

Machine Learning, Fibre Bundles and Biological Morphology

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What this talk is about

Background

- ▶ motivation: morphometrics
- ▶ previous work: continuous Procrustes distance

Learning from Correspondences

- ▶ diffusion geometry
- ▶ fibre bundles
- ▶ horizontal random walks

Results

- ▶ biological applications
- ▶ mathematical theory

Collaborators



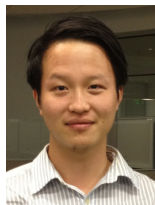
Rima Alaifari
ETH Zürich



Doug Boyer
Duke



Ingrid Daubechies
Duke



Tingran Gao
Duke



Yaron Lipman
Weizmann



Roi Poranne
ETH Zürich



Jesús Puente
J.P. Morgan



Robert Ravier
Duke

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

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

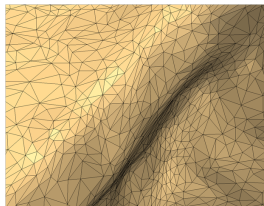
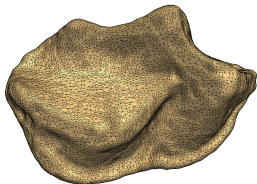


Landmarked Teeth \longrightarrow

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

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

Examples: finely discretized triangulated surfaces

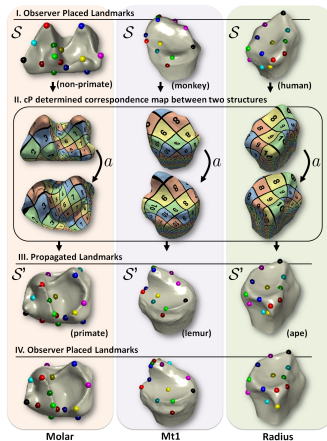
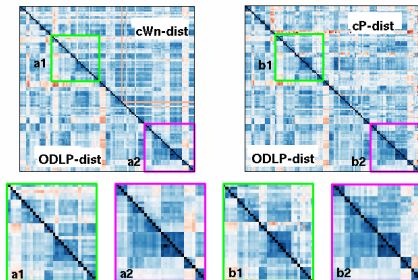


We defined 2 different distances

$d_{cWn}(S_1, S_2)$: conformal flattening
 comparison of neighborhood geometry
 optimal mass transport

$d_{cP}(S_1, S_2)$: continuous Procrustes distance

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

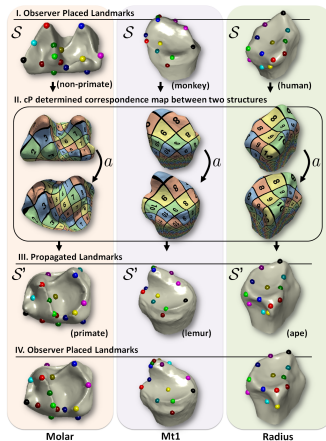


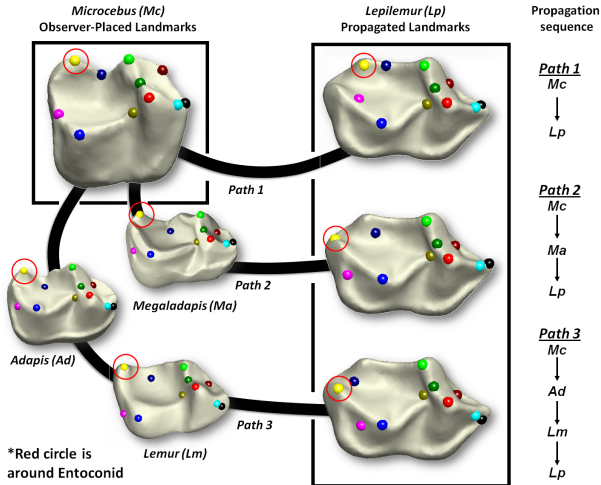
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Even mistake made by d_{CP} were similar to biologists' mistakes

small distances between $S_1, S_2 \rightarrow$ OK maps
larger distances \rightarrow not OK

Biologists' "wish list" changed...

... as they learned our language and saw our methods

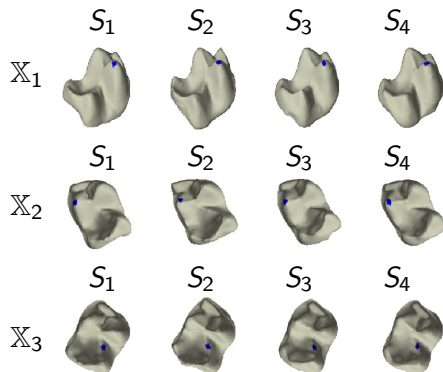
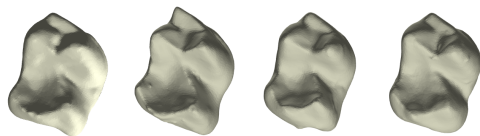
- ▶ **mappings** more important to them than distances
(\rightarrow discussion of variability in individuals or between species, locally)
- ▶ no *holonomy!*

Our formulation of problem changed too

Tingran Gao \rightarrow reformulate as connection on fibre bundle
+ horizontal diffusion

Even before this...

biological content in large concatenated matrix



$$\begin{aligned} \min \quad & \|M\mathbb{X} - \mathbb{X}\|_2^2 + \lambda \|\mathbb{X}\|_1 \\ \text{s.t.} \quad & \|\mathbb{X}\|_2 = 1. \end{aligned}$$

Resulting minimizers \mathbb{X}
supported on union of 4
surfaces

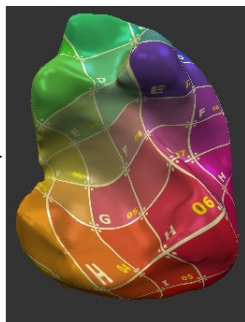
Use the Information in the Maps!

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

S_1



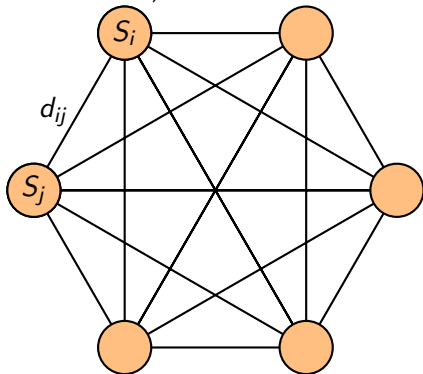
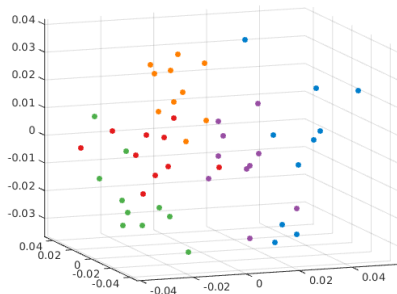
$\xrightarrow[\quad f_{12}]{d_{12}}$



S_2

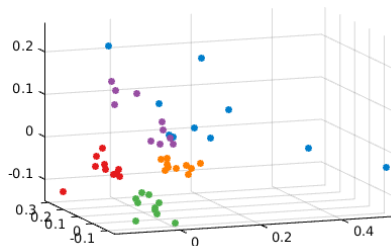
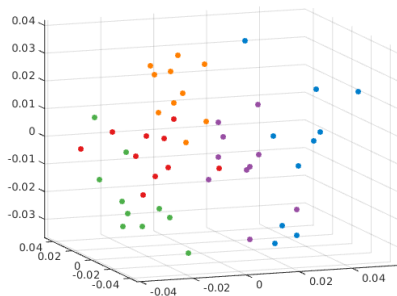
Learning from Distances

$$\begin{pmatrix} d_{11} & d_{12} & \cdots & d_{1N} \\ d_{21} & d_{22} & \cdots & d_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ d_{N1} & d_{N2} & \cdots & d_{NN} \end{pmatrix}$$



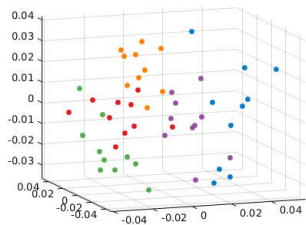
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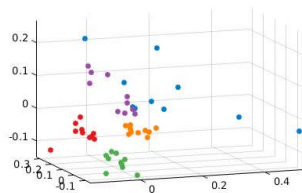


Diffusion Distance

MDS for CPD & DD

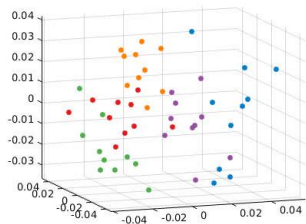


CPD

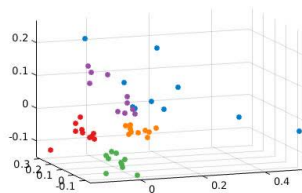


DD

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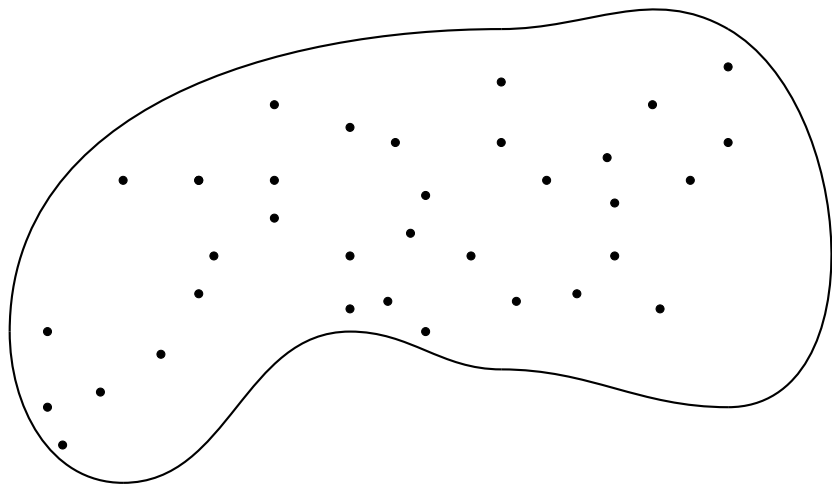


CPD

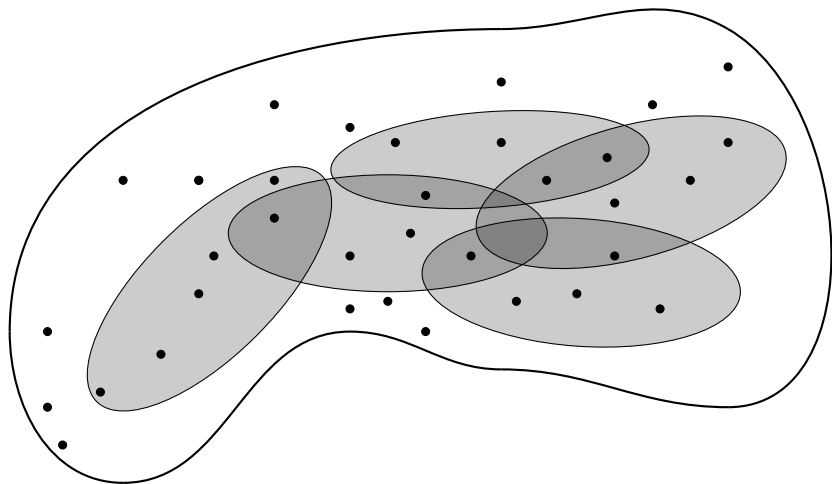


DD

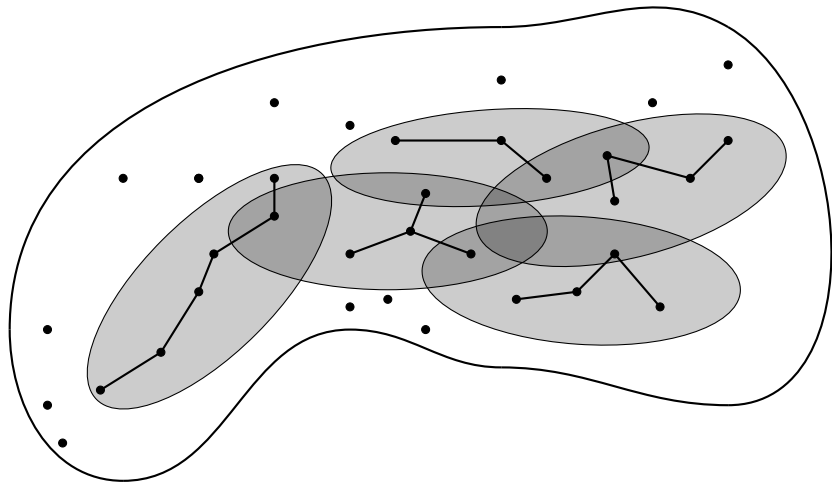
Diffusion Maps: “Knit Together” Local Geometry



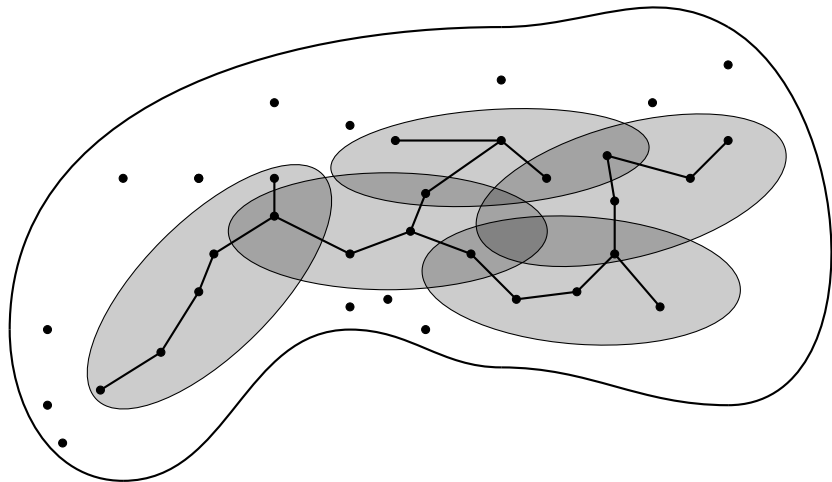
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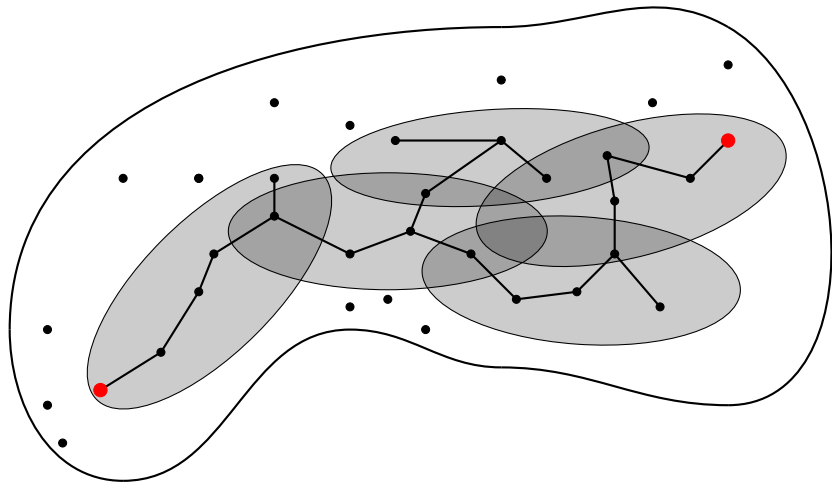
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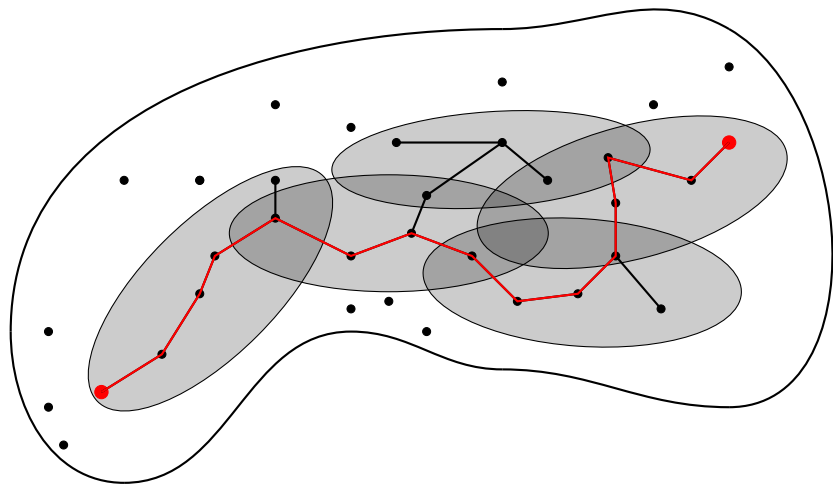
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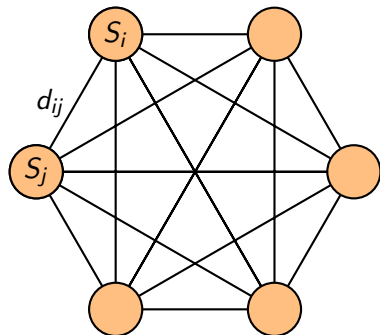


Diffusion Maps: “Knit Together” Local Geometry



Small distances are much more reliable!

Diffusion Maps: “Knit Together” Local Geometry



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

$$Pu_j = \lambda_j u_j, \quad j = 1, 2, \dots, m$$

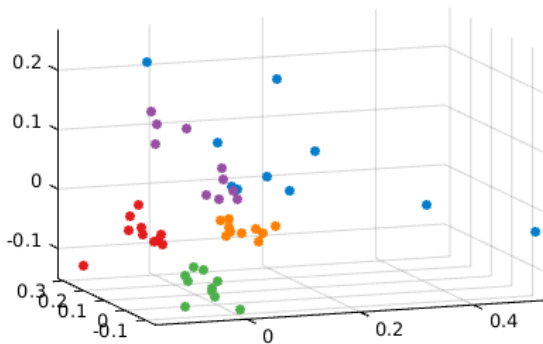
and represent each individual shape S_j as an m -vector

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

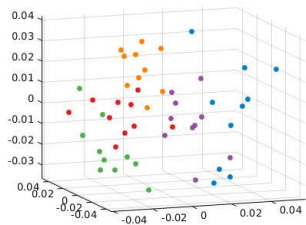
Diffusion Distance (DD)

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

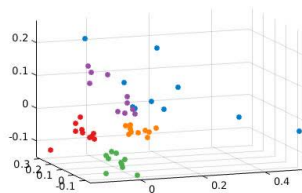
$$D_m^t(S_i, S_j) = \left(\sum_{k=1}^m \lambda_k^t (u_k(i) - u_k(j))^2 \right)^{\frac{1}{2}}$$



MDS for CPD & DD

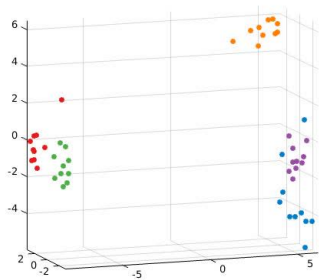


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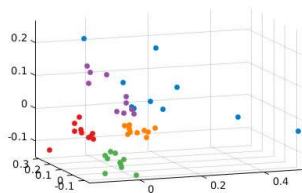


DD

Even Better: More Information!

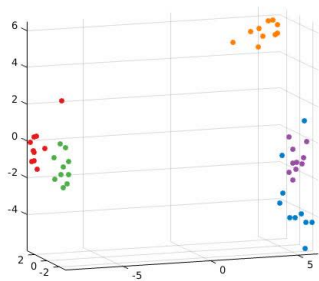


HBDD

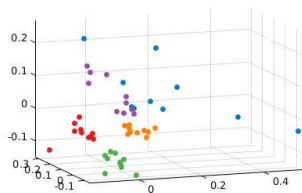


DD

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HBDD



DD

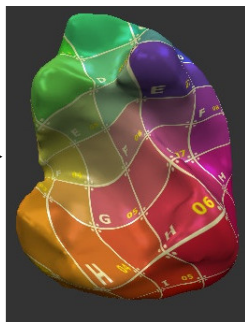
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S_1

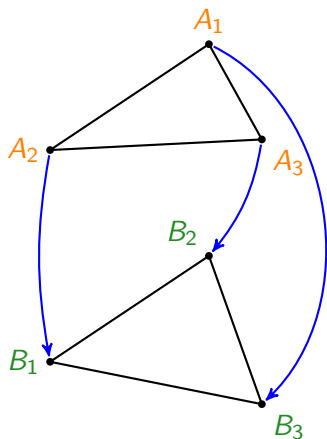


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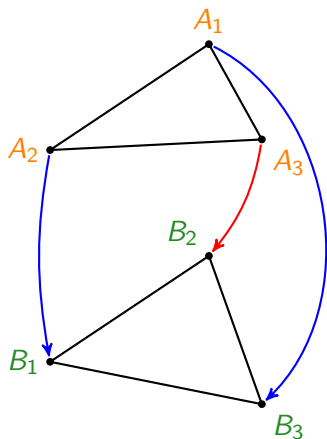
S_2

Correspondences Between Triangular Meshes



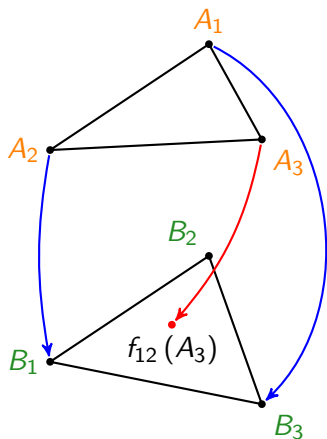
$$S_1 \begin{matrix} \vdots \\ A_1 \\ A_2 \\ A_3 \\ \vdots \end{matrix} \begin{matrix} \xrightarrow{S_2} \\ \dots & B_1 & B_2 & B_3 & \dots \\ \left(\begin{array}{ccccc} \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & 0 & 0 & 1 & \dots \\ \dots & 1 & 0 & 0 & \dots \\ \dots & 0 & 1 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{array} \right) \end{matrix}$$

Correspondences Between Triangular Meshes



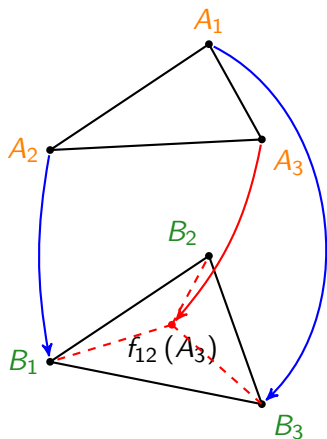
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Correspondences Between Triangular Meshes



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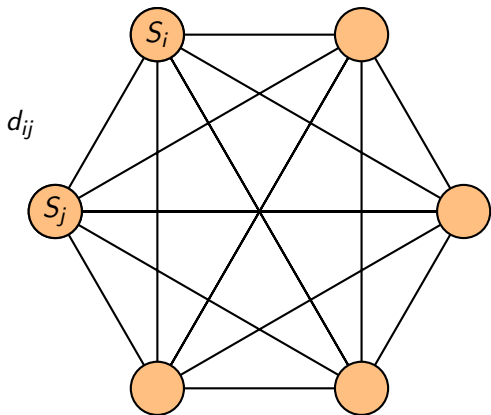
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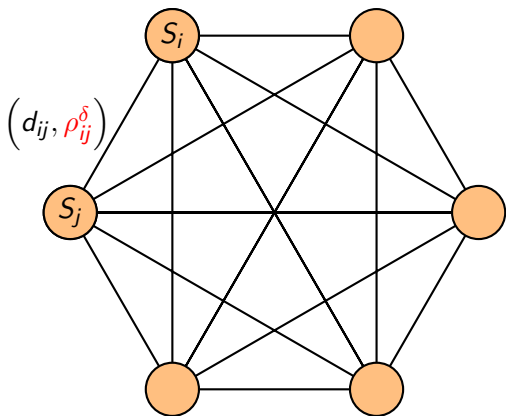
$$S_1 \downarrow \begin{matrix} \vdots \\ A_1 \\ A_2 \\ A_3 \\ \vdots \end{matrix} \left(\begin{array}{cccc} & \xrightarrow{S_2} & & & \\ \cdots & B_1 & B_2 & B_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \\ \cdots & 0 & 0 & 1 & \cdots \\ \cdots & 1 & 0 & 0 & \cdots \\ \cdots & \boxed{0.91} & \boxed{0.95} & \boxed{0.88} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{array} \right)$$

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

Distance Graph



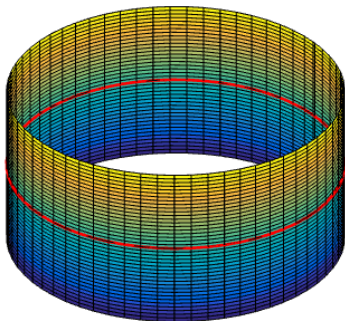
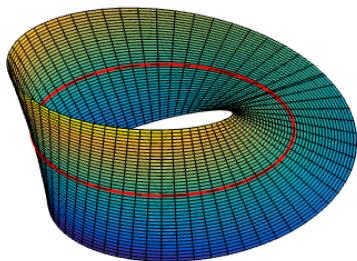
Augmented Distance Graph



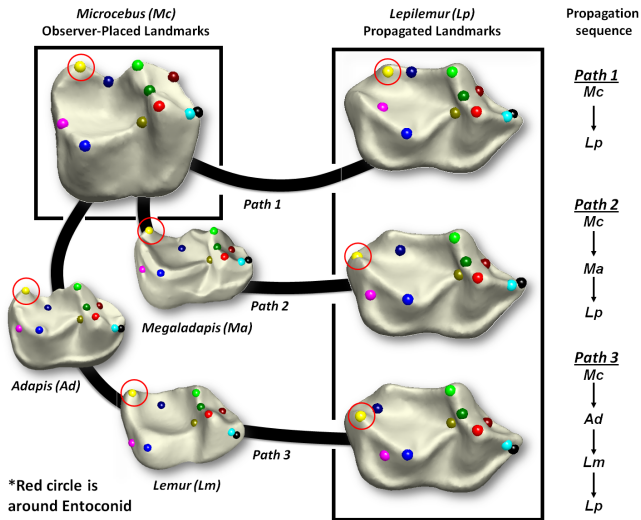
Horizontal Random Walk on a Fibre Bundle

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
- ▶ *local triviality*: for "small" open set $U \subset M$, $\pi^{-1}(U)$ is diffeomorphic to $U \times F$



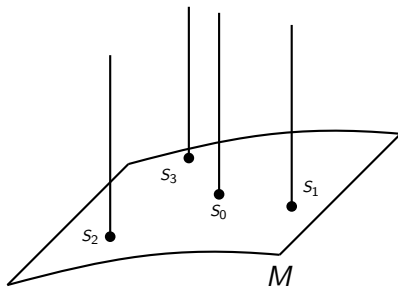
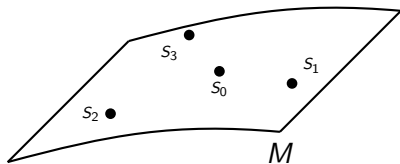
Shape Space is NOT a Trivial Fibre Bundle



Horizontal Random Walk on a Fibre Bundle

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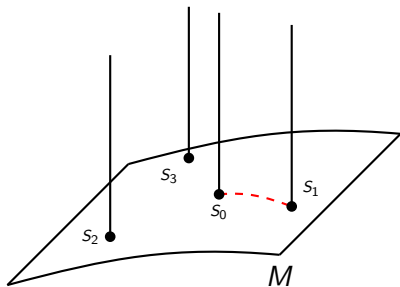
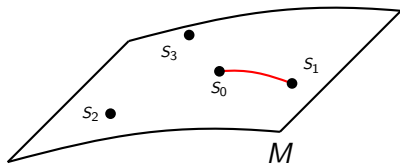
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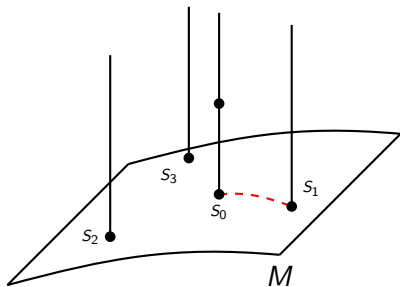
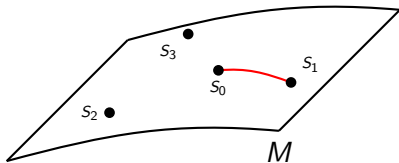
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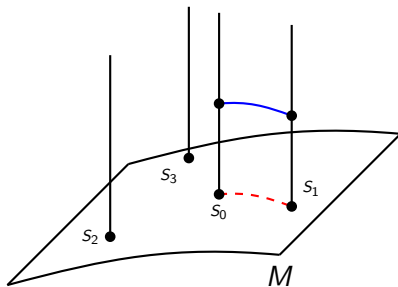
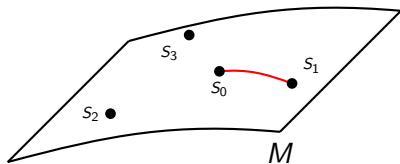
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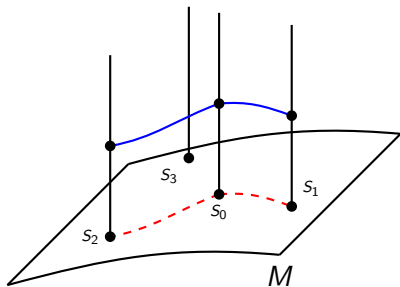
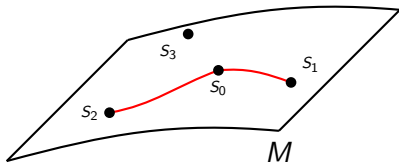
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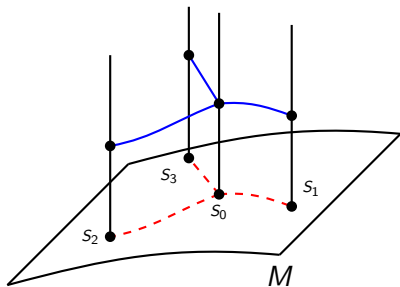
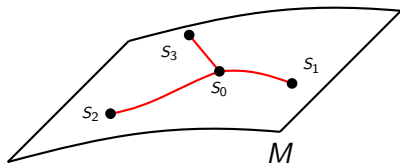
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Towards *Horizontal* Diffusion Maps

Diffusion Maps

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

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

Towards *Horizontal* Diffusion Maps

Horizontal Diffusion Maps

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

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

Towards *Horizontal* Diffusion Maps

Horizontal Diffusion Maps

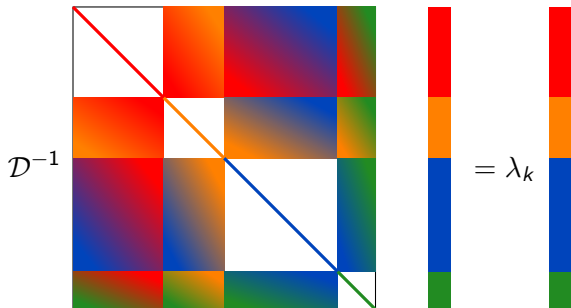
$$\mathcal{D}^{-1}\mathcal{W}u_k = \lambda_k u_k, \quad 1 \leq k \leq \kappa$$

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

Towards *Horizontal* Diffusion Maps

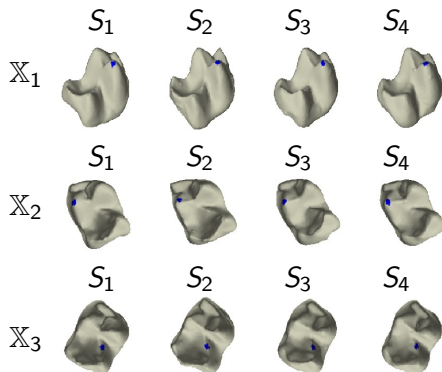
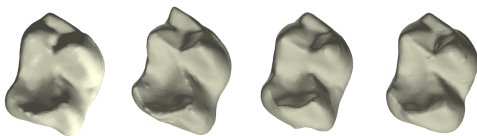
Horizontal Diffusion Maps

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



Even before this...

biological content in large concatenated matrix



$$\begin{aligned} \min \quad & \|M\mathbb{X} - \mathbb{X}\|_2^2 + \lambda \|\mathbb{X}\|_1 \\ \text{s.t.} \quad & \|\mathbb{X}\|_2 = 1. \end{aligned}$$

Resulting minimizers \mathbb{X}
supported on union of 4
surfaces

Towards *Horizontal* Diffusion Maps

Horizontal Diffusion Maps

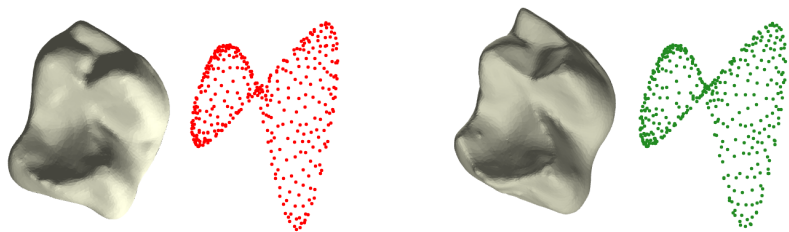
$$\mathcal{D}^{-1}\mathcal{W}u_k = \lambda_k u_k, \quad 1 \leq k \leq \kappa$$

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

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

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

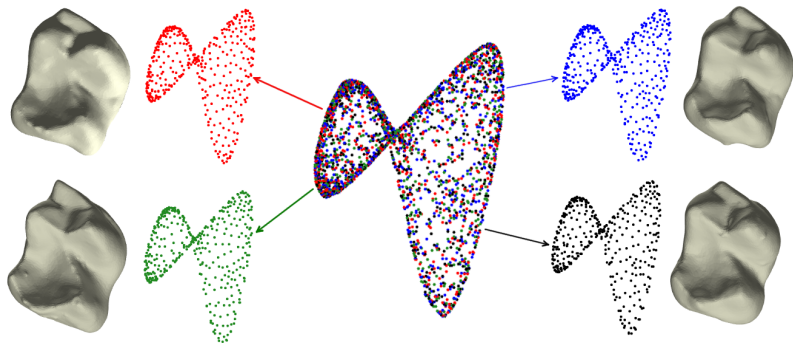
Horizontal Diffusion Maps



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

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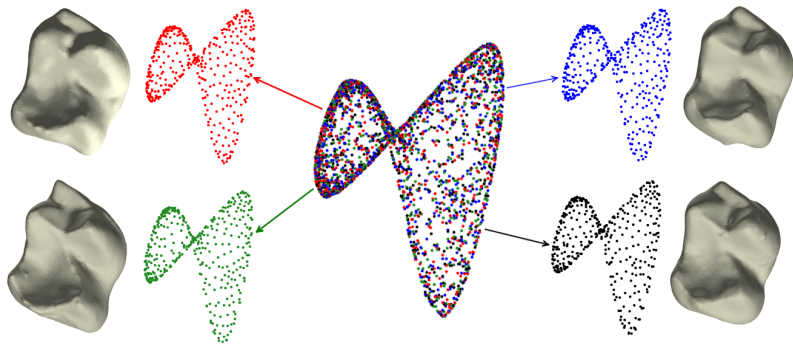
Horizontal Diffusion Maps



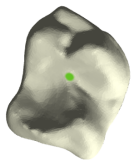
HDM: Application in Geometric Morphometrics

1. Global Registration
2. Automatic Landmarking
3. Species Classification

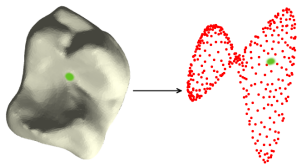
1. Global Registration



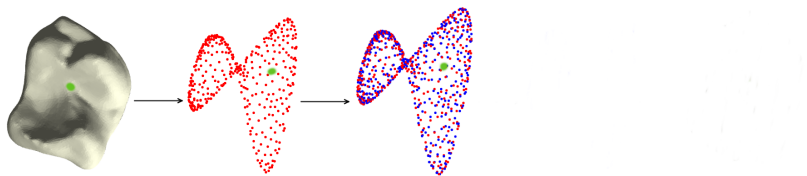
1. Global Registration



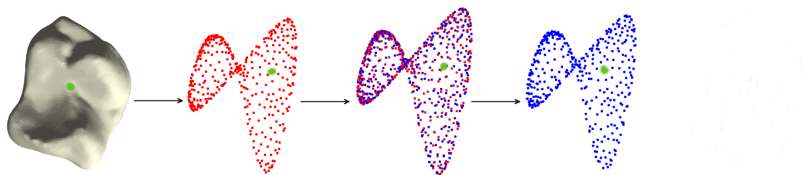
1. Global Registration



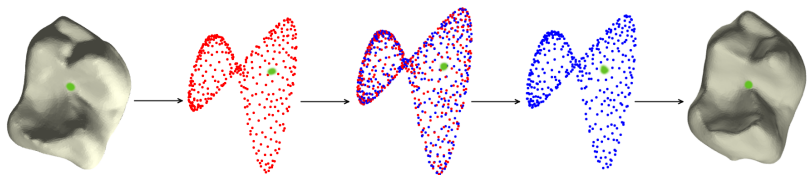
1. Global Registration



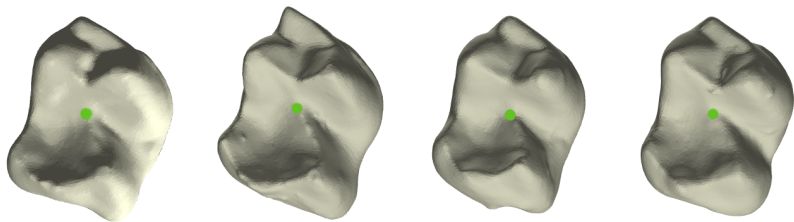
1. Global Registration



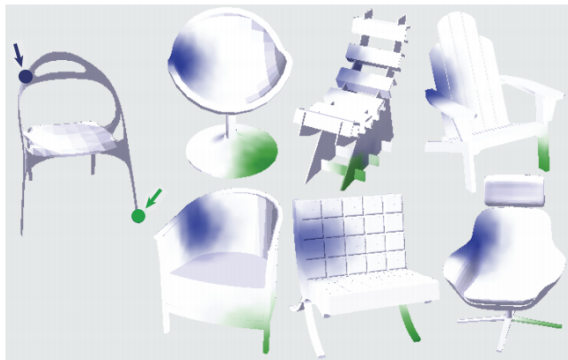
1. Global Registration



1. Global Registration

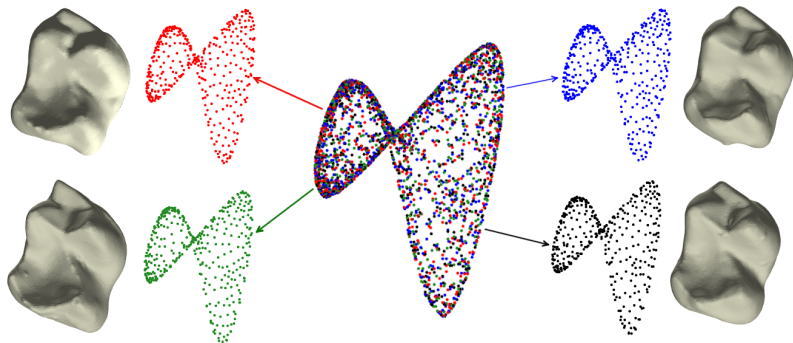


1. Global Registration: A Tool of Visual Exploration

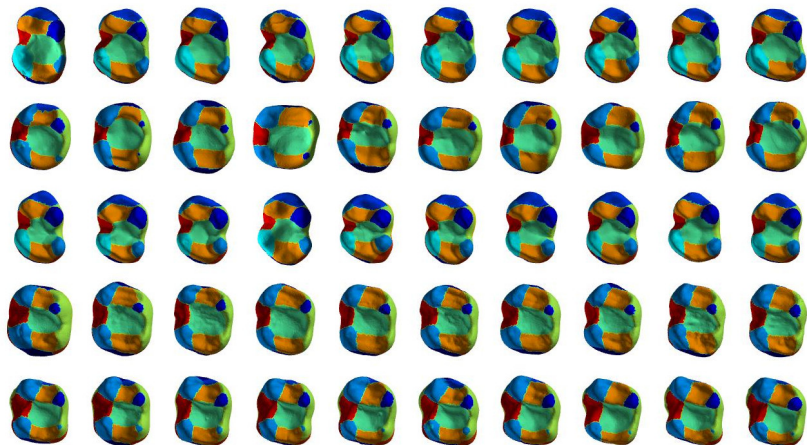


Kim et al. *Exploring Collections of 3D Models using Fuzzy Correspondences*. SIGGRAPH 2012.

2. Automatic Landmarking: *Spectral Clustering*



2. Automatic Landmarking: *Spectral Clustering*



3. Species Classification: HBDM & HBDD

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

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

Horizontal Base Diffusion Maps (HBDM): For fixed $1 \leq m \leq \kappa$, $t \geq 0$, represent S_j as a $\binom{m}{2}$ -dimensional vector

$$\left(\lambda_\ell^{t/2} \lambda_k^{t/2} \langle u_{\ell[j]}, u_{k[j]} \rangle \right)_{1 \leq \ell < k \leq m}$$

3. Species Classification: HBDM & HBDD

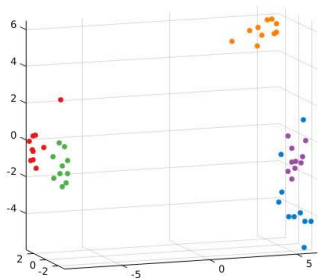
Horizontal Base Diffusion Distance (HBDD): For fixed $1 \leq m \leq \kappa$, $t \geq 0$,

$$D_{HB}^t(S_i, S_j) = \left(\sum_{1 \leq \ell < k \leq m} \lambda_\ell^t \lambda_k^t (\langle u_{\ell[i]}, u_{k[i]} \rangle - \langle u_{\ell[j]}, u_{k[j]} \rangle)^2 \right)^{\frac{1}{2}}$$

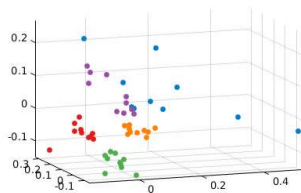
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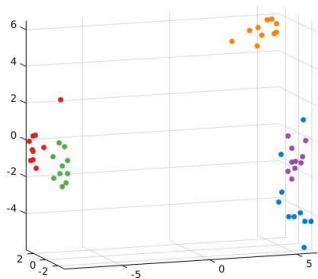


HBDD

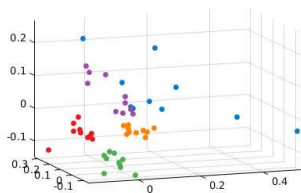


DD

3. Species Classification: HBDM & HBDD

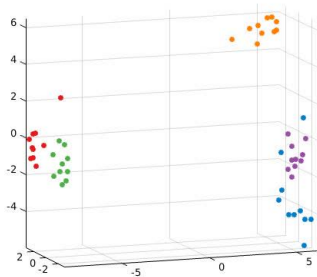


HBDD

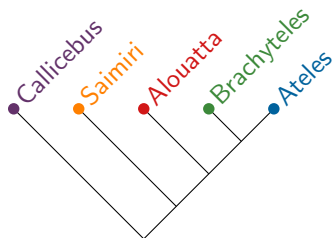


DD

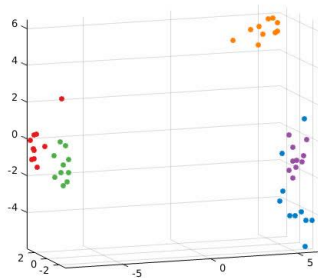
3. Species Classification: HBDM & HBDD



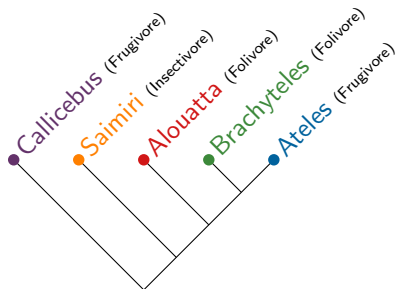
HBDD



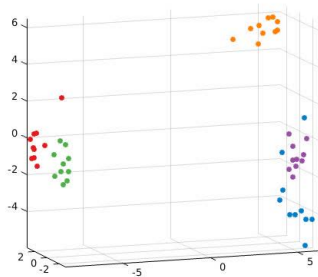
3. Species Classification: HBDM & HBDD



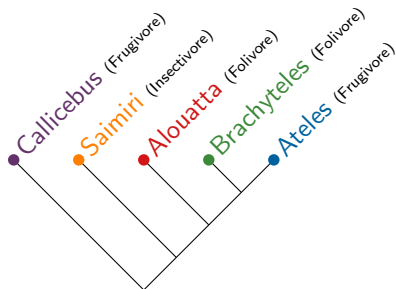
HBDD



3. Species Classification: HBDM & HBDD



HBDD

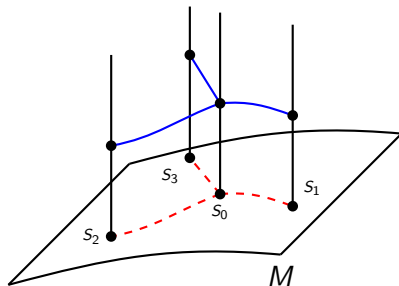
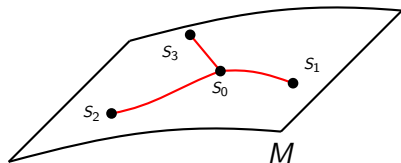


"Form Follows Function"

HDM: Horizontal Random Walk on a *Fibre Bundle*

$$P_{\epsilon}^{(\alpha)} = \left(D_{\epsilon}^{(\alpha)} \right)^{-1} W_{\epsilon}^{(\alpha)}$$

$$H_{\epsilon, \delta}^{(\alpha)} = \left(\mathcal{D}_{\epsilon, \delta}^{(\alpha)} \right)^{-1} \mathcal{W}_{\epsilon, \delta}^{(\alpha)}$$



Asymptotic Theory for Diffusion Maps

Theorem (Belkin-Niyogi 2005). Let data points x_1, \dots, x_n be sampled from a **uniform** distribution on M . Under mild technical assumptions, there exist a sequence of real numbers $t_n \rightarrow 0$ and a constant C such that in probability

$$\lim_{n \rightarrow \infty} C \frac{(4\pi t_n)^{-\frac{k+2}{2}} P_{t_n} - I}{n t_n} f(x) = \Delta_M f(x), \quad \forall x \in M.$$

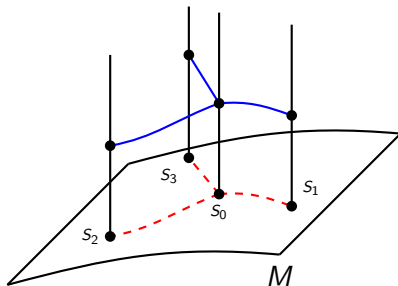
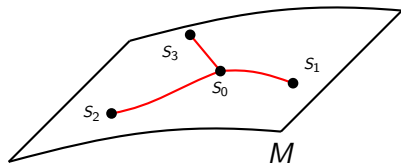
Theorem (Coifman-Lafon 2006). As $\epsilon \rightarrow 0$, for any $f \in C^\infty(M)$ and $x \in M$,

$$\begin{aligned} & P_\epsilon^{(\alpha)} f(x) \\ &= f(x) + \epsilon \frac{m_2}{2m_0} \left[\frac{\Delta_M [f p^{1-\alpha}](x)}{p^{1-\alpha}(x)} - f(x) \frac{\Delta_M p^{1-\alpha}(x)}{p^{1-\alpha}(x)} \right] + O(\epsilon^2). \end{aligned}$$

HDM: Horizontal Random Walk on a *Fibre Bundle*

$$P_{\epsilon}^{(\alpha)} = \left(D_{\epsilon}^{(\alpha)} \right)^{-1} W_{\epsilon}^{(\alpha)}$$

$$H_{\epsilon, \delta}^{(\alpha)} = \left(\mathcal{D}_{\epsilon, \delta}^{(\alpha)} \right)^{-1} \mathcal{W}_{\epsilon, \delta}^{(\alpha)}$$



Asymptotic Theory for HDM on (E, M, F, π)

Theorem (G. 2016). If $\delta = O(\epsilon)$ as $\epsilon \rightarrow 0$, then for any $f \in C^\infty(E)$ and $(x, v) \in E$, as $\epsilon \rightarrow 0$,

$$\begin{aligned} & H_{\epsilon, \delta}^{(\alpha)} f(x, v) \\ &= f(x, v) + \epsilon \frac{m_{21}}{2m_0} \left[\frac{\Delta_H (fp^{1-\alpha})(x, v)}{p^{1-\alpha}(x, v)} - f(x, v) \frac{\Delta_H p^{1-\alpha}(x, v)}{p^{1-\alpha}(x, v)} \right] \\ &+ \delta \frac{m_{22}}{2m_0} \left[\frac{\Delta_E^V (fp^{1-\alpha})(x, v)}{p^{1-\alpha}(x, v)} - f(x, v) \frac{\Delta_E^V p^{1-\alpha}(x, v)}{p^{1-\alpha}(x, v)} \right] \\ &+ O(\epsilon^2 + \epsilon\delta + \delta^2). \end{aligned}$$

Asymptotic Theory for HDM on (E, M, F, π)

Theorem (G. 2016). If $\delta = O(\epsilon)$ as $\epsilon \rightarrow 0$, then for any $f \in C^\infty(E)$ and $(x, v) \in E$, as $\epsilon \rightarrow 0$,

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- ▶ Δ_E^V is the vertical Laplacian on E
- ▶ Δ_H is the Bochner horizontal Laplacian on E
- ▶ in general $\Delta_H + \Delta_E^V \neq \Delta_E$, true if and only if π is *harmonic*

HDM on Unit Tangent Bundles ($\pi : UTM \rightarrow M$)

Corollary. If $\alpha = 1$, then

(i) If $\delta = O(\epsilon)$ as $\epsilon \rightarrow 0$, then for any $f \in C^\infty(UTM)$, as $\epsilon \rightarrow 0$,

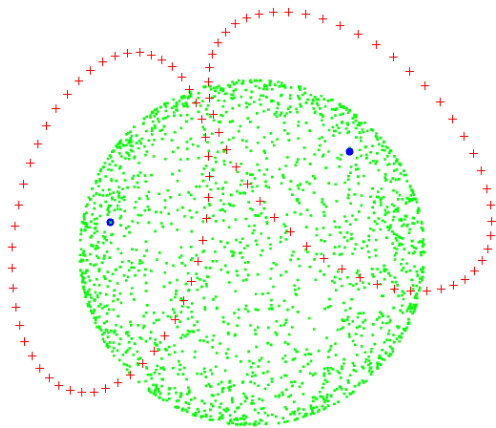
$$H_{\epsilon, \delta}^1 f(x, v) = f(x, v) + \epsilon \frac{m_{21}}{2m_0} \Delta_{UTM}^H f(x, v) \\ + \delta \frac{m_{22}}{2m_0} \Delta_{UTM}^V f(x, v) + O(\epsilon^2 + \epsilon\delta + \delta^2);$$

(ii) If $\delta = \gamma\epsilon$, then for any $f \in C^\infty(UTM)$,

$$\lim_{\gamma \rightarrow \infty} H_{\epsilon, \gamma\epsilon}^1 f(x, v) = \langle f \rangle(x) + \epsilon \frac{m'_2}{2m'_0} \Delta_M \langle f \rangle(x) + O(\epsilon^2),$$

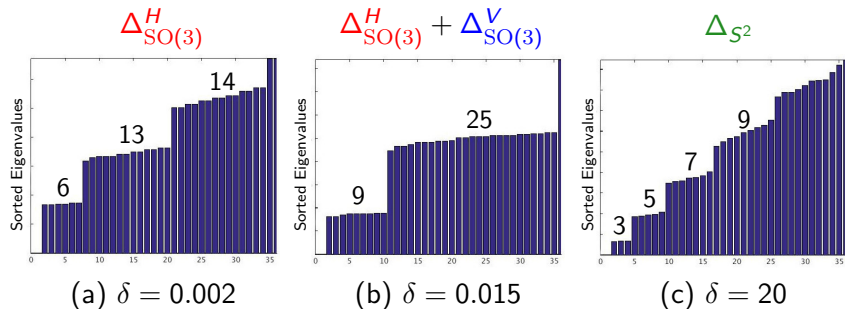
where $\langle f \rangle \in C^\infty(M)$ is the *average of f along the fibres*.

HDM on Unit Tangent Bundles: Validation on $SO(3)$



$SO(3)$ as the unit tangent bundle of $S^2 \subset \mathbb{R}^3$

HDM on Unit Tangent Bundles: Validation on $SO(3)$



Bar plots of the smallest 36 eigenvalues of *horizontal*, *total*, and *base* Laplacians on $SO(3)$, with fixed $\epsilon = 0.2$ and varying δ

The Convergence Rate: Diffusion Maps

Theorem (Singer 2006). Suppose N points are i.i.d. **uniformly** sampled from a d -dimensional Riemannian manifold M . The graph diffusion operator $P_{\epsilon, \alpha}$ converges to its smooth limit at rate

$$O\left(N^{-\frac{1}{2}}\epsilon^{\frac{1}{2}-\frac{d}{4}}\right).$$

Corollary. Under the same assumption, **non-uniform** sampling has convergence rate

$$O\left(N^{-\frac{1}{2}}\epsilon^{-\frac{d}{4}}\right).$$

The Convergence Rate: HDM on Unit Tangent Bundles

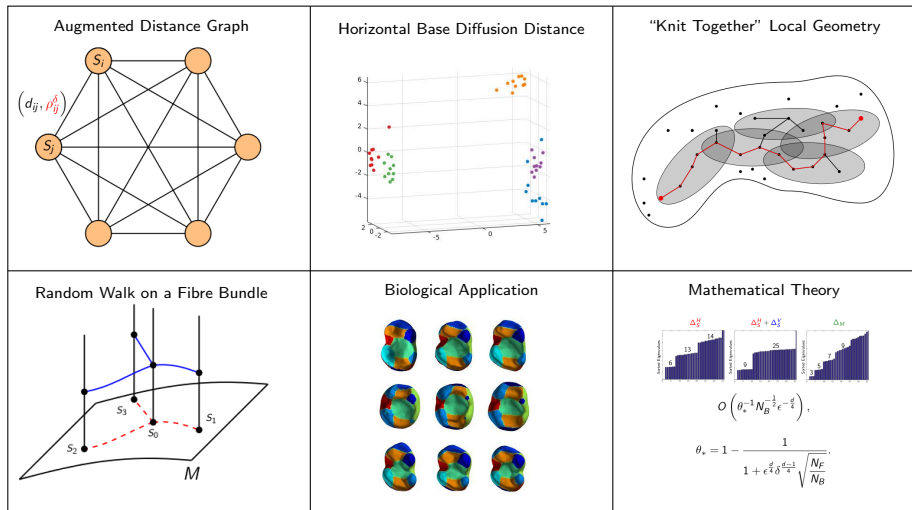
Theorem (G. 2015). Suppose N_B points are i.i.d. sampled from a d -dimensional Riemannian manifold M , and N_F unit tangent vectors are i.i.d. sampled at each of the N_B samples. The graph horizontal diffusion operator $H_{\epsilon, \delta}^\alpha$ converges to its smooth limit at rate

$$O\left(\theta_*^{-1} N_B^{-\frac{1}{2}} \epsilon^{-\frac{d}{4}}\right),$$

where

$$\theta_* = 1 - \frac{1}{1 + \epsilon^{\frac{d}{4}} \delta^{\frac{d-1}{4}} \sqrt{\frac{N_F}{N_B}}}.$$

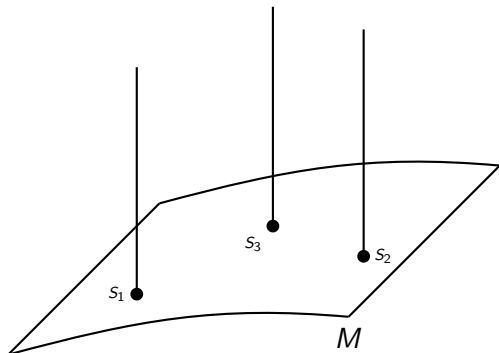
Summary and Future Work



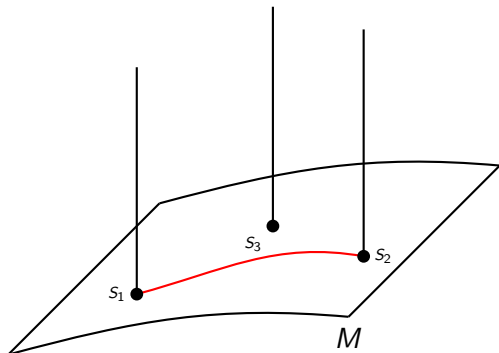
HDM: Random Walk on a *Fibre Bundle*



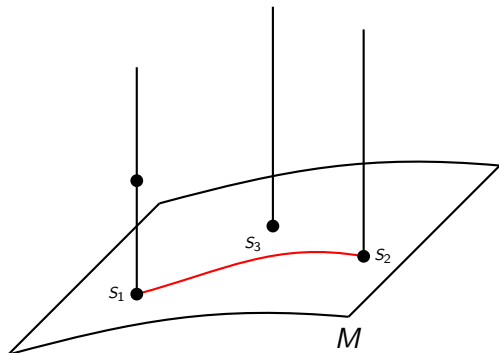
HDM: Random Walk on a *Fibre Bundle*



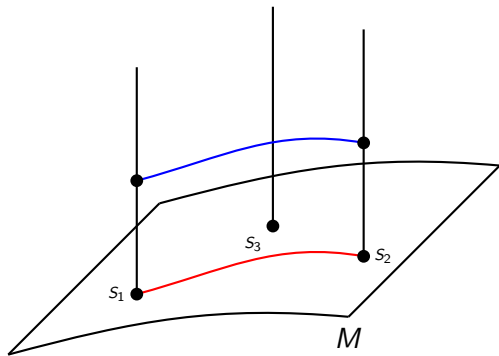
HDM – Parallel Transport



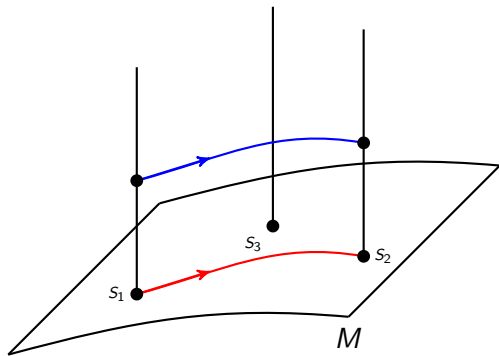
HDM – Parallel Transport



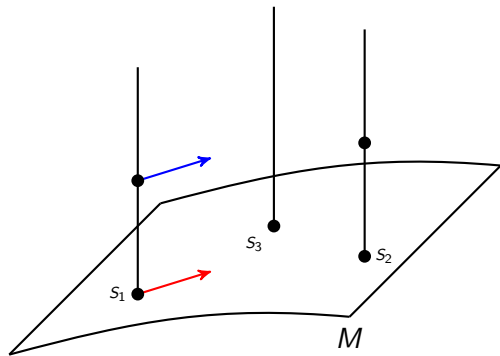
HDM – Parallel Transport



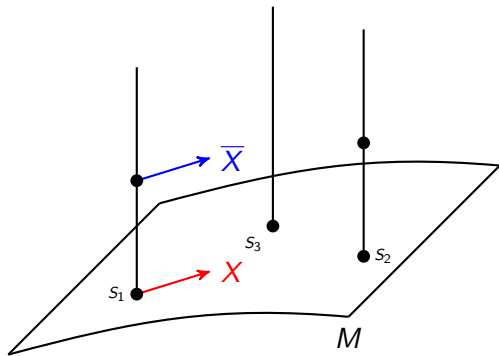
HDM – Connection



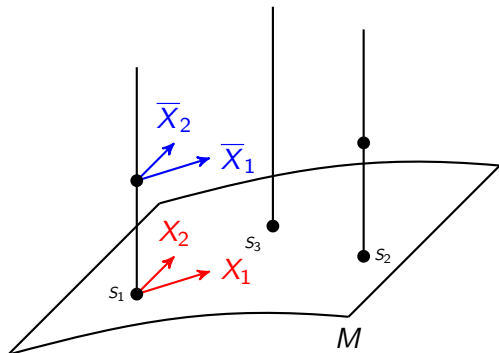
HDM – Connection



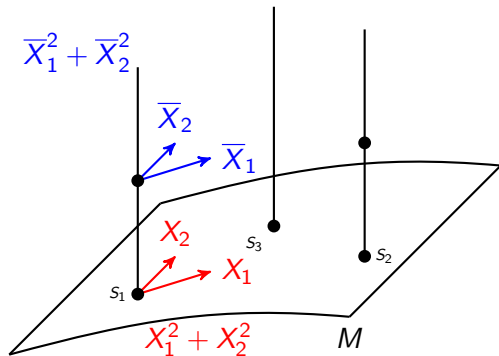
HDM – Connection



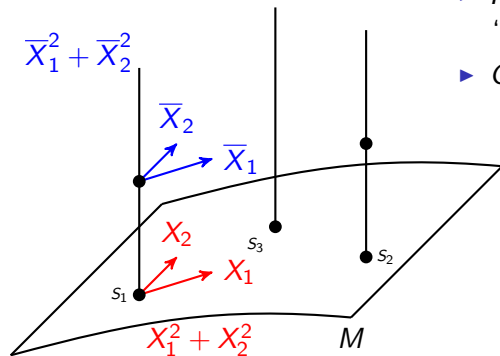
HDM – Connections



HDM – Hypocoellipticity



HDM – Hypoellipticity

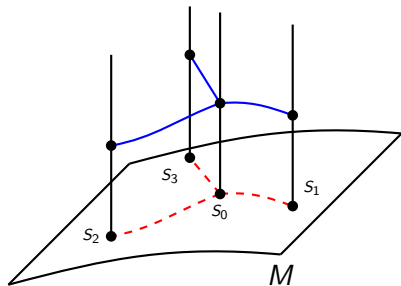
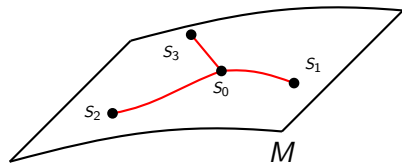


- ▶ Hörmander's Condition or "Bracket Generating"
- ▶ Chow-Rashevskii Theorem

HDM: Random Walk on a *Fibre Bundle*

$$P_{\epsilon, \alpha} = D_{\epsilon, \alpha}^{-1} W_{\epsilon, \alpha}$$

$$H_{\epsilon, \delta}^{(\alpha)} = \left(\mathcal{D}_{\epsilon, \delta}^{(\alpha)} \right)^{-1} \mathcal{W}_{\epsilon, \delta}^{(\alpha)}$$



Asymptotic Theory for HDM on (E, M, F, π)

Definition (G. 2015). For any $f \in C^\infty(E)$, $(x, v) \in E$,

$$\begin{aligned} & H_{\epsilon, \delta}^{(\alpha)} f(x, v) \\ &= \frac{\int_M \int_{F_y} K_{\epsilon, \delta}^{(\alpha)}(x, v; y, w) f(y, w) p(y, w) d\text{vol}_{F_y}(w) d\text{vol}_M(y)}{\int_M \int_{F_y} K_{\epsilon, \delta}^{(\alpha)}(x, v; y, w) p(y, w) d\text{vol}_{F_y}(w) d\text{vol}_M(y)} \end{aligned}$$

where

$$\begin{aligned} K_{\epsilon, \delta}^{(\alpha)}(x, v; y, w) &= \frac{K_{\epsilon, \delta}(x, v; y, w)}{p_{\epsilon, \delta}^\alpha(x, v) p_{\epsilon, \delta}^\alpha(y, w)}, \\ K_{\epsilon, \delta}(x, v; y, w) &= K \left(\frac{d_M^2(x, y)}{\epsilon}, \frac{d_{F_y}^2(P_{yx}v, w)}{\delta} \right). \end{aligned}$$