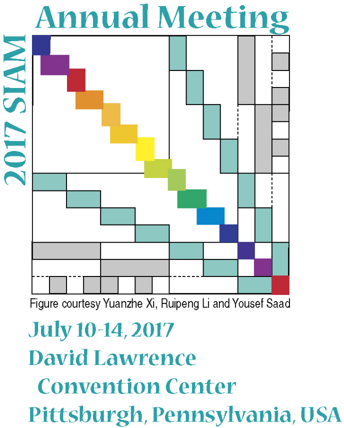
Geometry and Computational Challenges in Data Science (GCCDS)



Diffusion Geometry and Manifold Learning on Fibre Bundles

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Geometry and Computational Challenges in Data Science (GCCDS)
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Outline

Background & Motivations

- Graph Synchronization Problems

Manifold Learning on Fibre Bundles

- Diffusion Geometry
- Fibre Bundles
- Horizontal Diffusion Maps

Applications

- Evolutionary Anthropology

Graph Synchronization Problems

- Data:
  - graph $\Gamma = (V, E)$
  - matrix group G, equipped with a norm $\|\cdot\|$
  - **edge potential** $\rho : E \to G$ satisfying $\rho_{ij} = \rho_{ji}^{-1}, \; \forall (i,j) \in E$

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  - find a **vertex potential** $f : V \to G$ such that

$$f_i = \rho_{ij} f_j, \quad \forall (i,j) \in E$$

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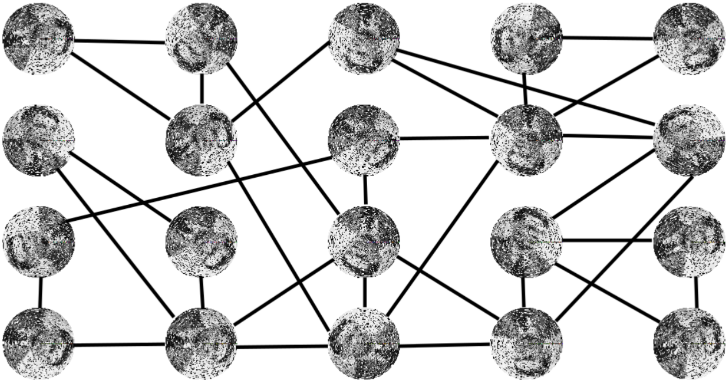
- The goal can be achieved if and only if $\rho_{ij} = f_i f_j^{-1}$
- **Not** always feasible!
- If infeasible, find the "closest solution" in the sense of

$$\min_{\substack{f:V\to G \\ \|f\|\neq 0}} \frac{1}{2} \frac{\sum_{i,j\in V} \|f_i - \rho_{ij} f_j\|^2}{\sum_{i\in V} \|f_i\|^2} (=: \eta(f))$$

A Toy Example

$$y_i = R_i x + \xi_i$$
$$R_i \in O(d), \quad \xi_i \sim \text{i.i.d. noise}$$



Afonso S. Bandeira. "Ten Lectures and Forty-Two Open Problems in the Mathematics of Data Science." (2015).

$$\boxed{\begin{array}{c} y_i = R_i x + \xi_i \\ R_i \in O(d), \quad \xi_i \sim \text{i.i.d. noise} \end{array}}$$

$$\begin{aligned} \text{Measurement:} \quad & R_{ij} \approx R_i^\top R_j \\ \text{Recover:} \quad & R_1, R_2, \cdots \end{aligned}$$

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$$\begin{aligned} \text{Measurement:} \quad & R_{ij} \approx R_i^\top R_j \\ \text{Recover:} \quad & R_1, R_2, \cdots \end{aligned}$$

$\Rightarrow$ Solve the minimization problem

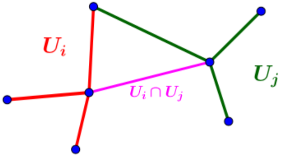
$$\min_{R_1, R_2, \cdots \in O(d)} \sum_{(i,j) \in E} w_{ij} \left\| R_{ij} - R_i^\top R_j \right\|_{\mathrm{F}}^2$$

Synchronization Problems: Examples

- Manifold Orientability [Singer, Wu (2011)]: $G = O(1)$
- Angular Synchronization [Singer (2011)]: $G = U(1)$
- Vector Diffusion Maps [Singer, Wu (2012)]: $G = O(d)$
- Multireference Alignment [Bandeira et al. (2014)]: $G = \{\text{cyclic shifts}\}$
- Global Registration of Point Clouds [Chaudhury (2015)]: $G = \mathbb{E}_d$
- Collection Shape Matching [Nguyen et al. (2011)], [Huang, Guibas (2013)], [Chen et al. (2014)], [Maron et al. (2016)]: $G = S_n$ (symm. group of n elements)
- Cryo-EM Structural Reconstruction [Singer et al. (2011)], [Shkolnisky, Singer (2012)], [Zhao, Singer (2014)], [Bandeira et al. (2015)]: $G = SO(3)$
- Cartan Motion Groups [Ozyesil et al. (2016)]: $G = K \ltimes V$ (more about this soon — in Nir Sharon's talk)

The Geometry of Synchronization Problems

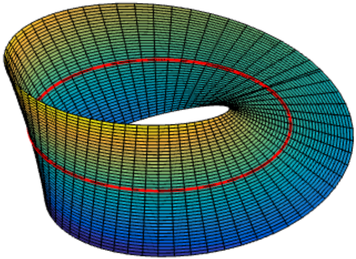
- Data:
  - graph $\Gamma = (V, E)$
  - linear algebraic group G, equipped with a norm $\|\cdot\|$
  - **edge potential** $\rho : E \to G$ satisfying $\rho_{ij} = \rho_{ji}^{-1}, \ \forall (i,j) \in E$
- Observation:
  - Let $\mathfrak{U} = \{U_i \mid 1 \leq i \leq |V|\}$ be an open cover of Γ (viewed as a 1-dimensional simplicial complex), where U_i is the *(open) star neighborhood* of vertex i.

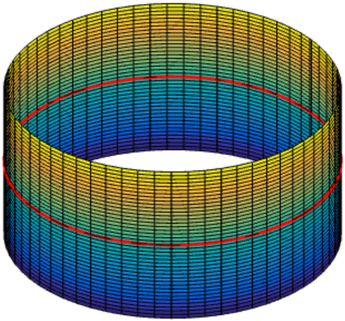


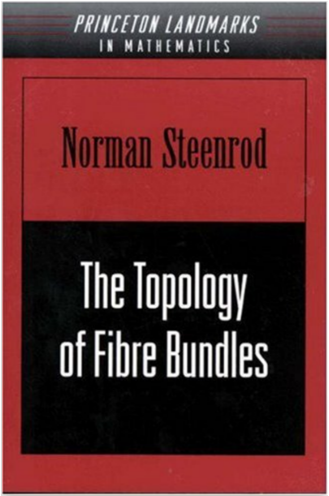
  - The ρ defines a *flat principal G-bundle* over Γ (denoted as $\mathscr{B}_\rho$).

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

- E: total manifold
- M: base manifold
- F: fibre
- E is "locally equivalent" to $M \times F$, but not necessarily so globally!



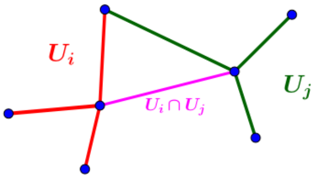




Theorem (Steenrod 1951, §2).
If topological group G acts on F and $\{U_i\}$, $\{\rho_{ij}\}$ is a system of coordinate transformations in the space M such that

$$\rho_{ii} = e \in G \quad \text{for all } U_i$$
$$\rho_{ij} = \rho_{ji}^{-1} \quad \text{if } U_i \cap U_j \neq \emptyset$$
$$\rho_{ij}\rho_{jk} = \rho_{ik} \quad \text{if } U_i \cap U_j \cap U_k \neq \emptyset$$

then there exists a fibre bundle $\mathscr{B}$ with base space M, fibre F, group G, and coordinate transforms $\{\rho_{ij}\}$.



No triple intersections!

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Geometric Observations

- Denote

$$C^0(\Gamma; G) := \{f : V \to G\} \text{ vertex potentials}$$
$$C^1(\Gamma; G) := \left\{\rho : E \to G \mid \rho_{ij} = \rho_{ji}^{-1}, \forall (i,j) \in E\right\} \text{ edge potentials}$$

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- Consider the right action of $C^0(\Gamma; G)$ on $C^1(\Gamma; G)$:

$$C^1(\Gamma; G) \times C^0(\Gamma; G) \to C^1(\Gamma; G)$$
$$(\rho, f) \longmapsto \tau_\rho f$$

defined as $(\tau_f \rho)_{ij} := f_i^{-1} \rho_{ij} f_j, \quad \forall (i,j) \in E$.

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  defined as $(\tau_f \rho)_{ij} := f_i^{-1} \rho_{ij} f_j, \quad \forall (i,j) \in E$.

- ρ synchronizable $\Leftrightarrow$ $\tau_f \rho$ synchronizable for all $f \in C^0(\Gamma;G)$, i.e. synchronizability is defined at the level of equivalence classes $C^1(\Gamma;G) / C^0(\Gamma;G)$

Moduli Space of Synchronization Data

Theorem (G., Brodzki, Muhkerjee (2016)). There exists a one-to-one correspondence (between *sets*)

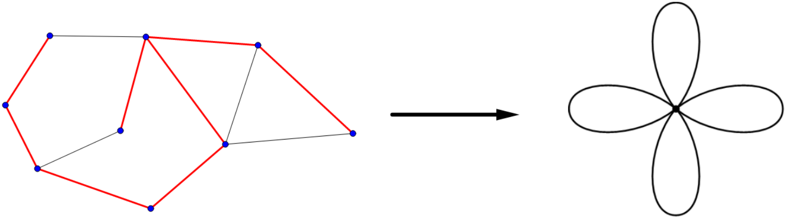
$$C^1(\Gamma; G) / C^0(\Gamma; G) \cong \mathrm{Hom}(\pi_1(\Gamma), G) / G$$

where G acts on $\mathrm{Hom}(\pi_1(\Gamma), G)$ by conjugations:

$$\begin{aligned} \mathrm{Hom}(\pi_1(\Gamma), G) \times G &\longrightarrow \mathrm{Hom}(\pi_1(\Gamma), G) \\ (\phi, g) &\longmapsto g^{-1}\phi g \end{aligned}$$

Tingran Gao, Jacek Brodzki, Sayan Mukherjee. "The Geometry of Synchronization Problems and Learning Group Actions." *submitted.* arXiv:1610.09051, 2016

Fundamental Group of a Graph?



$$\pi_1(\Gamma) = \bigvee_{k=1}^{|E|-|V|+1} S^1$$

$$\mathrm{Hom}(\pi_1(\Gamma), G) = \underbrace{G * G * G * \cdots * G * G * G}_{(|E|-|V|+1)\text{-copy free product}}$$

$$\boxed{C^0(\Gamma; G)/C^1(\Gamma; G) \cong \mathrm{Hom}(\pi_1(\Gamma), G)/G}$$

- Proof builds upon construction of a *holonomy homomorphism*
- The orbit space $C^0(\Gamma; G)/C^1(\Gamma; G)$ is exactly the *first cohomology set* $\check{H}^1((\Gamma, \mathfrak{U}), \underline{G})$
- "Synchronizability" is a property at the level of equivalence classes $\left[f_i^{-1}\rho_{ij}f_j\right]_{(i,j)\in E}$
- $\rho \in C^1(\Gamma; G)$ synchronizable
  $\Leftrightarrow [\rho] = [e]$ as equivalence classes in $C^0(\Gamma; G)/C^1(\Gamma; G)$
  $\Leftrightarrow$ the principal G-bundle $\mathscr{B}_\rho$ is trivial
- Future work: study synchronization problems through the geometry of the moduli space/character variety

Quick Aside: A Twisted De Rham-Hodge Theory

- Combinatorial Hodge Theory:

$$0 \rightleftarrows \Omega^0(\Gamma) \underset{\delta}{\overset{d}{\rightleftarrows}} \Omega^1(\Gamma) \rightleftarrows 0,$$

- *Twisted* Combinatorial Hodge Theory:

$$0 \rightleftarrows C^0(\Gamma; F) \underset{\delta_\rho}{\overset{d_\rho}{\rightleftarrows}} \Omega^1(\Gamma; \mathscr{B}_\rho[F]) \rightleftarrows 0.$$

- **Theorem (G., Brodzki, Muhkerjee (2016)).** Define

$$\Delta_\rho^{(0)} := \delta_\rho d_\rho, \quad \Delta_\rho^{(1)} := d_\rho \delta_\rho$$

then the following Hodge-type decomposition holds:

$$C^0(\Gamma; F) = \ker \Delta_\rho^{(0)} \oplus \operatorname{im} \delta_\rho = \ker d_\rho \oplus \operatorname{im} \delta_\rho,$$
$$\Omega^1(\Gamma; \mathscr{B}_\rho[F]) = \operatorname{im} d_\rho \oplus \ker \Delta_\rho^{(1)} = \operatorname{im} d_\rho \oplus \ker \delta_\rho.$$

Application: Evolutionary Anthropology

Doug Boyer

Jukka Jernvall

More Precisely: biological morphologists

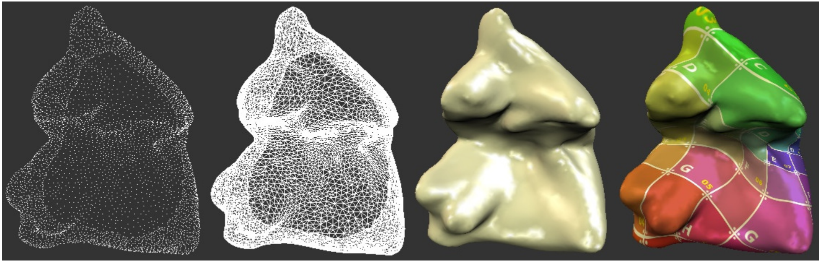
↓

Study Teeth & Bones of

extant & extinct animals

still live today   fossils

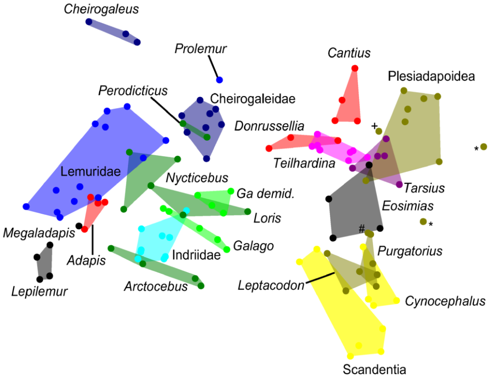
Data Acquisition: microCT (High Resolution X-ray CT)



Surface reconstructed from μCT-scanned voxel data

Landmarked Teeth $\longrightarrow$

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

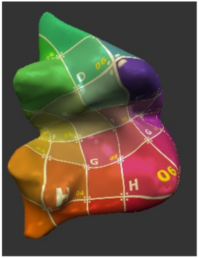


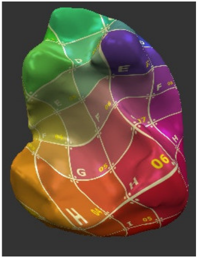
Boyer et al. "Algorithms to Automatically Quantify the Geometric Similarity of Anatomical Surfaces." *Proceedings of the National Academy of Sciences* 108.45 (2011): 18221-18226.

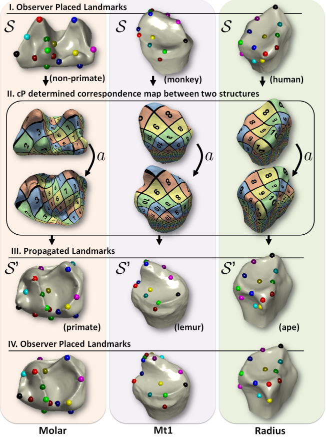
A Zoo of Shape Distances...

$d_{\mathrm{cWn}}(S_1, S_2)$: Conformal Wasserstein Distance (CWD)
$d_{\mathrm{cP}}(S_1, S_2)$: Continuous Procrustes Distance (CPD)
$d_{\mathrm{cKP}}(S_1, S_2)$: Continuous Kantorovich-Procrustes Distance (CKPD)

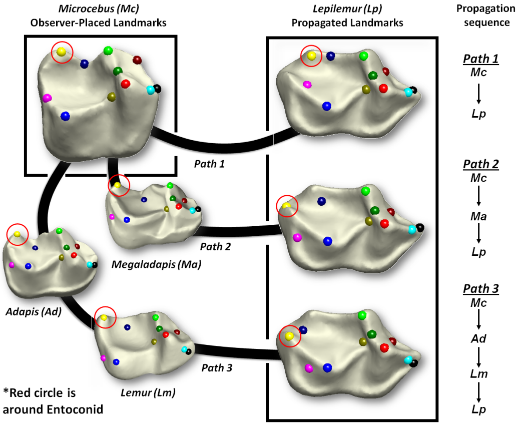
$$d_{\mathrm{cP}}(S_1, S_2) = \inf_{\mathcal{C} \in \mathcal{A}(S_1, S_2)} \inf_{R \in \mathbb{E}(3)} \left(\int_{S_1} \| R(x) - \mathcal{C}(x) \|^2 \, d\mathrm{vol}_{S_1}(x) \right)^{\frac{1}{2}}$$





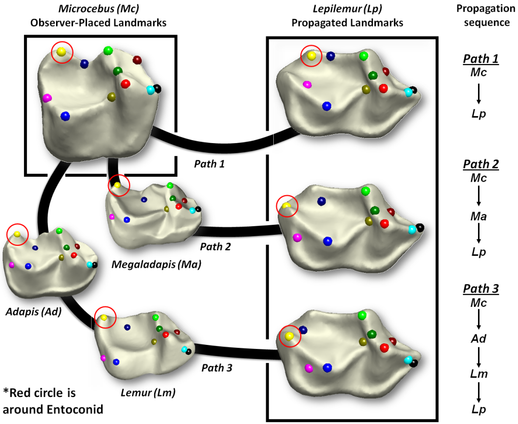


Interpretability Issue



Even mistakes made by CPD were similar to biologists' mistakes!

Resolving Interpretability Issue #1: Trust Small Distances



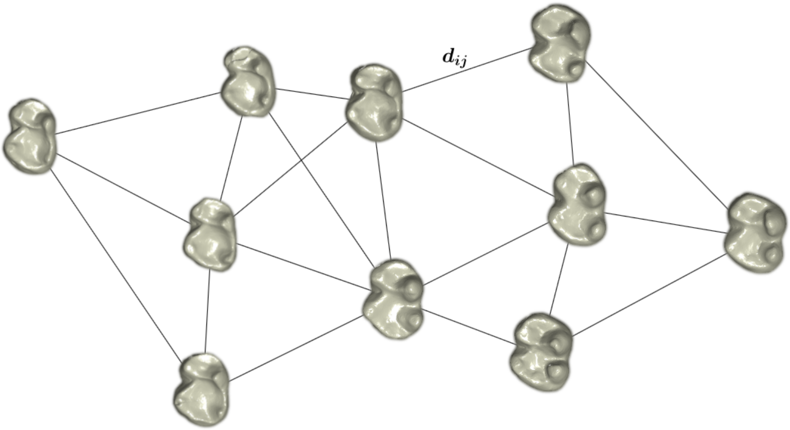
"Correct" like a biologist, but *automatically*?

small distances between $S_1, S_2 \longrightarrow$ OK maps

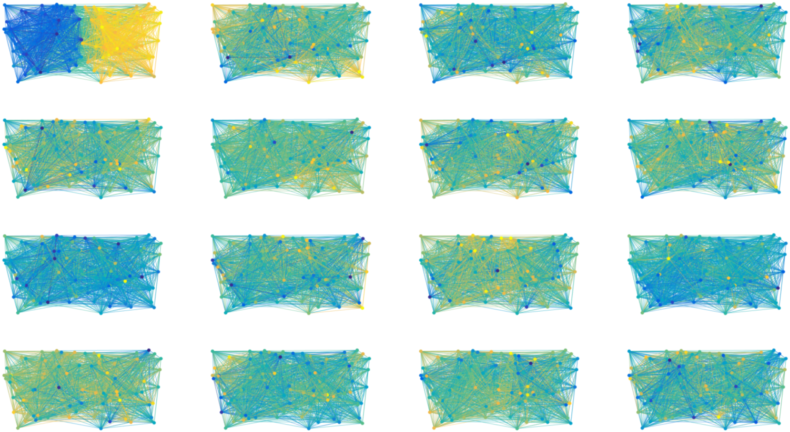
larger distances $\longrightarrow$ not OK

Gao et al. (2016) "Development and Assessment of Fully Automated and Globally Transitive Geometric Morphometric Methods." *submitted.* DOI: `http://dx.doi.org/10.1101/086280`

Trust Only *Small* Distances: *Geodesics* in Shape Space



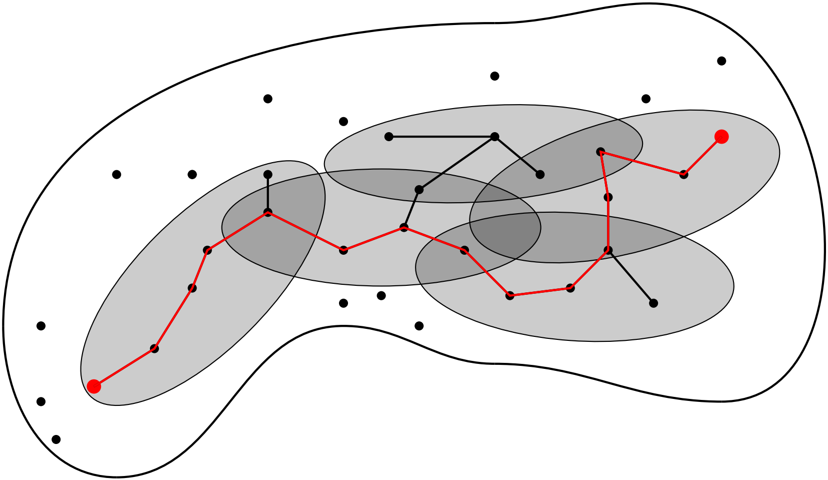
Diffusion Maps and Diffusion Distances



Diffusion Maps: Embedding Graphs into ℓ_2 using Eigenfunctions and the Heat Kernel of the Graph Laplacian

Coifman, R. R., and Lafon, S. "Diffusion Maps." *Appl. & Comput. Harmonic Analysis* 21, no. 1 (2006): 5-30.

Diffusion Maps: “Knit Together” Local Geometry

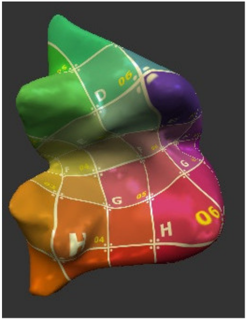


Small distances are much more reliable!

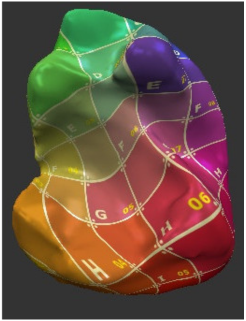
Resolving Interpretability Issue #2: Use Maps!

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

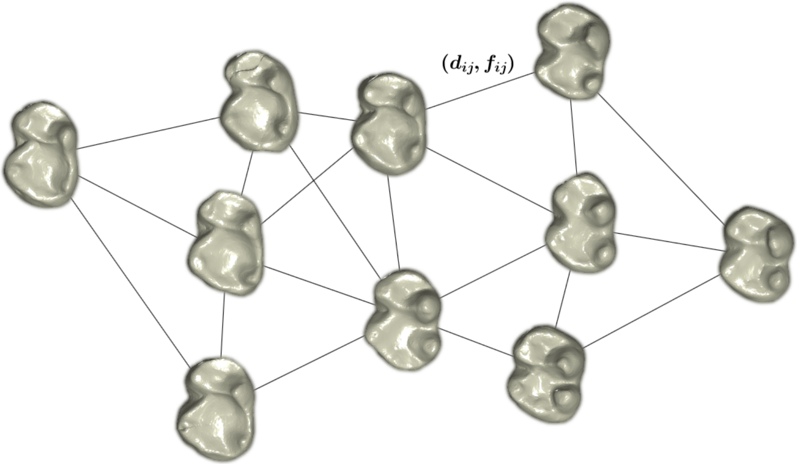
S_i

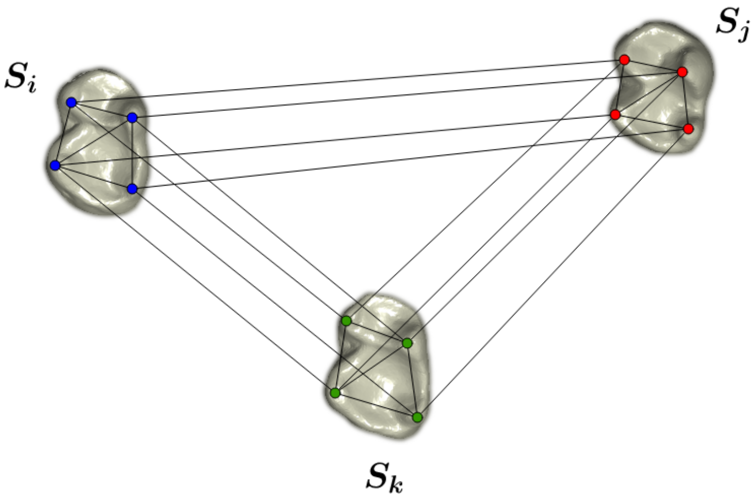


$\xrightarrow[f_{ij}]{d_{ij}}$



S_j


(d_{ij}, f_{ij})

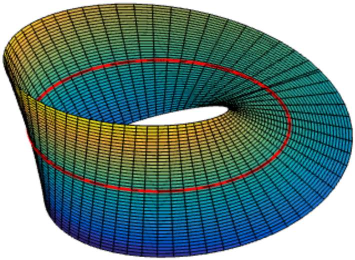


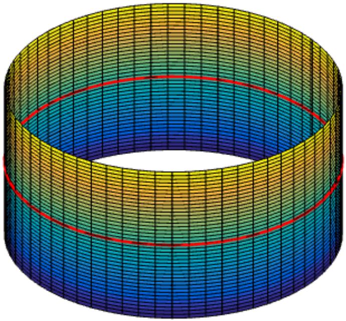
S_i
S_j
S_k

Geometric Model —— *Fibre Bundles*

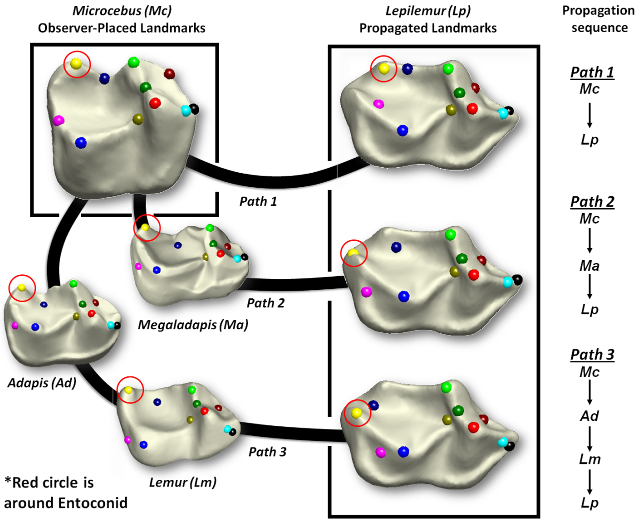
Fibre Bundle $\mathscr{E} = (E, M, F, \pi)$

- E: total manifold
- M: base manifold
- F: fibre
- E is "locally equivalent" to $M \times F$, but not necessarily so globally!

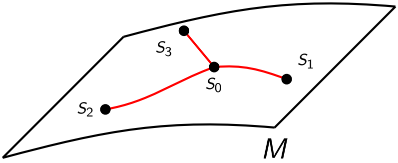


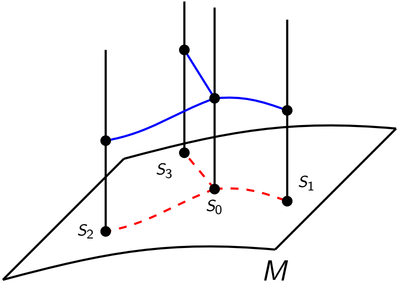


Shape Space is NOT a Trivial Fibre Bundle



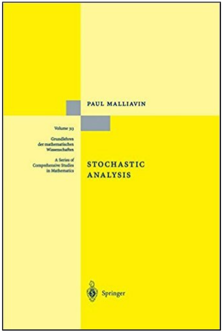
Horizontal Random Walk on a *Fibre Bundle*

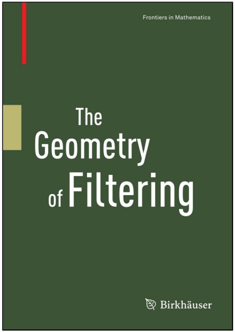


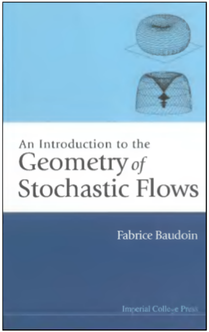


Horizontal Diffusion Process in Stochastic Geometry

- K.D. Elworthy, W.S. Kendall. "Factorization of Harmonic Maps and Brownian Motions." University of Warwick, 1985.
- M. Liao, "Factorization of Diffusions on Fibre Bundles." *Transactions of the American Mathematical Society.* 311.2 (1989): 813-827.
- M. Arnaudon, A. Thalmaier. "Horizontal Martingales in Vector Bundles." *Séminaire de Probabilits de Strasbourg.* 36 (2002): 419-456.
- K.D. Elworthy, Y. Le Jan, and X. Li. "The Geometry of Filtering." Springer Basel, 2010. 33-59.
- F. Baudoin. "An Introduction to the Geometry of Stochastic Flows." London: Imperial College Press, 2004.



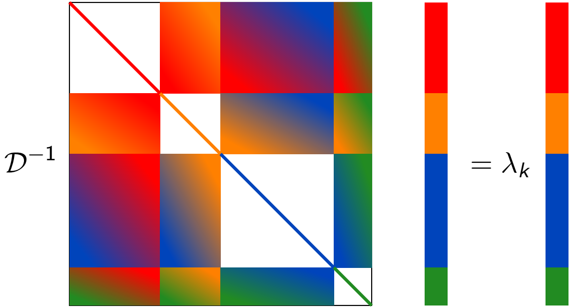




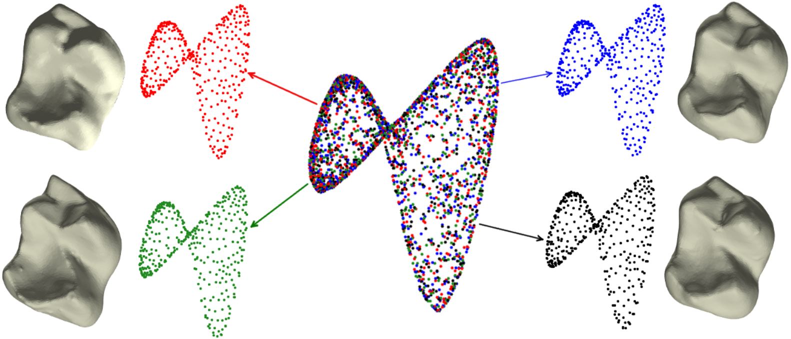
Horizontal Diffusion Maps

Horizontal Diffusion Maps

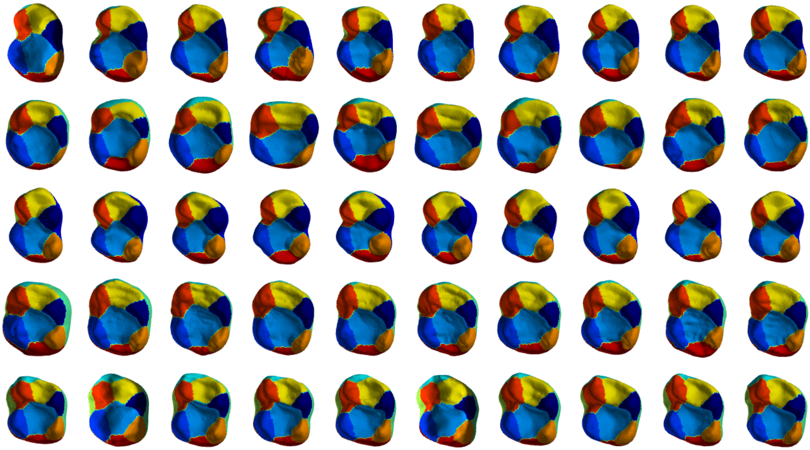
$$\mathcal{D}^{-1}\mathcal{W}u_k = \lambda_k u_k, \quad 1 \leq k \leq \kappa$$



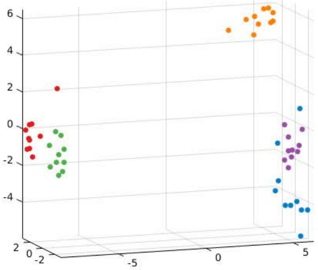
Horizontal Diffusion Maps



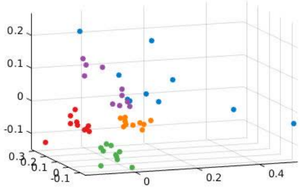
Automatic Landmarking — Interpretability



Species Clustering

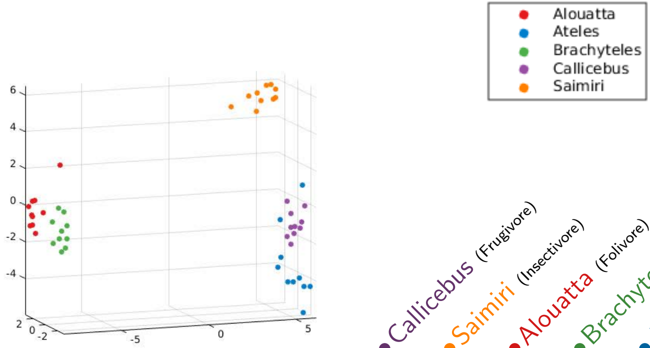


Horizontal Base Diffusion Distance (with Maps)

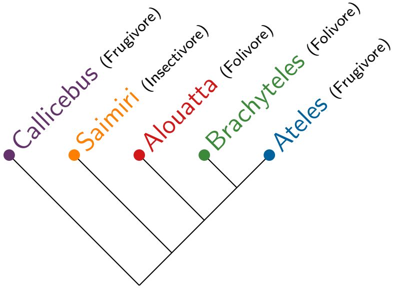


Diffusion Distance (without Maps)

Species Clustering



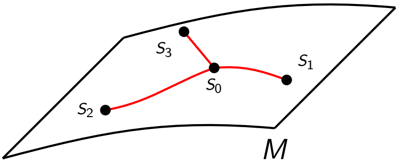
Horizontal Base Diffusion Distance (with Maps)

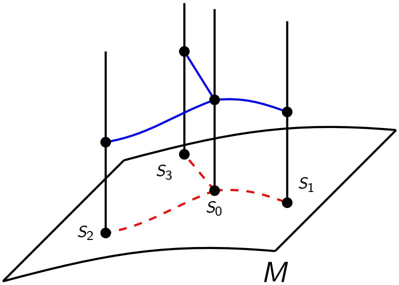


HDM: Mathematical Theory

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

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





Asymptotic Theory for Diffusion Maps

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

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

Theorem (Coifman-Lafon 2006). As $\epsilon \to 0$, for any $f \in C^\infty(M)$ and $x \in M$, if $\{x_i\}_{i=1}^n \sim p(x)\mathrm{dvol}_M(x)$, then w.h.p.

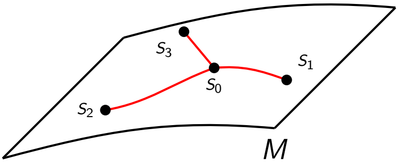
$$P_\epsilon^{(\alpha)} f(x)$$

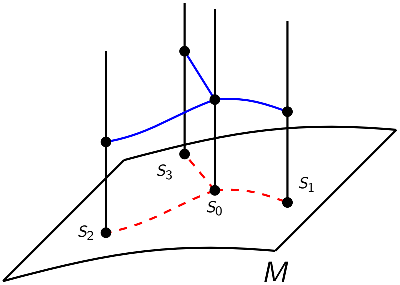
$$= f(x) + \epsilon \frac{m_2}{2m_0} \left[\frac{\Delta_M \left[f p^{1-\alpha} \right](x)}{p^{1-\alpha}(x)} - f(x) \frac{\Delta_M p^{1-\alpha}(x)}{p^{1-\alpha}(x)} \right] + O\left(\epsilon^2\right).$$

HDM: Horizontal Random Walk on a *Fibre Bundle*

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

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





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

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

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

Tingran Gao. *The Diffusion Geometry of Fibre Bundles.* arXiv:1602.02330, 2016

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

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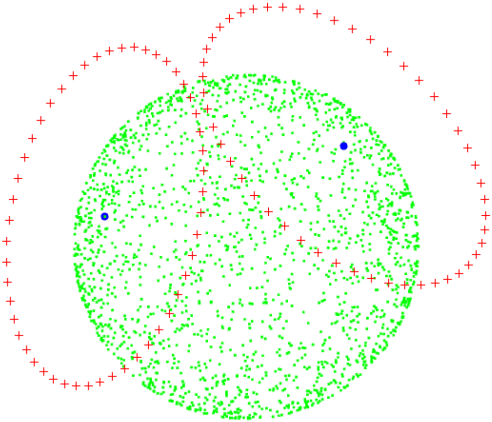
&= f(x, v) + \epsilon \frac{m_{21}}{2m_0} \left[\frac{\Delta_H \left(fp^{1-\alpha}\right)(x, v)}{p^{1-\alpha}(x, v)} - f(x, v) \frac{\Delta_H p^{1-\alpha}(x, v)}{p^{1-\alpha}(x, v)} \right] \\
&\quad + \delta \frac{m_{22}}{2m_0} \left[\frac{\Delta^V_E \left(fp^{1-\alpha}\right)(x, v)}{p^{1-\alpha}(x,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

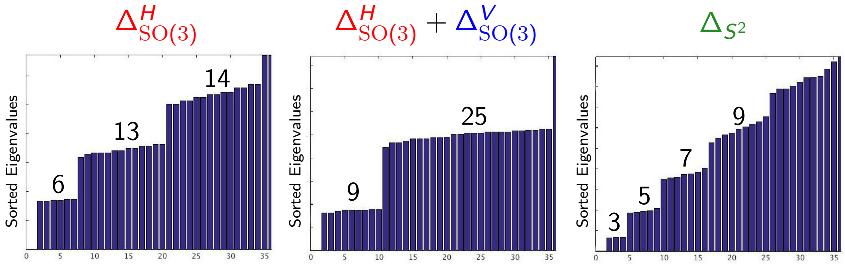
- Δ^V_E is the vertical Laplacian on E
- Δ_H is the Bochner horizontal Laplacian on E
- In general $\Delta_H + \Delta^V_E \neq \Delta_E$, true if and only if π is *harmonic*

HDM on Unit Tangent Bundles: Validation on $\mathrm{SO}(3)$



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

HDM on Unit Tangent Bundles: Validation on $\mathrm{SO}(3)$



(a) $\delta = 0.002$ (b) $\delta = 0.015$ (c) $\delta = 20$

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

Tingran Gao. *The Diffusion Geometry of Fibre Bundles.* arXiv:1602.02330, 2016

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. 2016). 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 $H^{\alpha}_{\epsilon,\delta}$ converges to its smooth limit at rate

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

where

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

Tingran Gao. "The Diffusion Geometry of Fibre Bundles." *submitted.* arXiv:1602.02330, 2016

Collaborators

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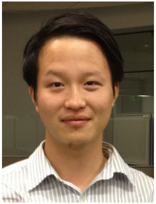

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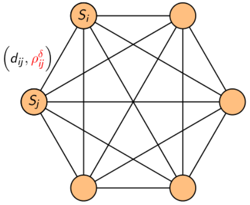
Jesús Puente
J.P. Morgan

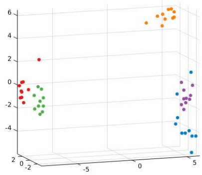
Robert Ravier
Duke

Thank You!

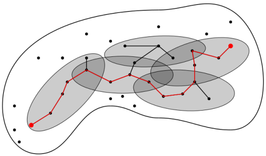
Augmented Distance Graph



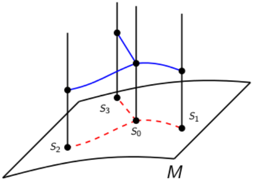
Horizontal Base Diffusion Distance



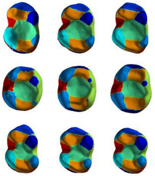
"Knit Together" Local Geometry



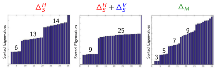
Random Walk on a Fibre Bundle



Biological Application



Mathematical Theory



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

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

Tingran Gao. "The Diffusion Geometry of Fibre Bundles." *submitted.* arXiv:1602.02330, 2016

Tingran Gao, Jacek Brodzki, Sayan Mukherjee. "The Geometry of Synchronization Problems and Learning Group Actions." *submitted.* arXiv:1610.09051, 2016