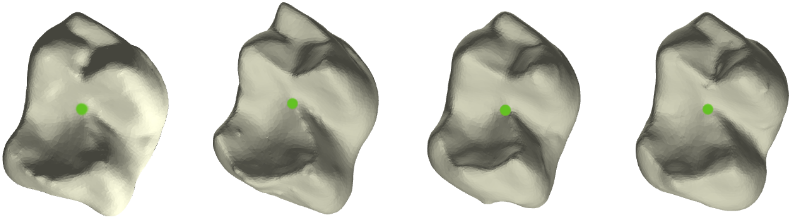
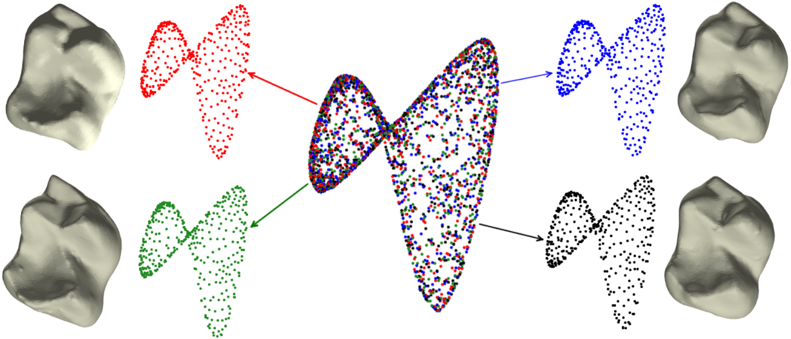


2. Automatic Landmarking: *Spectral Clustering*



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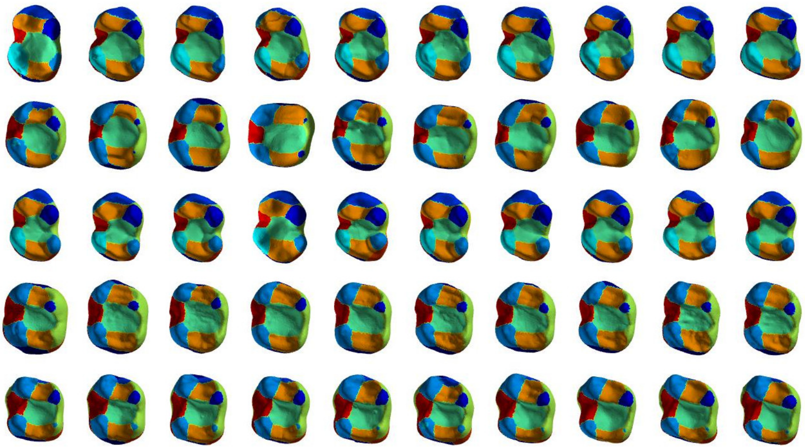
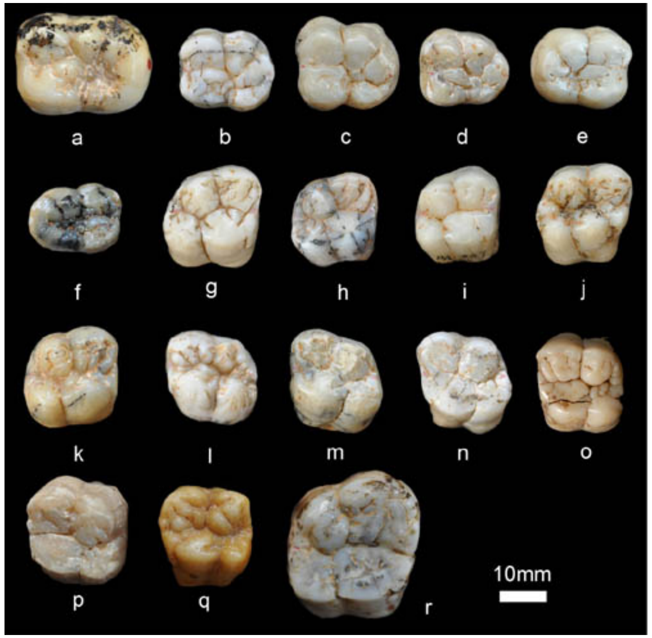


Ongoing and future directions.

- 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.

Connection is reasonable for bones/teeth of closely related species.



primate molars

crabeater seal molars