Teeth, Bones and Manifolds:

a meeting of mathematical

and biological minds

Ingrid Daubechies

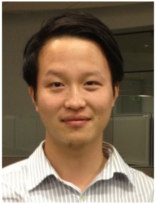
Inaugural Conference, IMSA, 2019

Collaborators

Rima Alaifari
ETH Zürich

Doug Boyer
Duke

Ingrid Daubechies
Duke



Tingran Gao
Duke

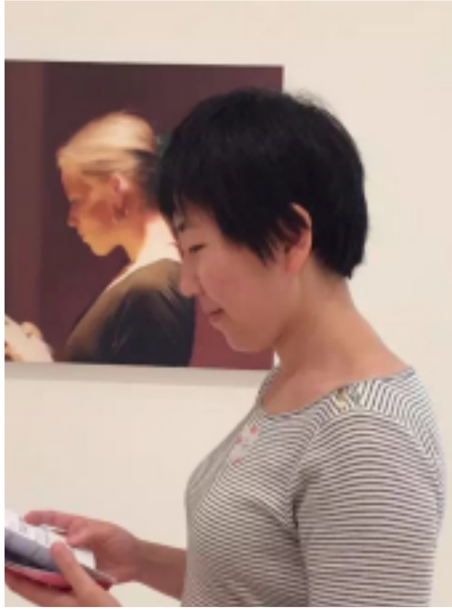
Yaron Lipman
Weizmann

Roi Poranne
ETH Zürich

Jesús Puente
J.P. Morgan

Robert Ravier
Duke

Shahar Kovalsky



Shan Shan

Panchali Nag

Chen-Yun Lin

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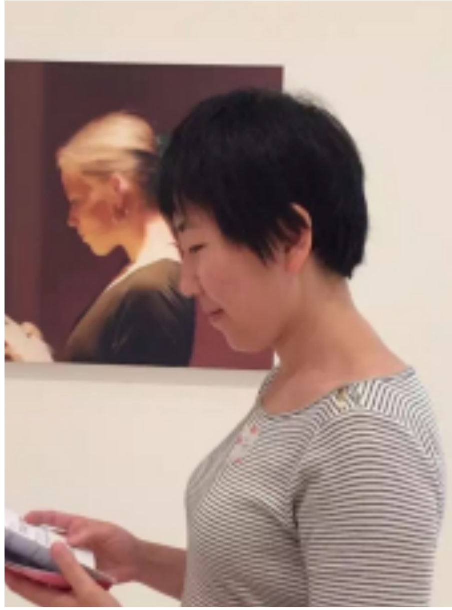

Shan Shan

Panchali Nag

Chen-Yun Lin

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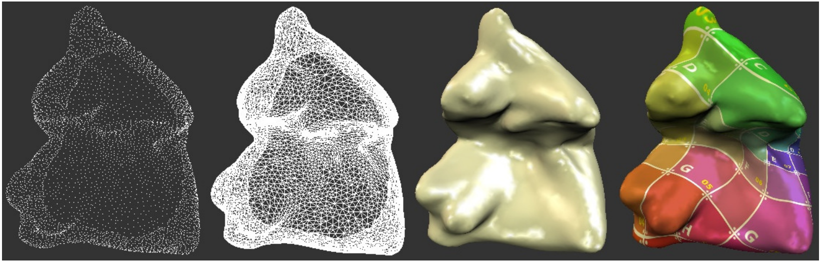
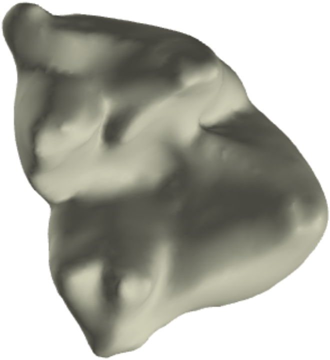
Then: find automatic way to compute Procrustes distances between surfaces — without landmarks

Data Acquisition



Surface reconstructed from μCT-scanned voxel data

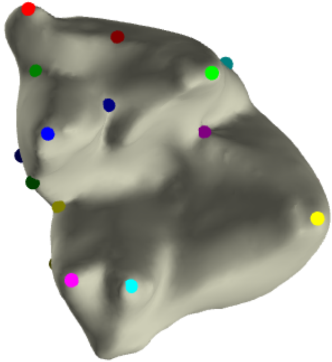
Geometric Morphometrics



second mandibular molar of a Philippine flying lemur

- Manually put k landmarks

Geometric Morphometrics



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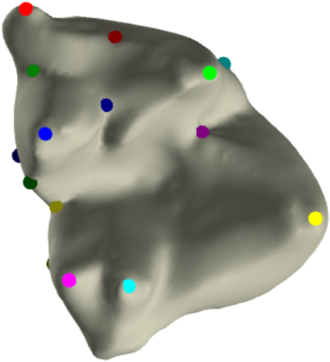
$$p_1, p_2, \cdots, p_k$$

Geometric Morphometrics



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- Use spatial coordinates of the landmarks as features

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

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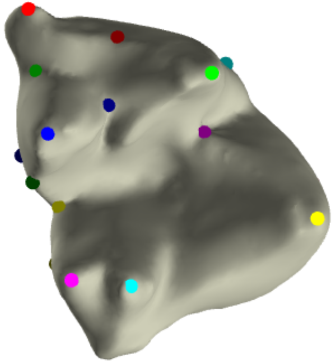

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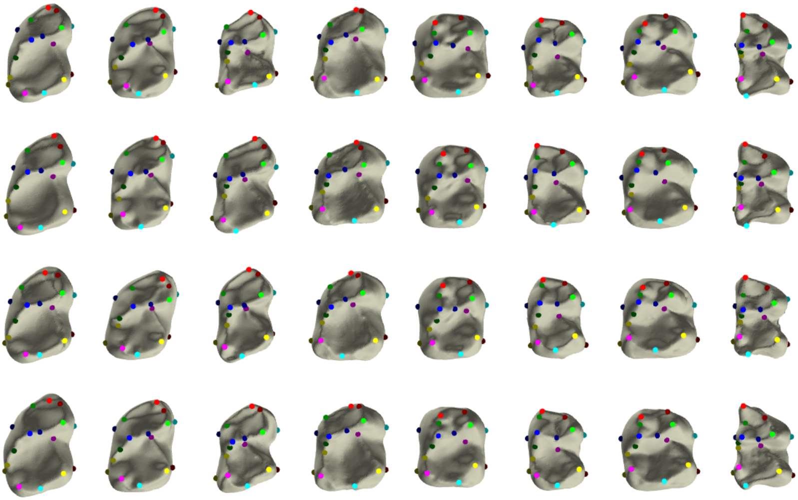
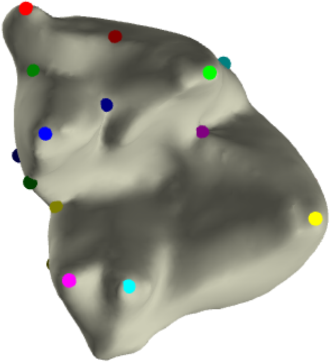
$$p_j = (x_j, y_j, z_j), \; j = 1, \cdots, k$$

- 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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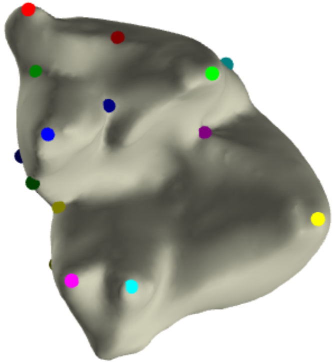
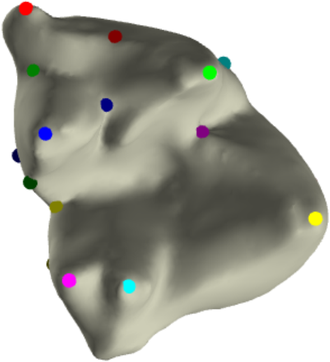


- Landmark Placement: tedious and time-consuming

Geometric Morphometrics: Limitation of Landmarks



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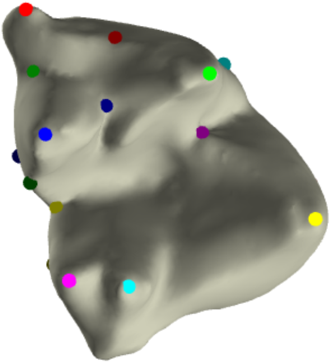

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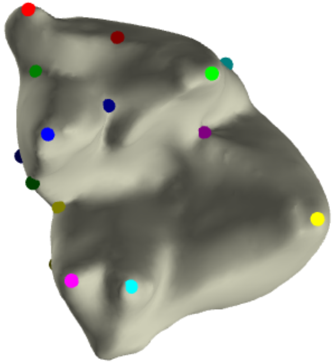
- Domain Knowledge: high degree of expertise needed, not easily accessible

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

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

Landmarked Teeth $\longrightarrow$

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

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Landmarked Teeth $\longrightarrow$

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

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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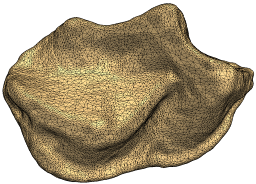
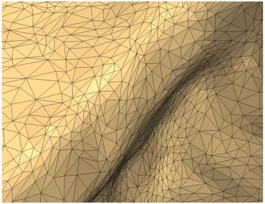
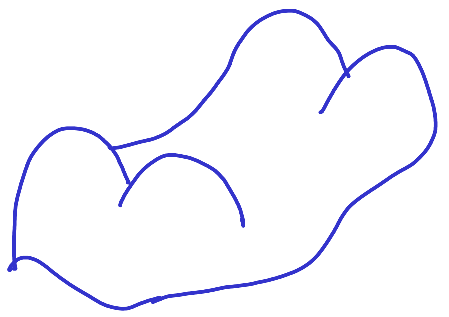
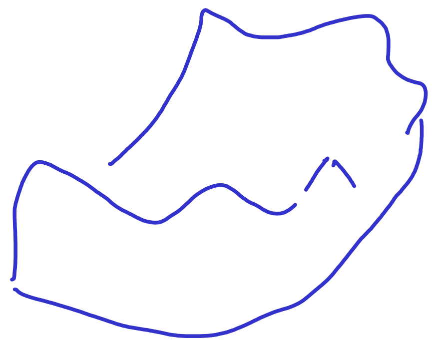
examples: finely discretized triangulated surfaces

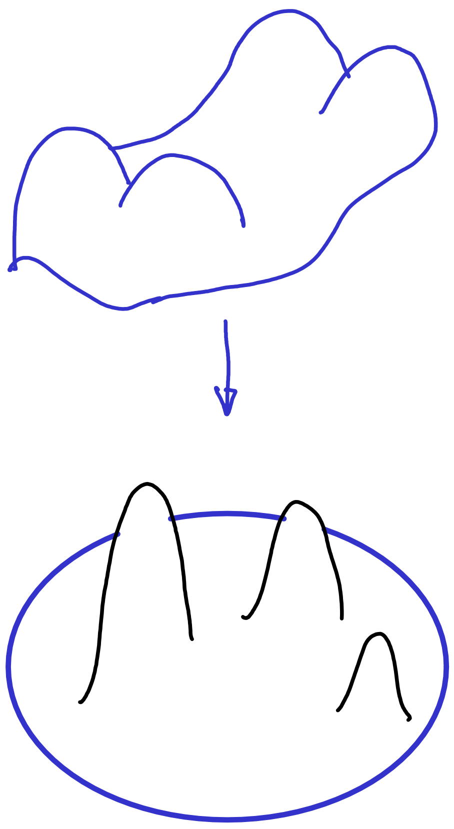


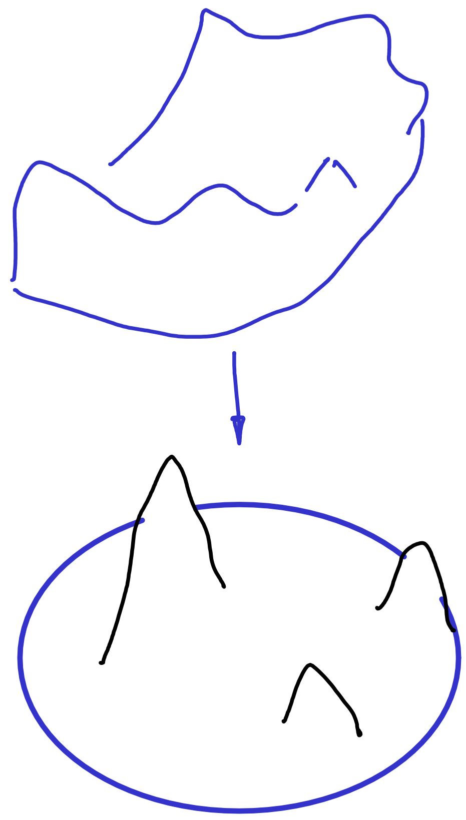


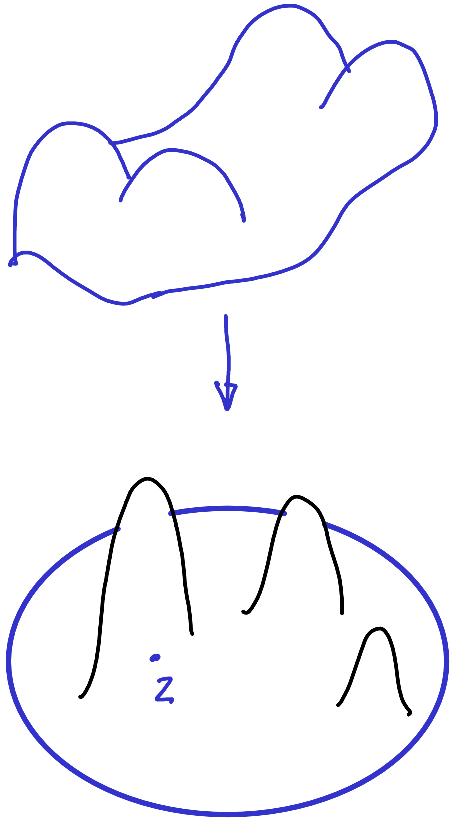
We defined 2 different distances

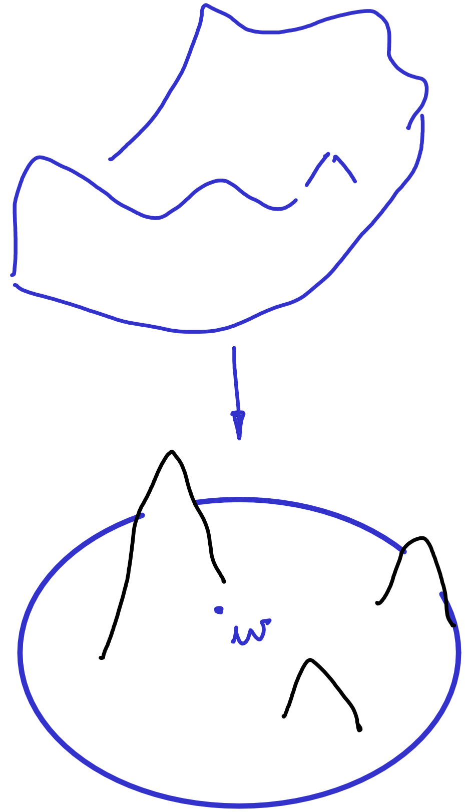
$d_{\mathrm{cWn}}(S_1, S_2)$:	conformal flattening
	comparison of neighborhood geometry
	optimal mass transport
$d_{\mathrm{cP}}(S_1, S_2)$:	continuous Procrustes distance

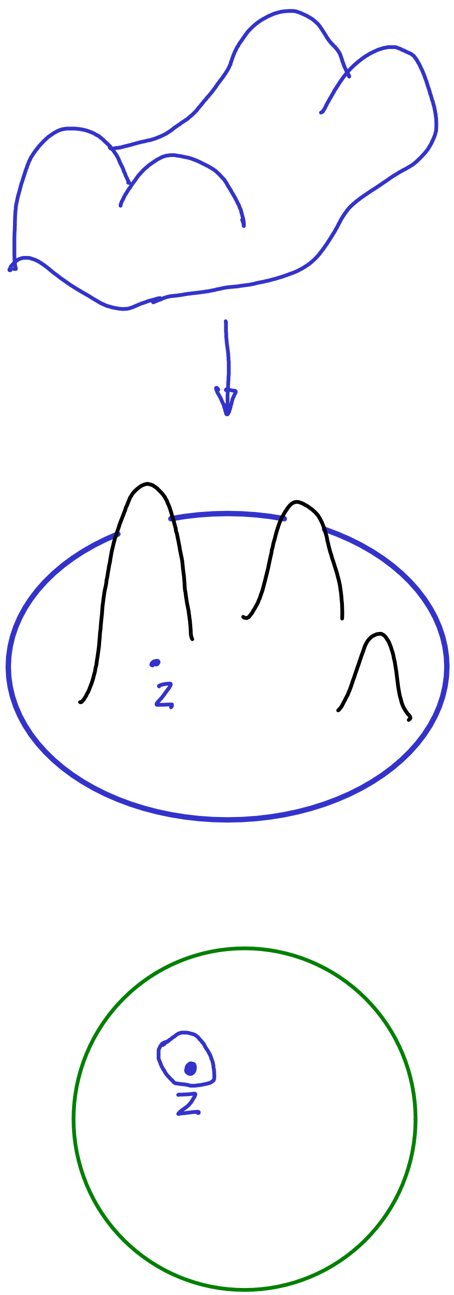





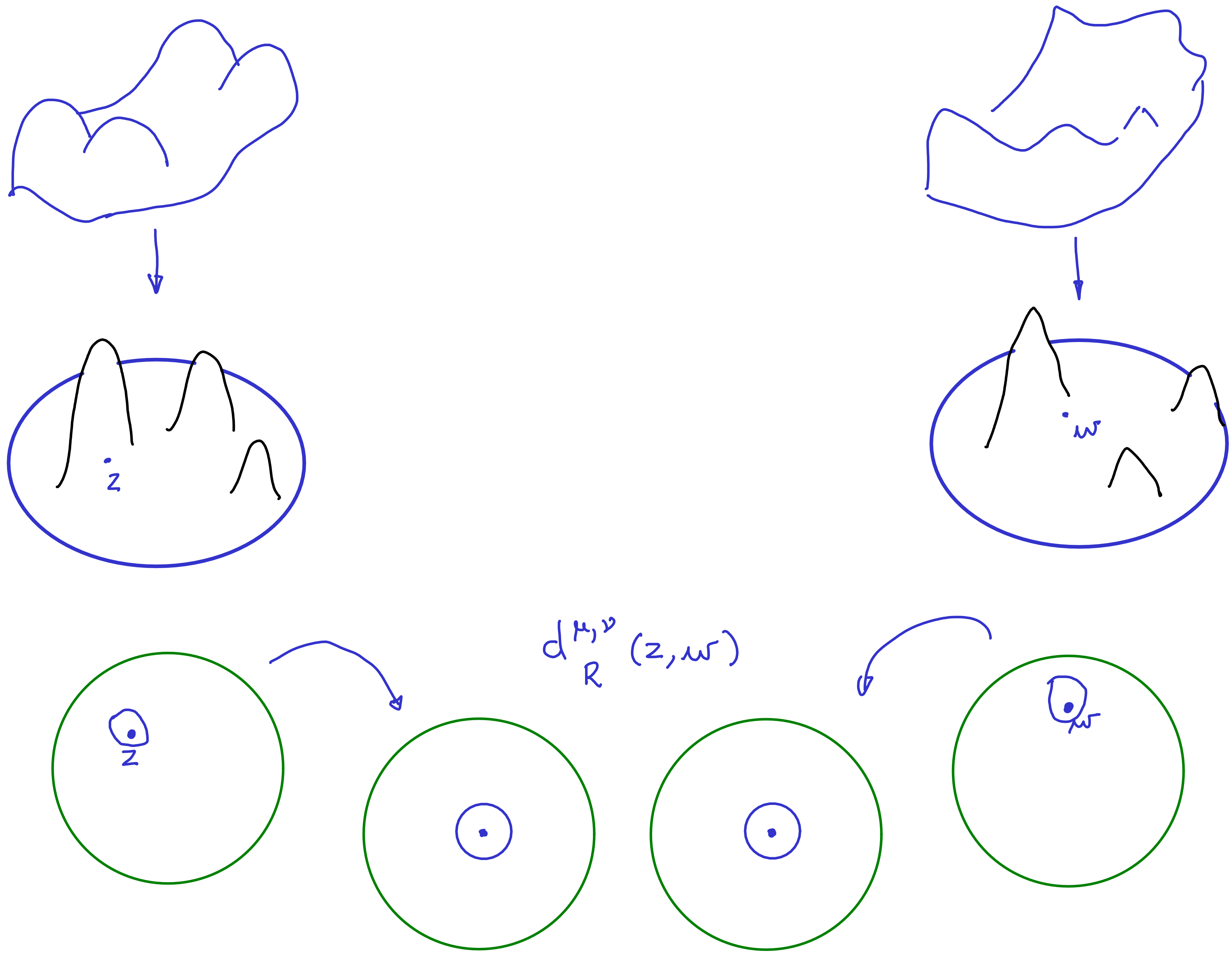



z

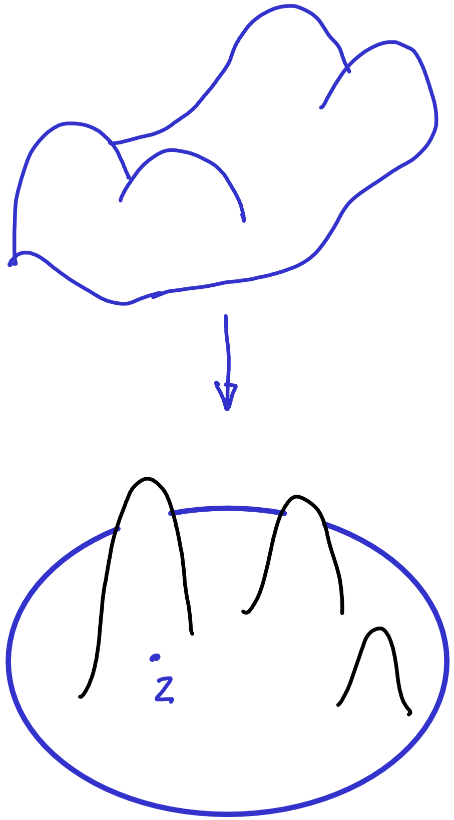

w


z
z

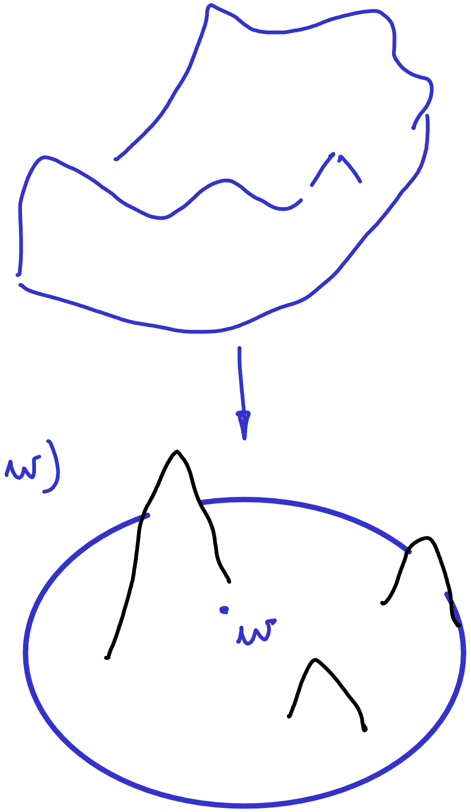

w
w

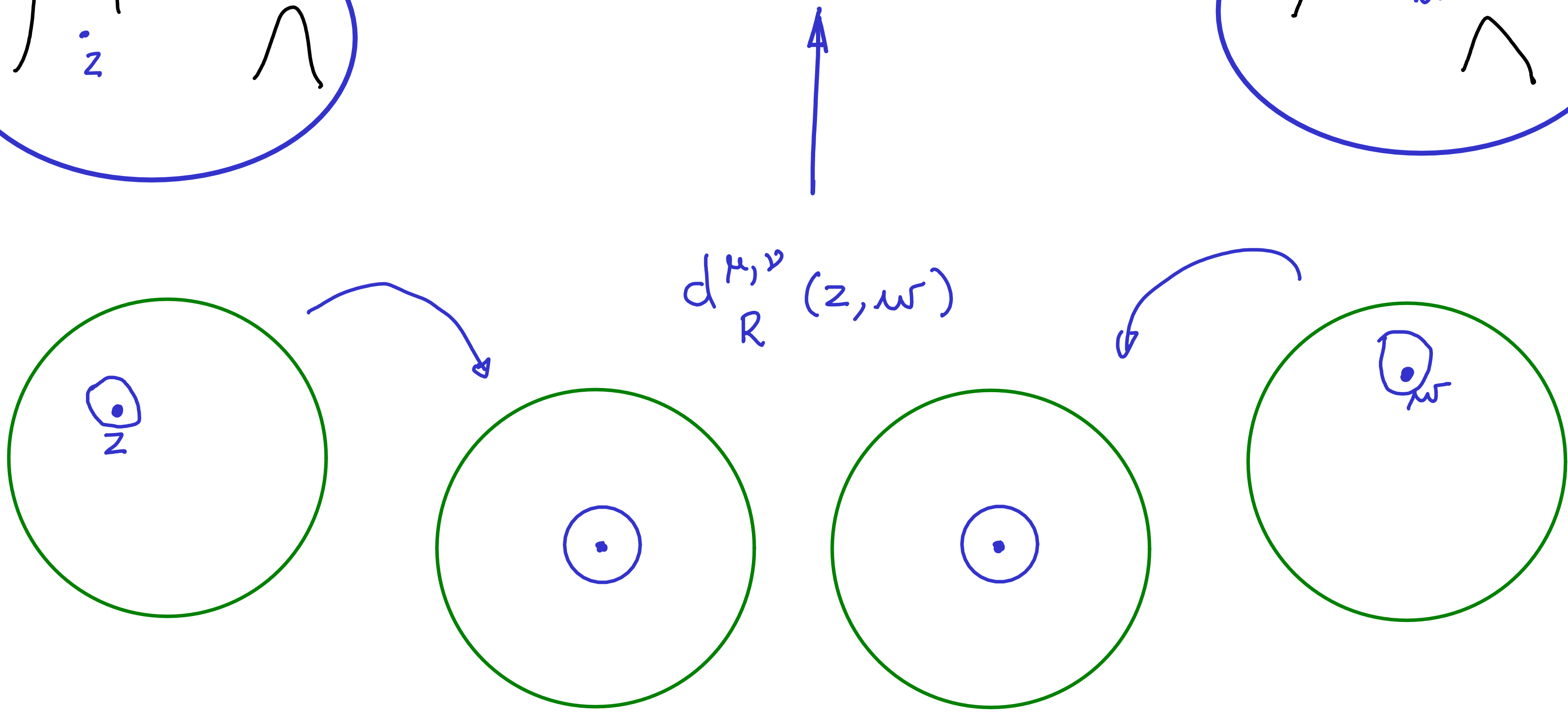


z
w
$d^{\mu,\nu}_{R}(z,w)$
z
w

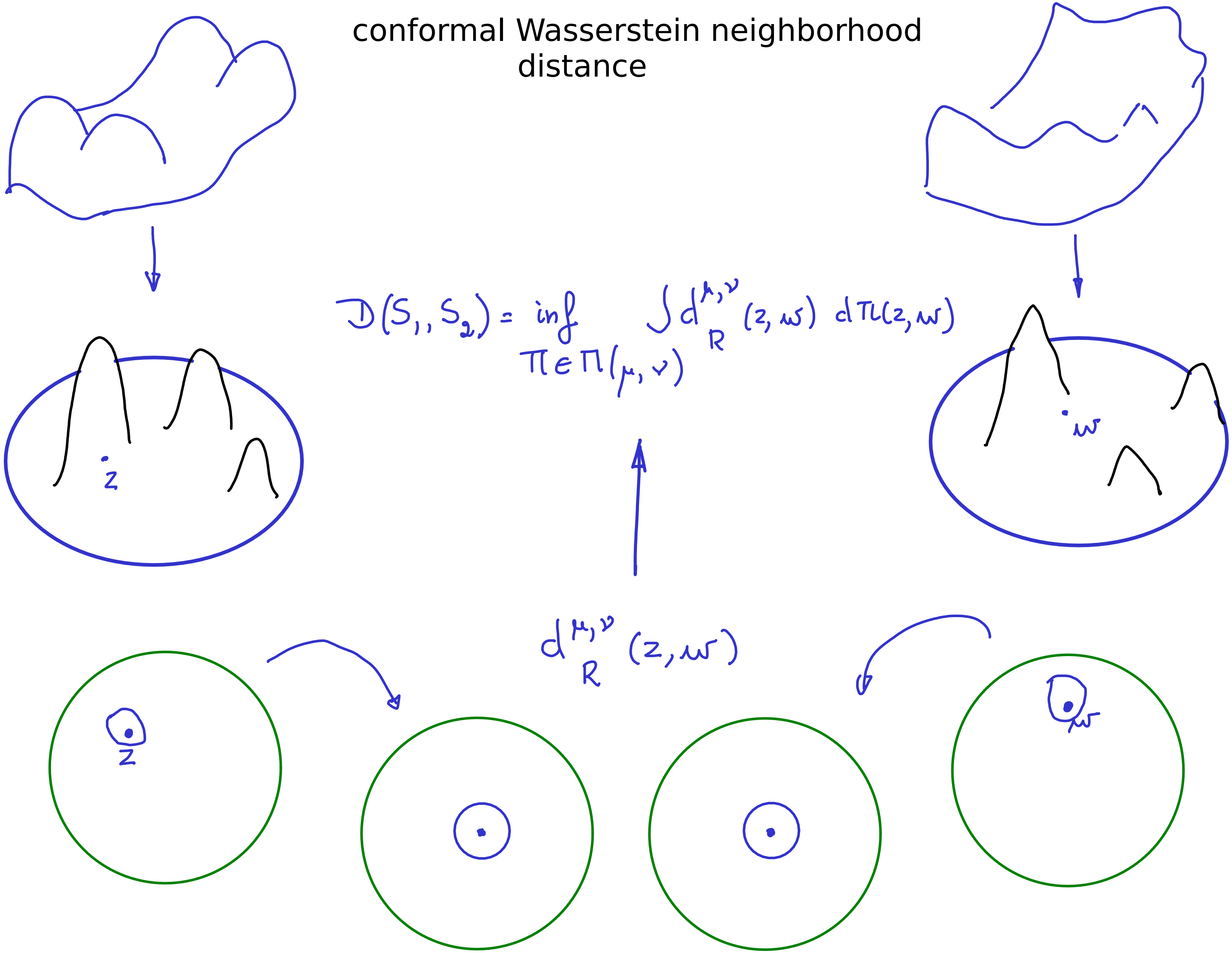


$$D(S_1, S_2) = \inf_{\pi \in \Pi(\mu,\nu)} \int d_R^{\mu,\nu}(z,w)\, d\pi(z,w)$$





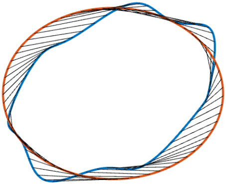
conformal Wasserstein neighborhood distance



Continuous Procrustes Distance (cPD)

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

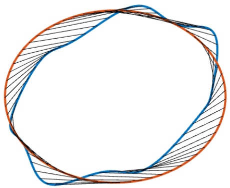
where $\mathcal{C} : S_1 \to S_2$ is an area-preserving diffeomorphism.

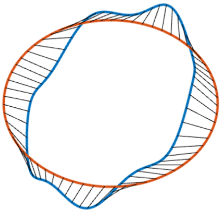


Continuous Procrustes Distance (cPD)

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

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

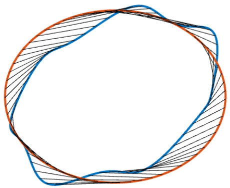
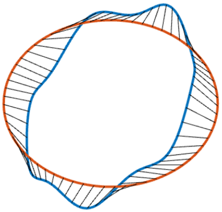
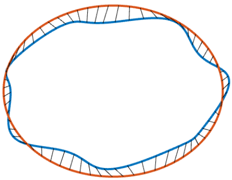




Continuous Procrustes Distance (cPD)

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

where $\mathcal{A}\left(S_1, S_2\right)$ 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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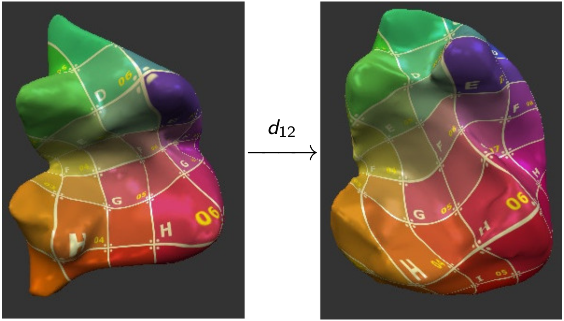
$$d_{cP}\left(S_1, S_2\right) = \inf_{\mathcal{C}\in\mathscr{A}} \inf_{R\in\mathbb{E}_3} \left(\int_{S_1} \| R(x) - \mathcal{C}(x) \|^2 \, d\mathrm{vol}_{S_1}(x) \right)^{1/2}$$



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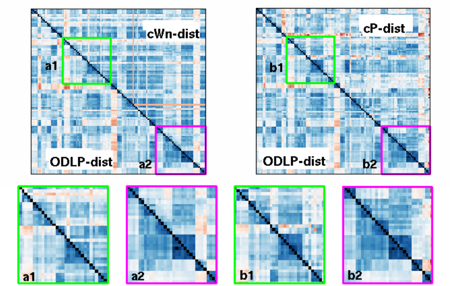
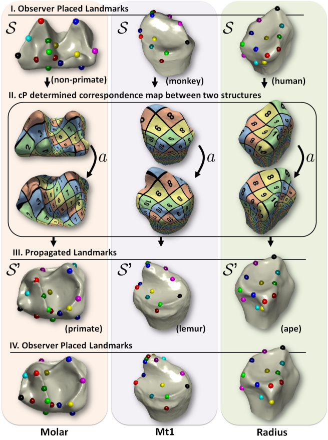
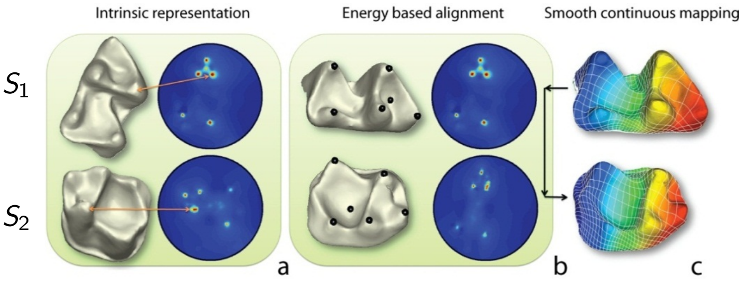
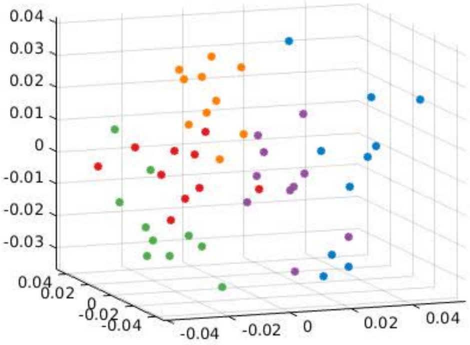




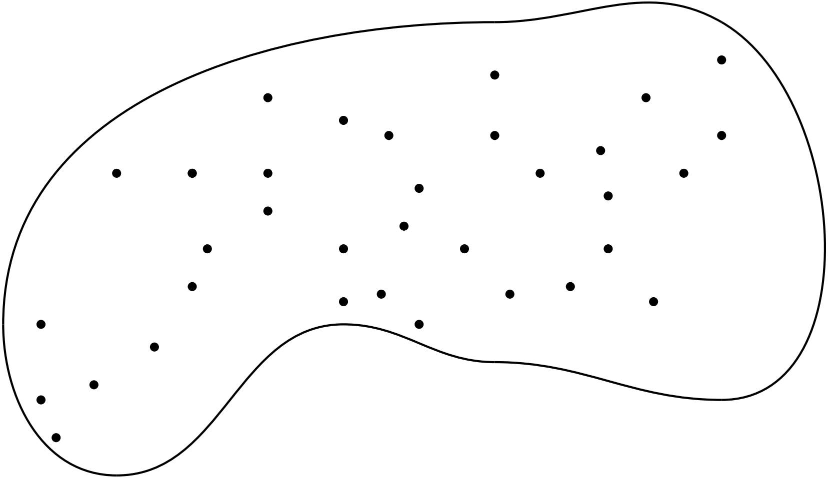
Bypass Explicit Feature Extraction



Multi-Dimensional Scaling (MDS) for cPD Matrix

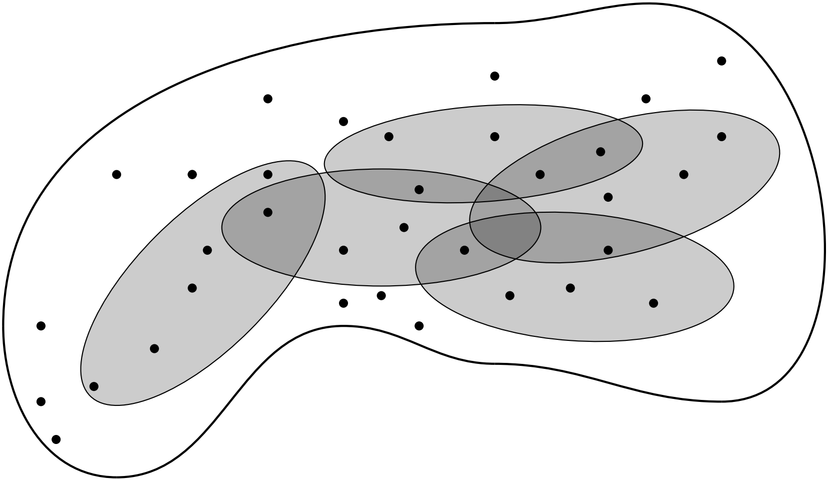


Diffusion Maps: “Knit together” local geometry to get “better” distances



Small distances are much more reliable!

Diffusion Maps: “knitting together” local geometry



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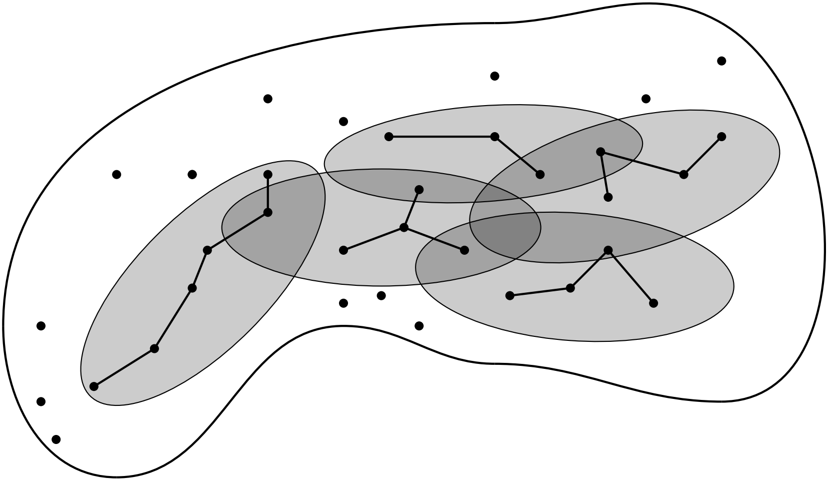

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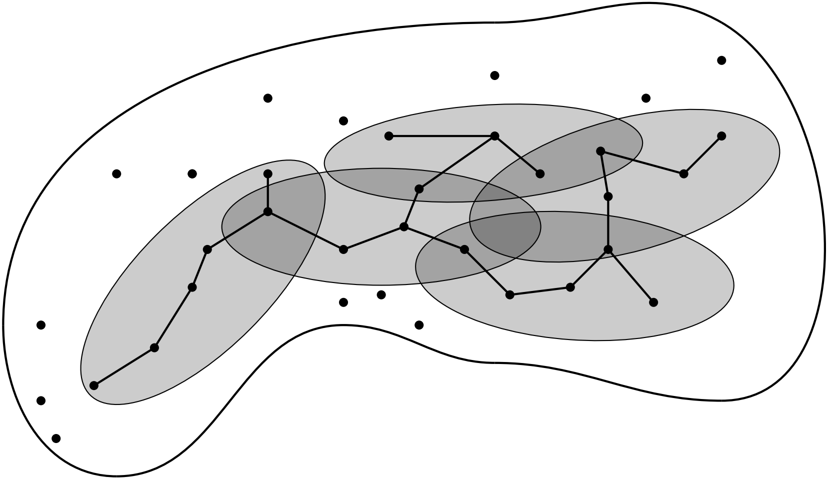

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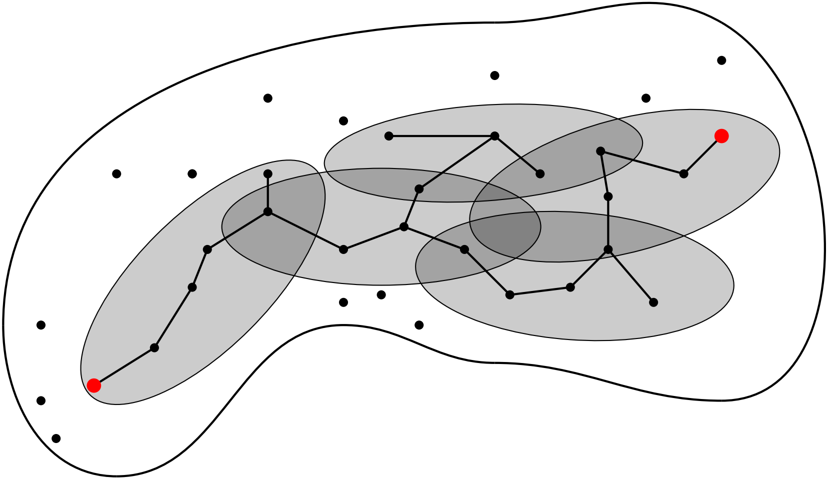

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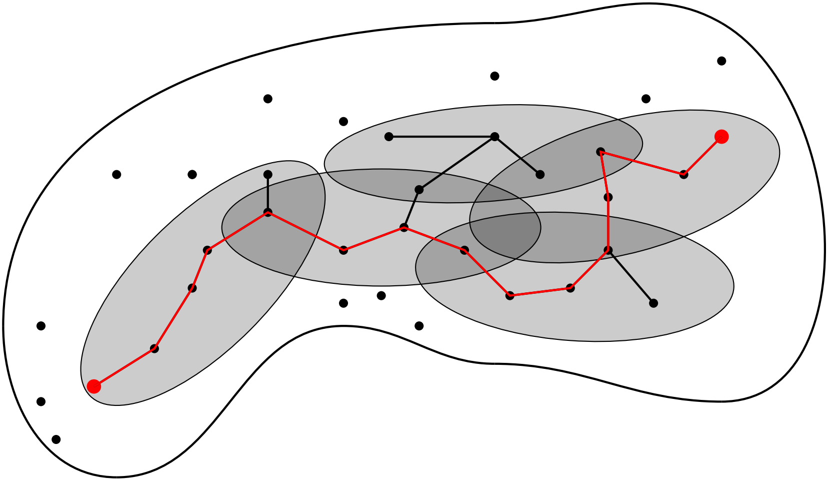

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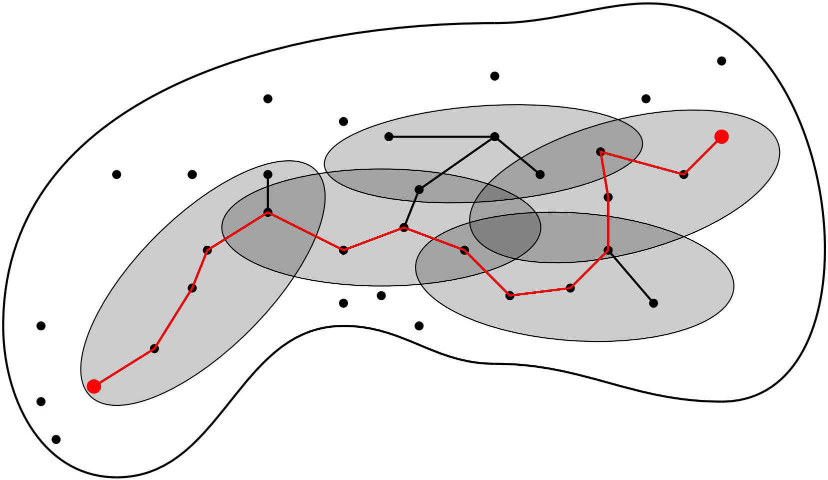

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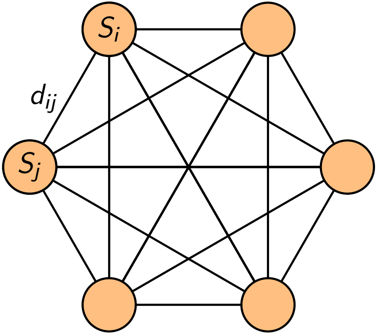

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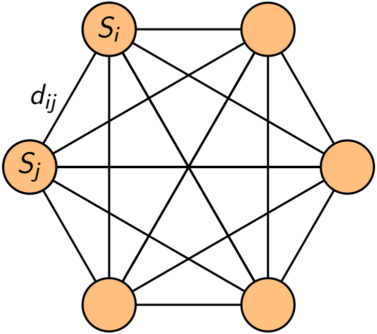

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- Solve eigen-problem

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

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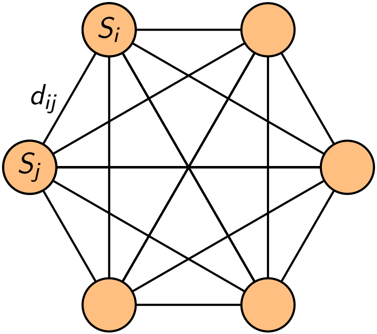

- $P = D^{-1}W$ defines a random walk on the graph
- Solve eigen-problem

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

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

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

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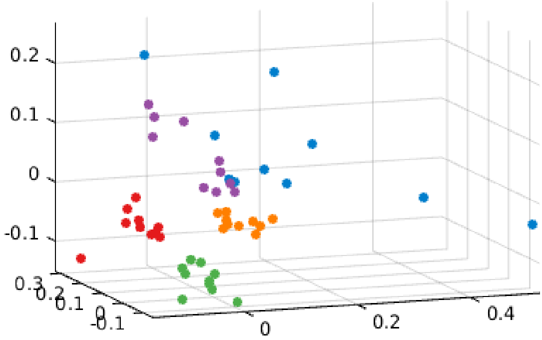
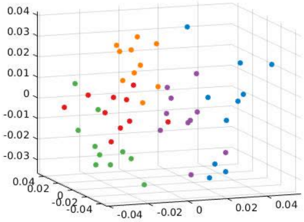
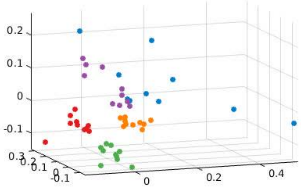


MDS for cPD & DD

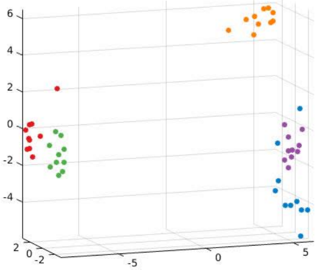


cPD

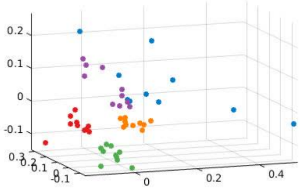


DD

Even better can be obtained!

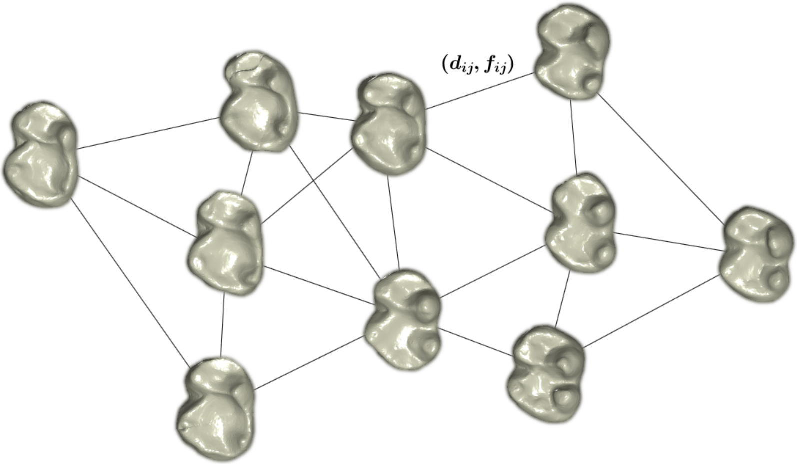


HBDD



DD

to get Diffusion Distance : used local distances
knitted together
→ spectral parametrization
→ distance.


(d_{ij}, f_{ij})

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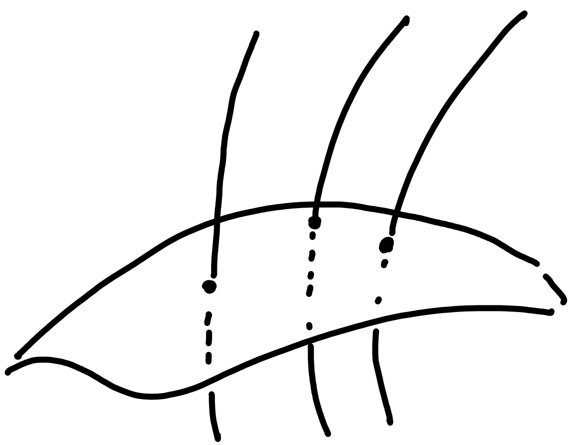
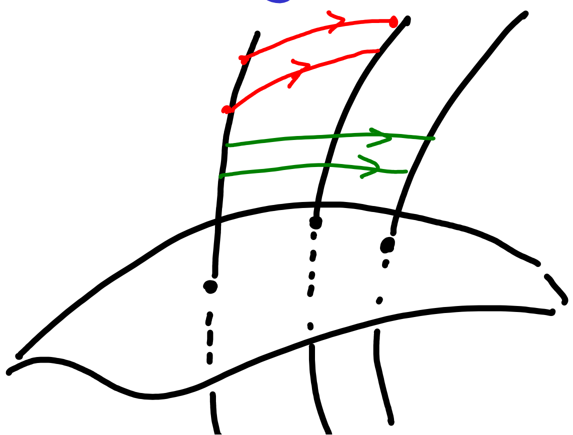
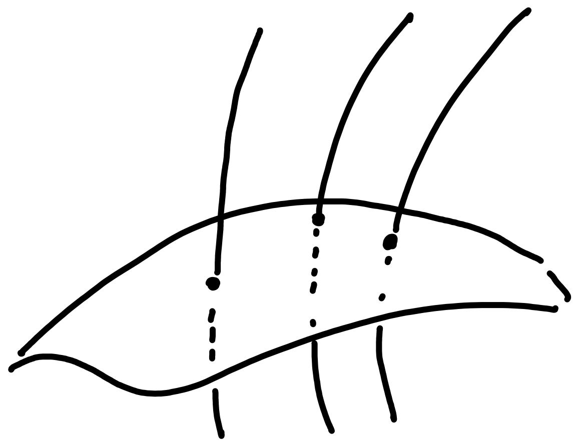
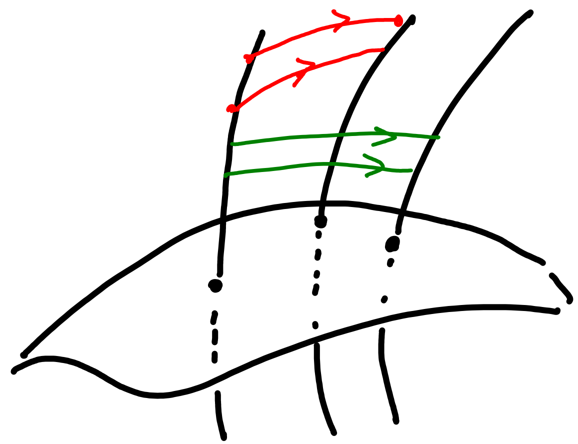




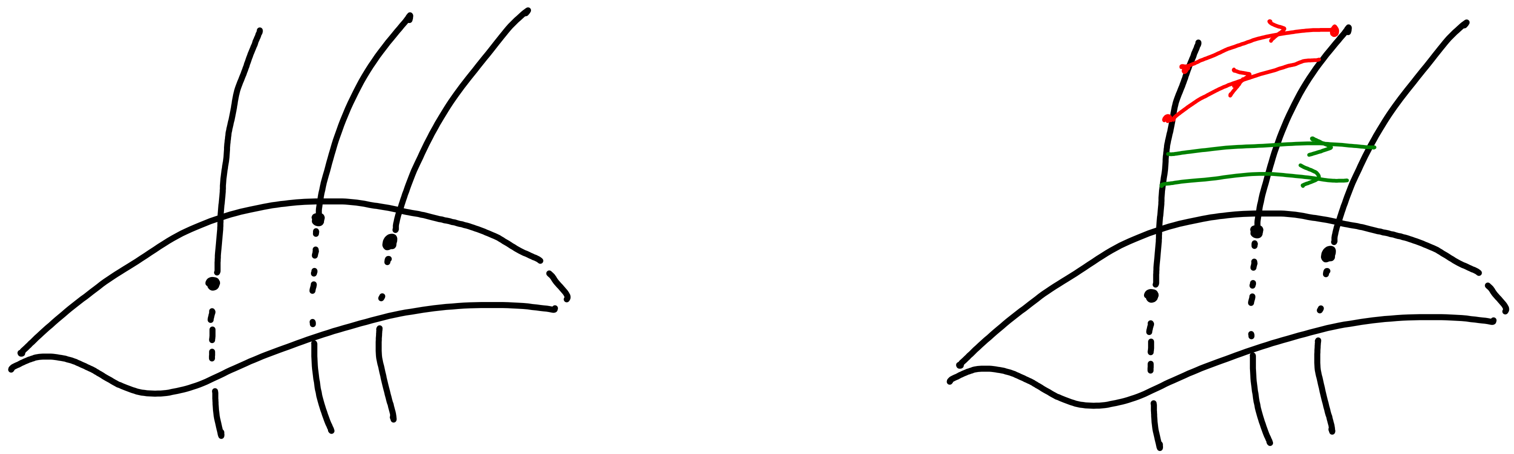




Connection.

↓

family of mappings between fibers



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

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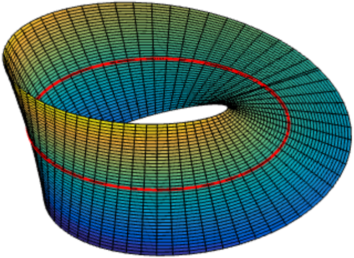

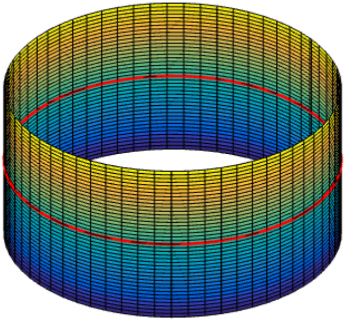

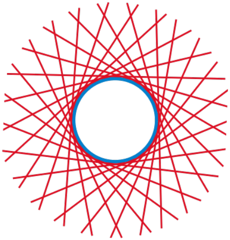

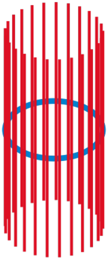

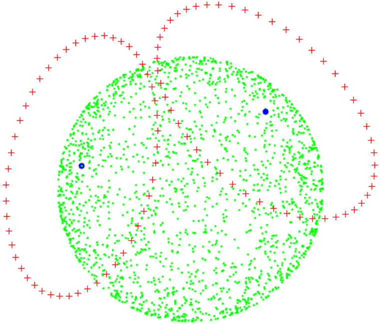

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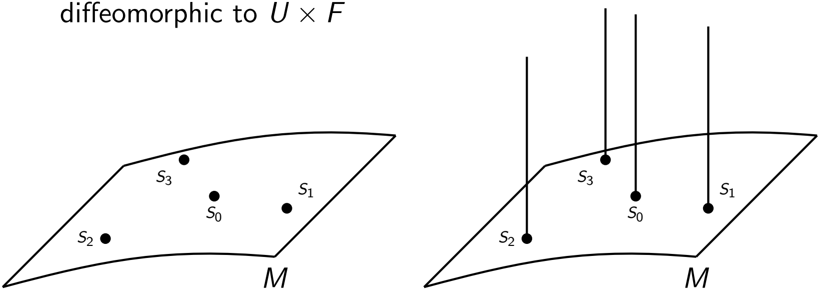

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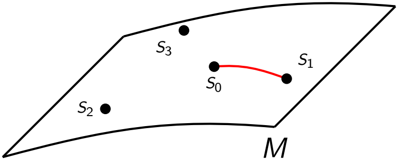

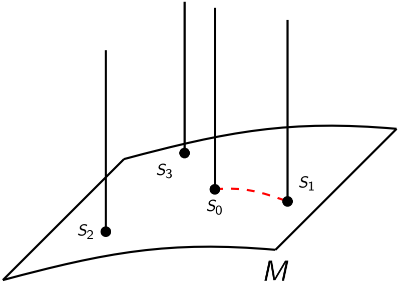

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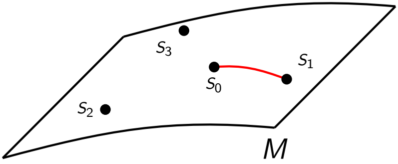

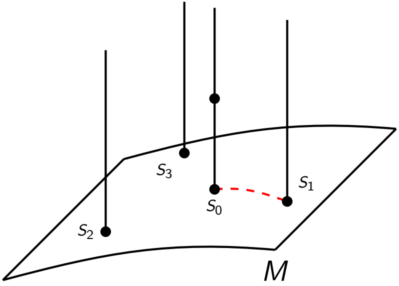

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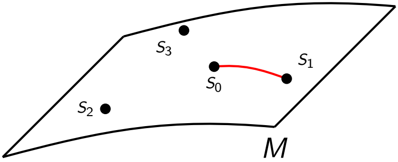

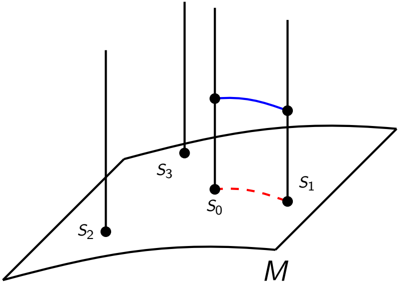

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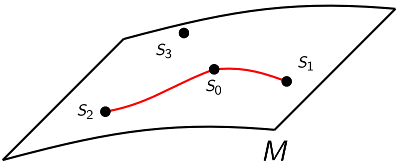

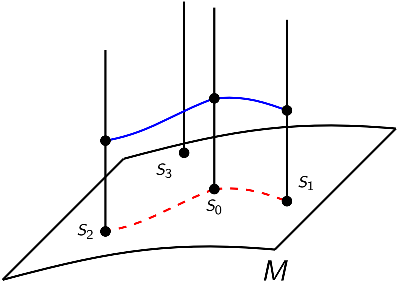

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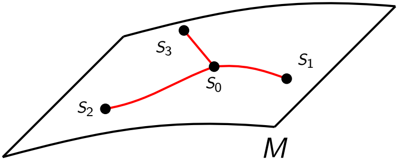
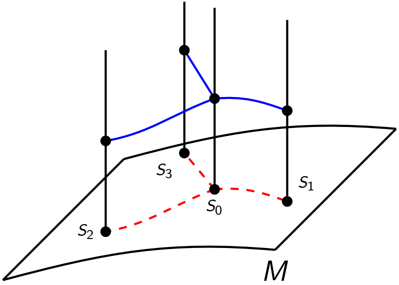
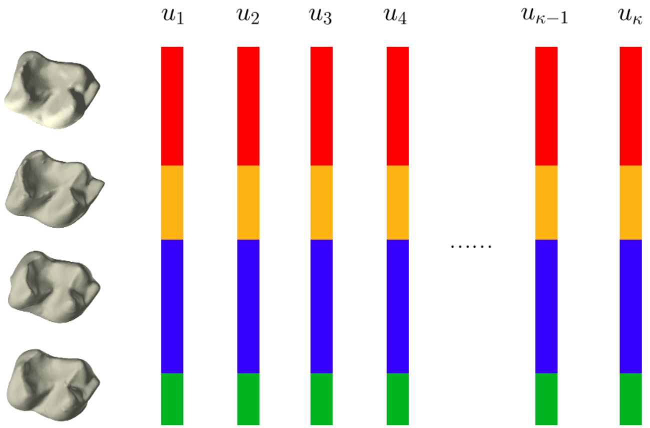




Horizontal Diffusion Maps: Embedding the Entire Bundle



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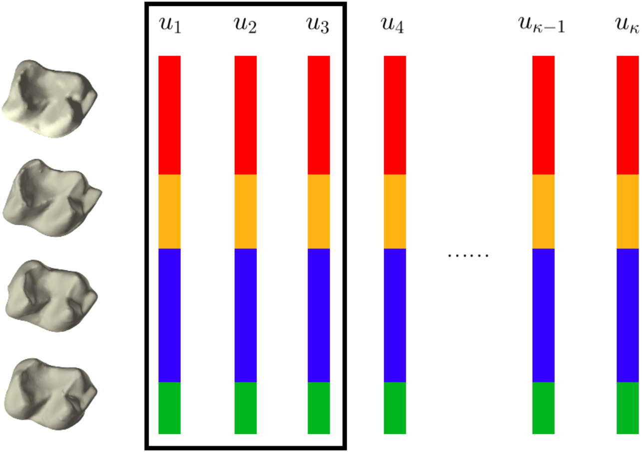

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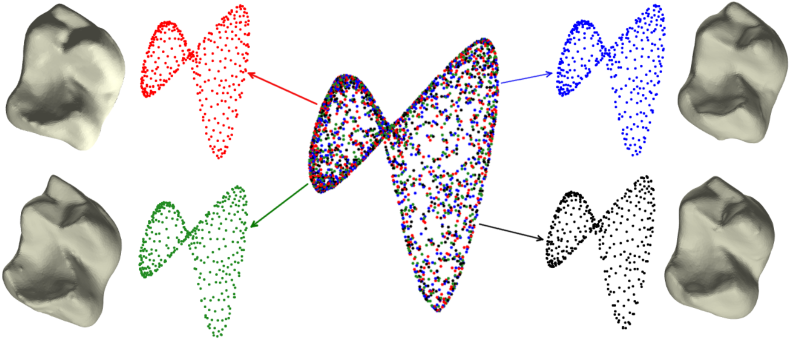
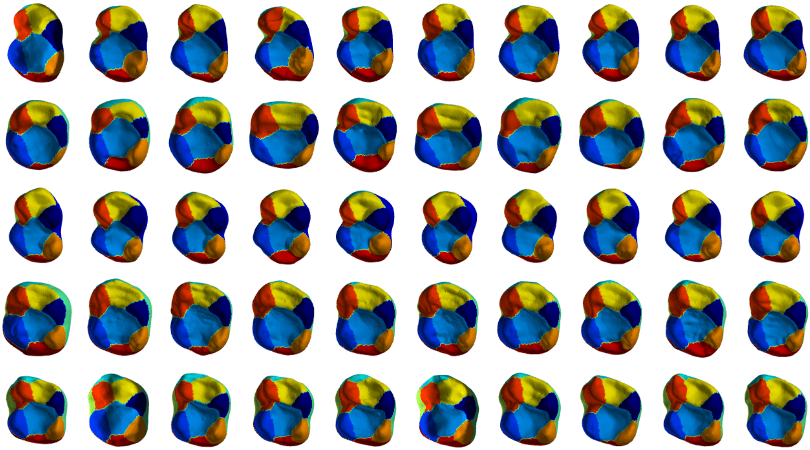
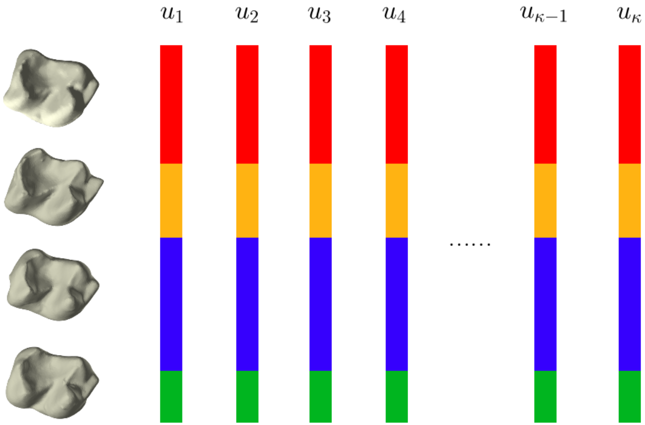


Automatic Landmarking — Interpretability



Horizontal Diffusion Maps: Embedding the Base Manifold



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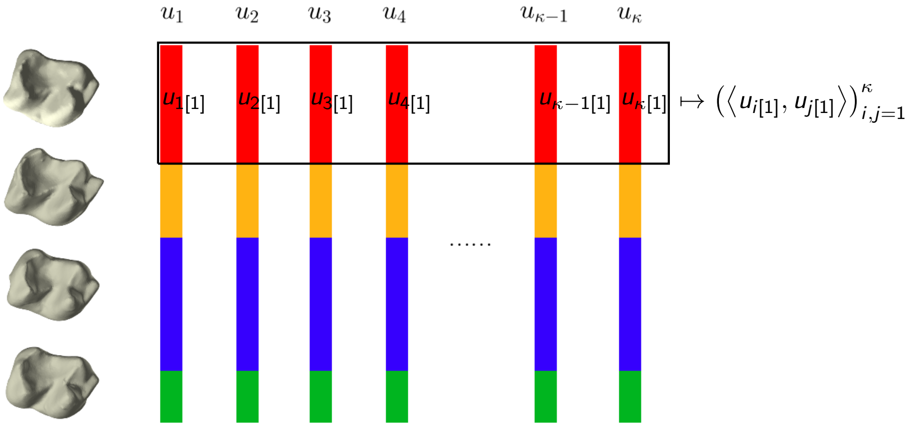

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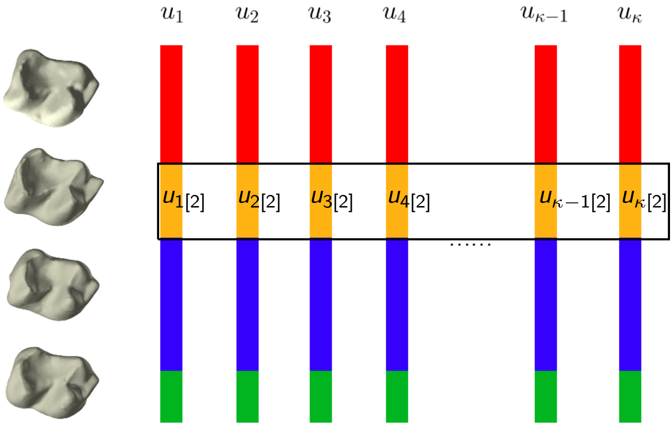

$$\mapsto \left(\left\langle u_{i[2]}, u_{j[2]} \right\rangle\right)_{i,j=1}^{\kappa}$$

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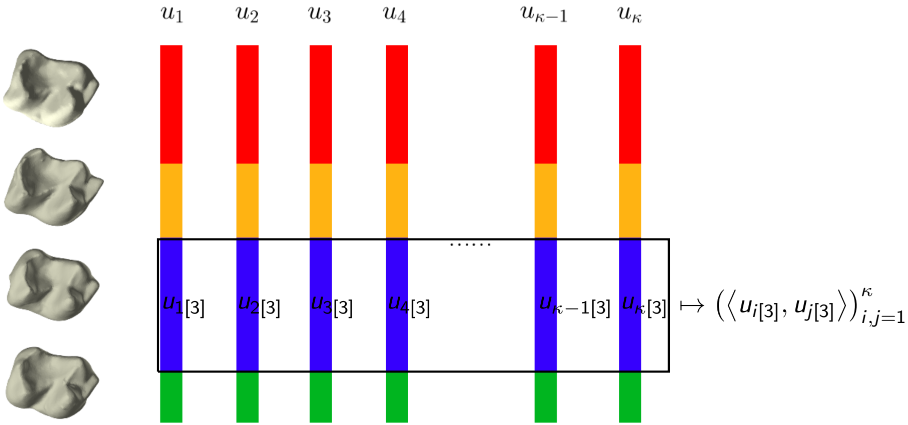

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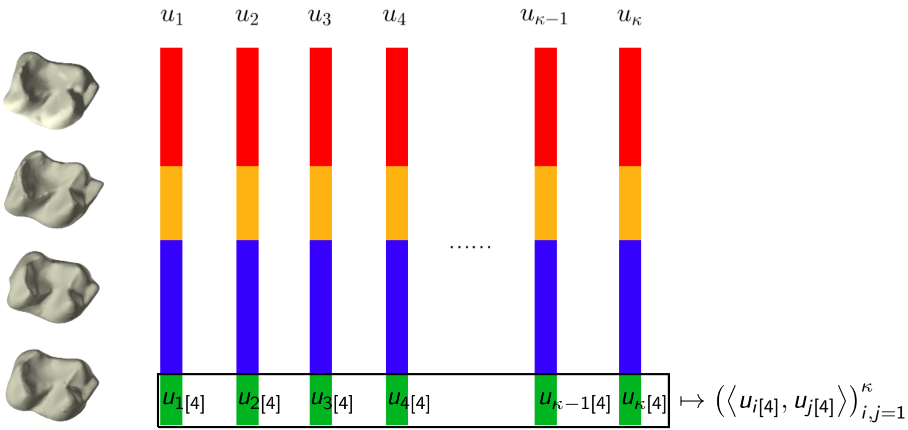
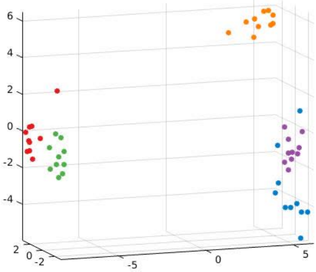
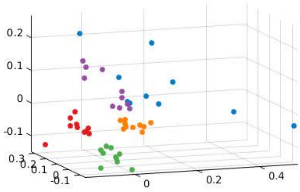


Species Clustering



Horizontal Base Diffusion Distance (with Maps)



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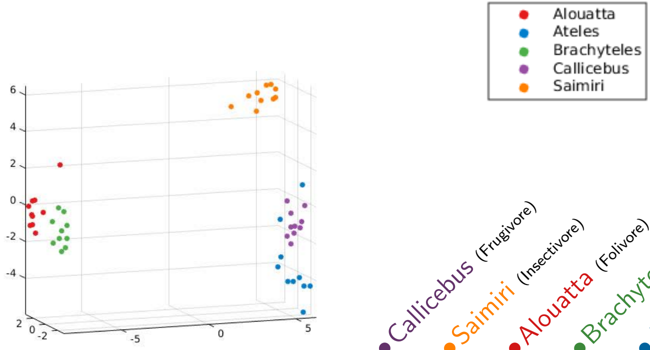

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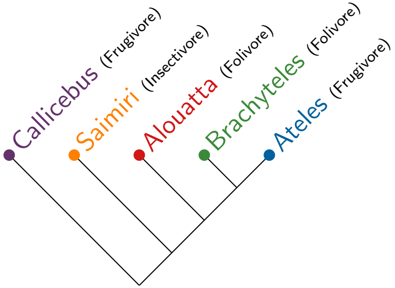

spectral coordinates for points in fiber bundle:

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

j ↔ S_j

p ← pt p on S_j

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j: S_j

p: pt p on S_j

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

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

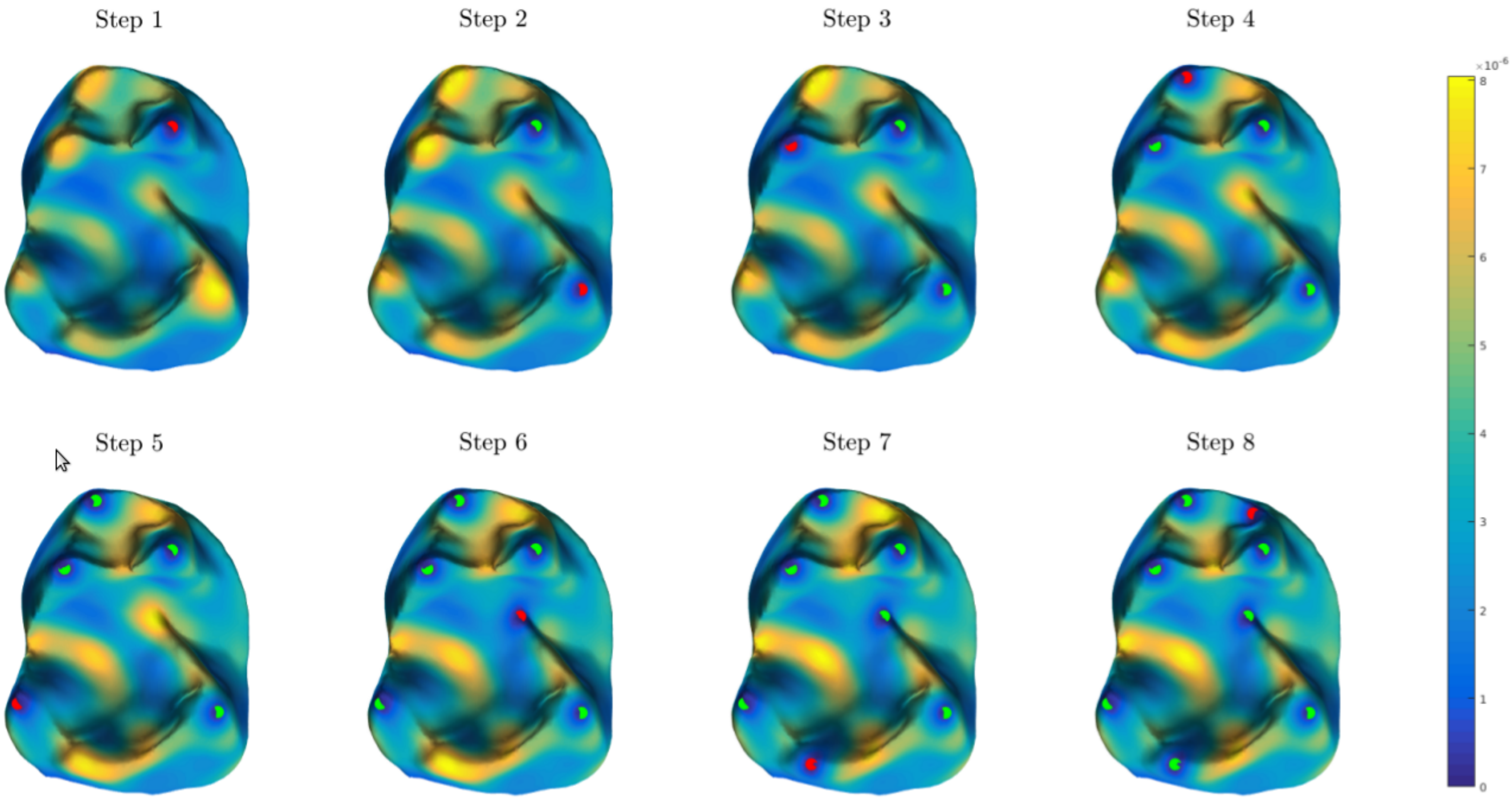
j ↝ S_j; p ← pt p on S_j

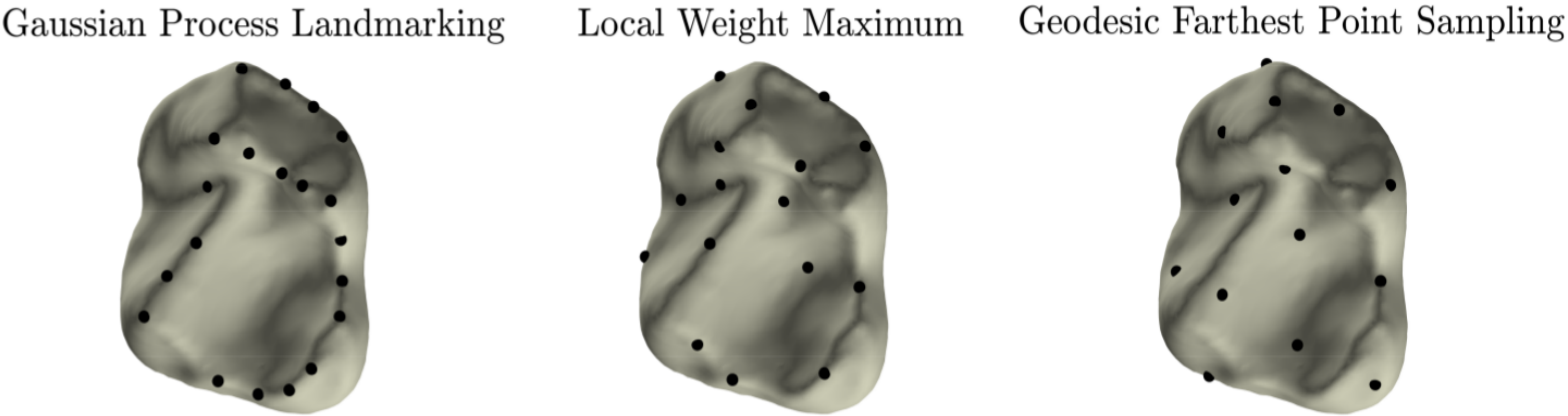
↓ "project" to geometry on base manifold

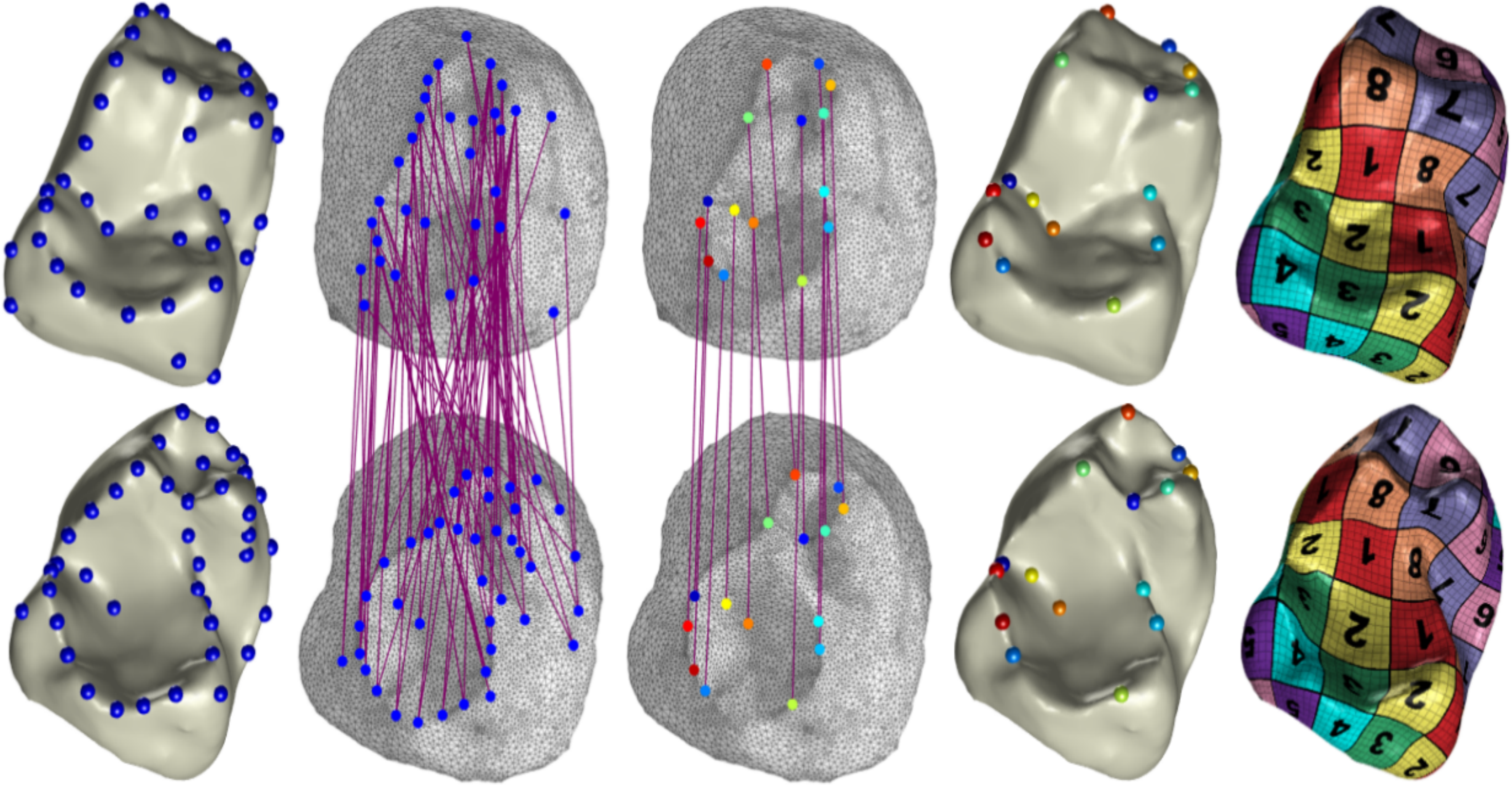
hor. dist (S_i, S_j)

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

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


Step 1
Step 2
Step 3
Step 4
Step 5
Step 6
Step 7
Step 8
×10^-6
8
7
6
5
4
3
2
1
0


Gaussian Process Landmarking
Local Weight Maximum
Geodesic Farthest Point Sampling



(a) (b) (c) (d) (e)

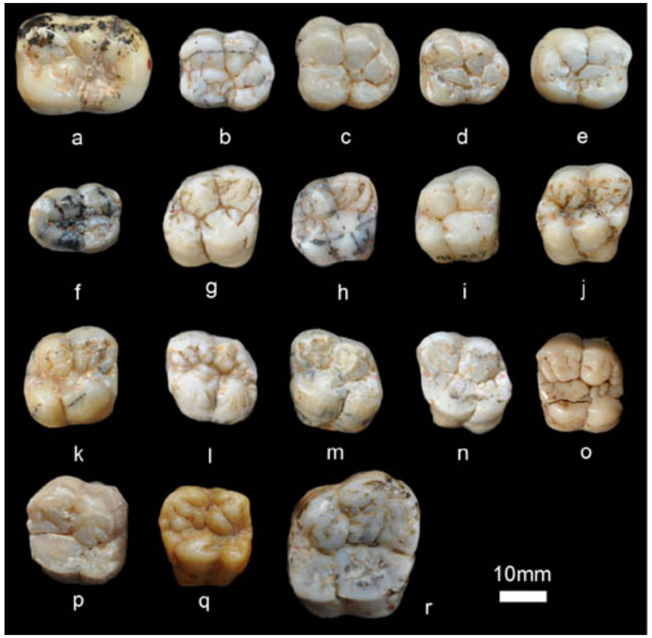

Source
GP-BD
0.096
0.059
0.083
CPM
0.185
0.092
0.099
(a)
(b)
(c)

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