FUNCTIONAL AND SHAPE DATA ANALYSIS

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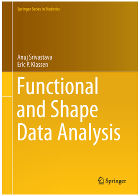
Presented at Texas A&M FIDS & TAMID on September 18, 2020



Srivastava & Klassen
Functional and Shape Data Analysis
Springer, 2016

Outline

1. Introduction, Motivation, and Background (1:00 - 1:30pm)
   - Introduction and Motivational Examples
   - Background: Shape Analysis
   - Background: Functional Data Analysis Using $\mathbb{L}^2$ Metric
2. Elastic Functional Data Analysis (1:30 - 2:15pm)
   - Registration Problem
   - Fisher-Rao Metric and Square-Root Velocity Function

——————— Coffee Break (15 mins) ———————-

3. Elastic Shape Analysis of Planar Curves (2:30 - 3:15pm)
   - Registration Problem
   - Elastic Metric and Square-Root Velocity Function
   - Shape Clustering, Summary, and Modeling
4. Matlab Code & Demo (3:15 - 3:45pm)
   - Alignment of Scalar Functions
   - Shapes of Planar, Closed Curves
5. Shape Analysis of Complex Objects (3:45 - 4:00pm)
   - Shape Analysis of Surfaces
   - Shape Analysis of Tree-like Structures

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Preface: Modern Statistical Data Analysis

- We are going through a remarkable period of transition and growth, reflecting large strides in data-driven methodologies – FIDS, TAMID.
- Where is data coming from? Imaging sensors and modalities are becoming a major source of data.
- From mega scale (e.g. satellite and space imaging) to human scale (cellphones, vehicular sensors, medical imaging, etc) to nanoscale (e.g. sub-cellular structures and electron microscopy imaging).
- Data is complex! It leads to newer challenges and inspires newer solutions. Data (images) contain objects of interest and we want to *understand and analyze roles of these objects* in larger systems.
- Our specific subgoals are to estimate, recognize, track, classify, and predict objects and their behaviors. We use shapes of objects as an important characteristic in working towards these goals.

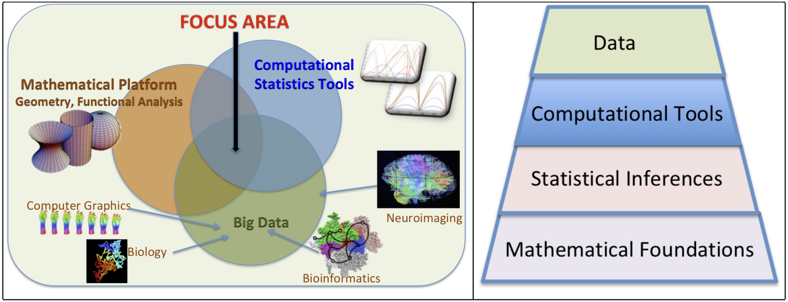
Preface: Modern Statistical Data Analysis

- Why the focus on shapes? Shapes (structures) and functionality of objects are highly interconnected. Structures both constrain and enable functionality of an object. Understanding functions demands understanding structures.

- Object data is highly structured. Traditional statistical tools are not directly applicable. We can add or subtract two vectors or two matrices, but how does one add or subtract two objects?

- These challenges are spawning a new age of structural data analysis, with a confluence of tools from geometry, topology, statistics and other several other domains.

- This topic area is multidisciplinary, or transdisciplinary, not just interdisciplinary:



- Statistical analyses have traditionally been performed in Euclidean spaces. Structured data is highly non-Euclidean. We need novel mathematical platforms that are more suited to our needs.

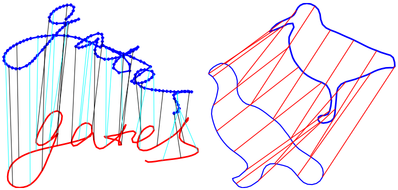
Intro: Functional and Shape Data Analysis

Historically:

- Functional Data Analysis (FDA):
  - The term was coined by Jim Ramsay and Bernard Silverman in late 80s.
  - Statistical analysis where variables of interest are functions – mostly, scalar functions on a fixed interval.
  - Mathematical platform was Hilbert space of square-integrable functions (will discuss this in detail later)
  - Using a (truncated) orthonormal basis, many statistical problems are converted to multivariate statistics. Replace functions by their coefficients.
- Shape Analysis:
  - Pioneered by D'Arcy Thompson (early 20th century), David Kendall (1980s), Ulf Grenander (1990s), and others.
  - Most of this analysis was performed assuming that objects were made up of a set of registered points – landmarks.
  - The main accomplishment were developing mathematical machinery that performs analysis while being invariant to rotations, translations, scale.

More recently:

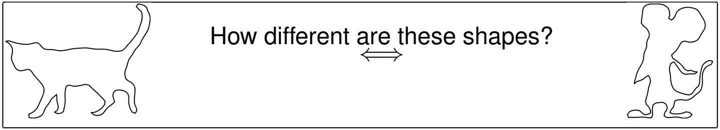
- Shape Analysis of Functional Data:
  - Objects are represented by functions (continuum) – scalar functions, curves, surfaces, etc.
- Challenges:
  - **Invariance**: A shape of the object does not change under rotation, translation and scaling. Analysis is invariant to rotations, translations, scale, etc.
  - **Registration**: Which point on one object is matched with which point on the other?
    We do not assume that the data is already registered. That is the biggest achievement of this theory. Registration is performed during shape analysis.



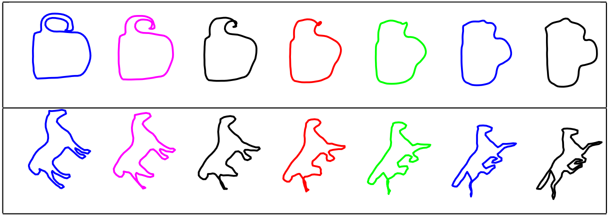
Typical Shape Analysis Tasks

A set of theoretical and computational tools that can provide:

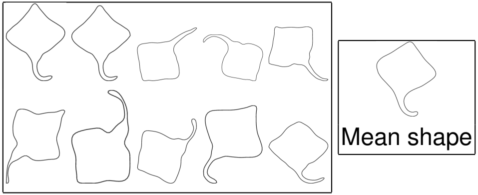
- Shape Metric: Quantify differences in any two given shapes.



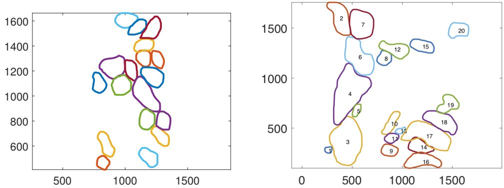
- Shape Deformation/Geodesic:
  How to optimally deform one shape into another?



- Shape summary: Compute sample mean, sample covariance, PCA, and principal modes of shape variability.



- Shape model and testing: Develop statistical models and perform hypothesis testing.



Running Mice

Sedentary Mice

- Related tools: ANOVA, two-sample test, k-sample test, etc.

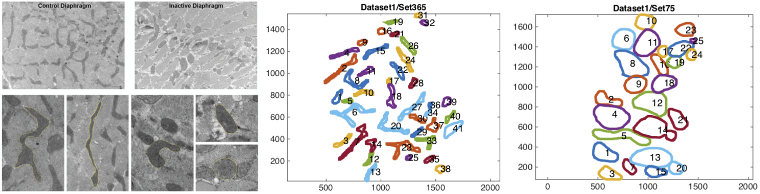
Motivations: Application Areas

Where do we need Functional and Shape Data Analysis?

Everywhere! If there is functional data, or image data, or object data!

- Biology & Bioinformatics
- Computer Vision & AI
- Meteorological, Atmospheric, Earth Sciences
- Medical Imaging Dianostics & Computational Anatomy
- Health, Lifestyle, Biometrics

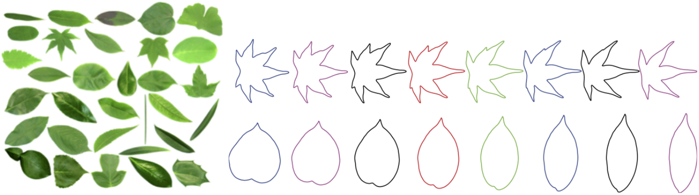
- Shapes of Mitochondria contours.



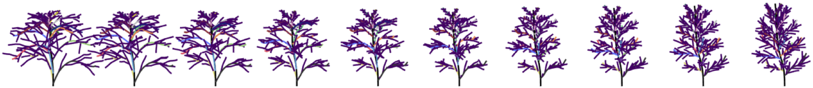
- Scientific questions: Does the amount of daily activity performed by an animal influence the shapes of mitochondria?

- ANOVA type problem: Factor – daily exercise, Response – mitochondria shapes. Decide significance of external factors.

- Leaves: Classification of leaves using shapes.

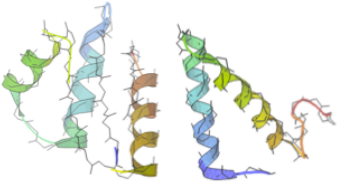


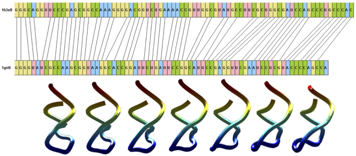
- Trees:



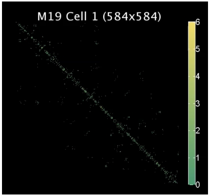
Bioinformatics

- Proteins, RNAs – Structure Analysis

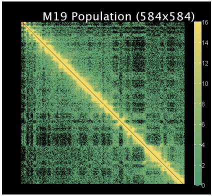




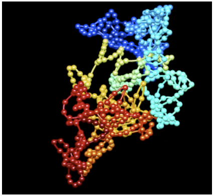
- Chromosome structure analysis using Hi-C data



Single Cell



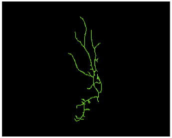
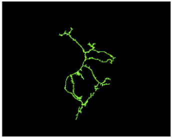
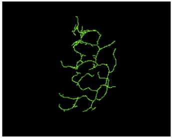
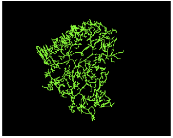
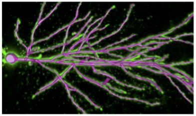
Ensemble



Estimation

Neuron Morphology

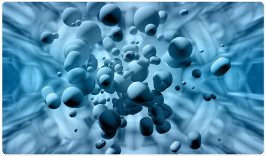
- Neurons, axons

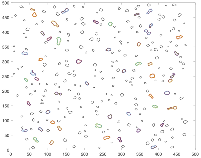







- Complex branching structures, different numbers and shapes of branches.
- Interested in neuron morphology for various medical reasons – cognition, genomic associations, diseases.

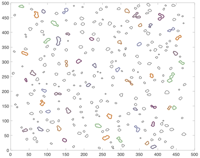
Nanoparticle Morphology

- Nanoimaging: Supervising material properties using EM

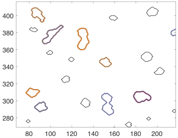




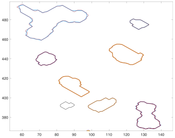
Frame i



Frame j



Zoom in 1

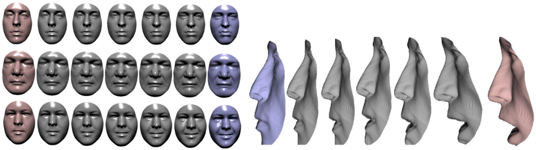


Zoom in 2

- Scientific: Compare populations of dynamic shapes, not just individual static shapes.

Biometrics - Human Body

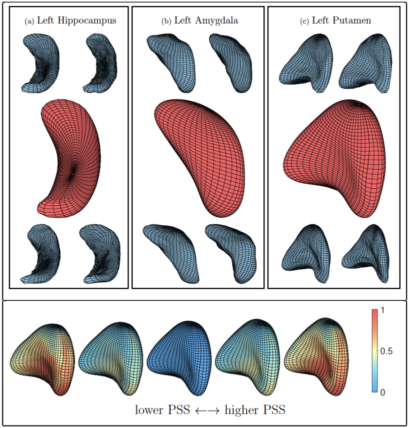
- Human biometrics is a fascinating problem area.
- Facial Surfaces: 3D face recognition for biometrics



- Human bodies: applications – medical (replace BMI), textile design.

- Shapes are represented by surfaces in $\mathbb{R}^3$

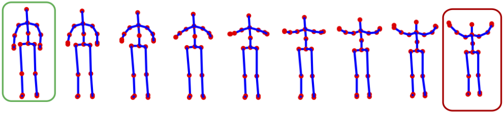
- Subcortical structures in human brain



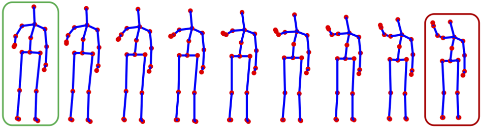
- Shapes are represented by surfaces in $\mathbb{R}^3$
- Goal is to analyze shapes of these structures in order to diagnose or predict onset of cognitive disorders – Alzheimers, Schizophrenia, ADHD, PTSD, etc.

- Human activity data using remote sensing — kinect depth maps

(a) Source and Target skeletons from Action#11 'Two Hand Wave'

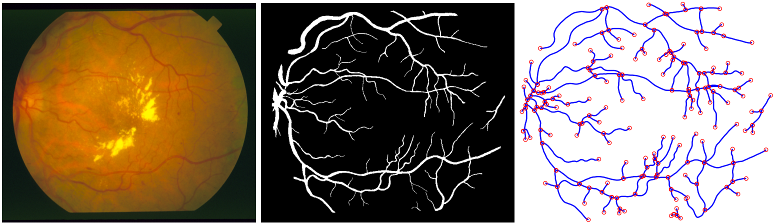


(b) Source and Target skeletons from Action#1 'High Arm Wave'



- Each sketelon is considered either as an element of $\mathbb{R}^{60}$ or Kendall's shape space (20 landmarks in $\mathbb{R}^3$).
- An action is then a curve on that representation space.
- Goal is action classification while being invariant to rate at which action is performed.

- Shape analysis of vasculature in retinal images.

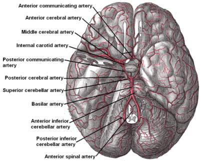


Original Image — Binary Segmentation — Graph Representation

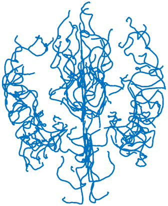
- The goal is to detect and diagnose different kinds of abnormalities associated with vision and eyes.

Brain Arterial Networks

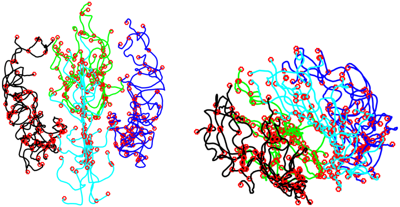
- Shape analysis of networks of arteries in human brain



Schematic



Dense Point Clouds



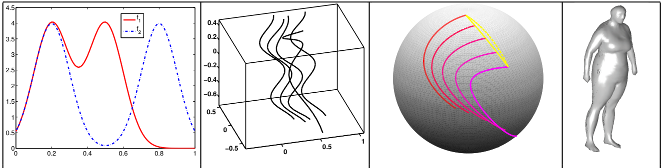
Network of 3D curves

- The goal is to study how arterial networks change with age, gender, disease, and injuries.

What is the Nature of Objects

Many objects can be represented as functions $f : D \to \mathbb{R}^k, M$

- 2D, 3D, or Euclidean Curves: For example, 2D closed curves forming silhouettes of objects.
- Collections of Curves: For example, neurons or botanical trees.
- Surfaces: Boundaries of 3D objects.



$D = [0, 1], k = 1$	$D = [0, 1], k = 3$	$D = [0, 1], M = \mathbb{S}^2$	$D = \mathbb{S}^2, k = 3$
functions	curves	trajectories	surfaces

- Tajectories on nonlinear manifolds. e.g. covariance trajectories, skeletal trajectories.
- Simplest example: scalar functions on $[0, 1]$. We are going to focus a lot on statistical analysis of scalar functions on a fixed interval.

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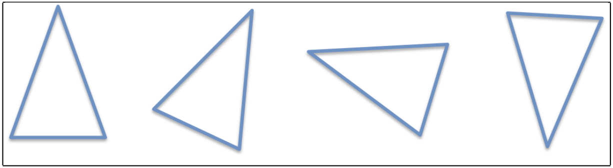
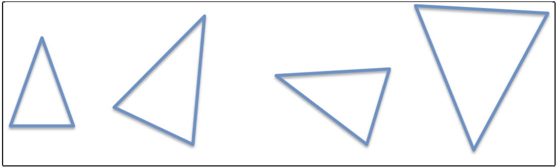
- Congruent Objects: If we rotate and translate an object, then it remains congruent to the original object.



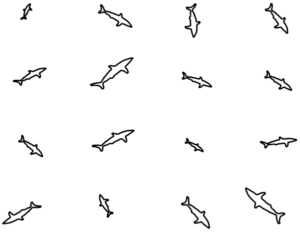
- Similar Objects: If we scale, rotate, and translate an object, then it remains similar to the original object.



These are called similarity or *shape-preserving* transformations.

Invariance in Shape Analysis

- General Objects: Shape is a property that is invariant to rotation, translation, and scaling of objects (Kendall, 84).



- An additional invariance for functional data:
  - In case we are working with continuous objects (curves, surfaces, etc), there is another transformation – re-parameterization – that leaves shapes unchanged.
  - For example, shape of a parametrized curve is also invariant to how it is parameterized.
  - This transformation has another role – it helps in registering points along two objects. (More on this later)

Shape-Preserving Transformations as Groups

- It is very useful to view these transformations as groups.

- What is a Group:
  A group G is a set having an associative binary operations, denoted by $\cdot$, such that:
  - there is an identity element $e \in G$ ($e \cdot g = g \cdot e = g$ for all $g \in G$.
  - for every $g \in G$, there is an inverse g^{-1} ($g \cdot g^{-1} = e$).

- Examples:
  - Translation Group: $\mathbb{R}^n$, group operation is addition, identity element is zero vector
  - Scaling Group: $\mathbb{R}_+$, group operation is multiplication, identity element is 1.
  - Rotation Group: $SO(n)$, group operation is matrix multiplication, identity element is I_n.
  - Diffeomorphism/Reparameterization Group: Define

    $$\Gamma = \{\gamma : [0,1] \to [0,1] | \gamma(0) = 0, \gamma(1) = 1, \gamma \text{ is a diffeo}\} .$$

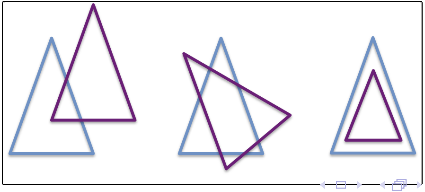
    Γ is a group, group operation is composition: $\gamma_1 \circ \gamma_2 \in \Gamma$
    Identity element is $\gamma_{id}(t) = t$.

Object Transformations as Group Actions

- Transformations (of an object) are viewed as actions of a group.

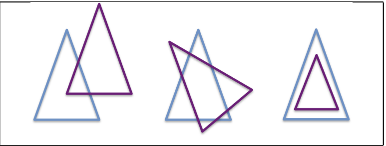
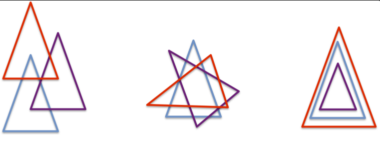
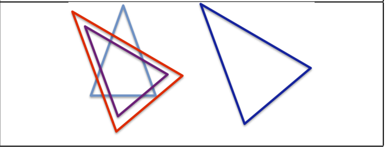
- What is a Group Action:
  Given a set M and a group G, the (left) group action of G on M is defined to be a map: $G \times M \to M$, written as (g, p) such that:
  - $(g_1, (g_2, p)) = (g_1 \cdot g_2, p)$, for all $g_1, g_2, \in G$, $p \in M$.
  - $(e, p) = p$, $\forall p \in M$

- Examples:
  - Translation Group: $\mathbb{R}^n$ with additions, $M = \mathbb{R}^n$:
    Group action $(y, x) = (x + y)$
  - Rotation Group: $SO(n)$ with matrix mulitplication, $M = \mathbb{R}^n$:
    Group action $(O, x) = Ox$
  - Scaling Group: $\mathbb{R}_+$ with multiplication, $M = \mathbb{R}^n$:
    Group action $(a, x) : ax$.



Object Transformations as Group Actions

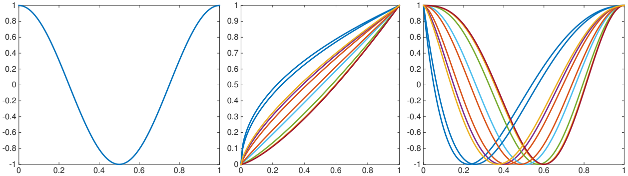
- What is the advantage of viewing transformations as group actions? One can compose these group elements to form composite transformations.

Single Transform	
Double Transform	
Composite Transform	

A Transformation of Functions: Time Warping

- Diffeo Group: Γ with compositions,
  $M = \mathcal{F}$, the set of smooth functions on $[0, 1]$.

  Group action: $(f, \gamma) = f \circ \gamma$, time warping!



f $\{\gamma_i\}$ $\{f \circ \gamma_i\}$

- We will use this group to register – align peaks and valleys – of scalar functions.

- Very important group in shape analysis of functional data.

Shapes are Represented by Orbits

- Shapes are not represented by single points in a space – they are represented by sets.

- What are Orbits:
  For a group G acting on a manifold M, and a point $p \in M$, the orbit of p:

$$[p] = \{(g, p) | g \in G\}$$

  If $p_1, p_2 \in [p]$, then there exists a $g \in G$ s. t. $p_2 = (g, p_1)$.

- Examples:
  - Translation Group: $\mathbb{R}^n$ with additions, $M = \mathbb{R}^n$
    $[x] = \mathbb{R}^n$: All possible translations of a point.
  - Rotation Group: $SO(n)$ with matrix mulitplication, $M = \mathbb{R}^n$
    $[x]$ is a sphere with radius $\|x\|$: All possible rotations of a point (a vector from origin).
  - Scaling Group: $\mathbb{R}_+$ with multiplication, $M = \mathbb{R}^n$
    $[x]$ = a half-ray almost reaching origin: All possible scalings of a vector from origin.
  - Time Warping Group Γ: $[f]$ is the set of all possible time warpings of $f \in \mathcal{F}$.

Shape Spaces are Quotient Spaces

- Two elements of an orbit have exactly the same shape. Orbits are either equal or disjoint. They partition the original space M.

Quotient Space M/G

The set of all orbits is called the quotient space of M modulo G.

$$M/G = \{[p] | \in p \in M\} \ .$$

Quotient Metric

Let d_m be a distance on M such that: (1) the action of G on M is by isometry under d_m, and (2) the orbits of G are closed sets, then:

$$\boxed{d_{m/g}([p],[q]) = \inf_{g \in G} d_m(p,(g,q)) = \inf_{g \in G} d_m((g,p),q)}$$

Group action is by isometry: $d_m(p,q) = d_m((g,p),(g,q))$. This forms the basis for all of shape analysis.

- The minimization over a group (usually rotation or reparameterization) is called alignment or registration.

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——————— Coffee Break (15 mins) ———————-

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Traditional Functional Analysis: Hilbert Structure

Let $\mathcal{F}$ be a function space.

- Vector Space: For any $f_1, f_2 \in \mathcal{F}$ and $a_1, a_2 \in \mathbb{R}$, we have $a_1 f_1 + a_2 f_2 \in \mathcal{F}$.
- Banach Space: $\mathcal{F}$ is complete, and there exists a norm on $\mathcal{F}$. (Recall the definition of a norm).
- Hilbert Space: $\mathcal{F}$ is a Banach space, and there is an inner product associated with the norm on $\mathcal{F}$.
  Example: Set of square-integrable functions
  - Standard $\mathbb{L}^2$ inner product: $\langle f_1, f_2 \rangle = \int_D \langle f_1(t), f_2(t) \rangle \, dt$.
  - $\mathbb{L}^2$ norm or $\mathbb{L}^2$ distance:
    $\|f_1 - f_2\| = \langle f_1 - f_2, f_1 - f_2 \rangle = \sqrt{\int_D \langle f_1(t) f_1 - f_2(t), f_1(t) - f_2(t) \rangle \, dt}$
  - Denote: $\mathbb{L}^2(D, \mathbb{R}^k) = \{f : D \to \mathbb{R}^k | \|f\| < \infty\}$. Often use $\mathbb{L}^2$ for the set.
  - Shortest path between any two points, f_1, f_2 in $\mathbb{L}^2$ is a straight line:
    $$\alpha(\tau) = (1 - \tau) f_1 + \tau f_2 \, .$$
    The length of this path is $\|f_1 - f_2\|$.
- This is the most common/convenient mathematical platform used in Functional Data Analysis.

Computing Data Summary:
Let $f_1, f_2, \ldots, f_n$ be data samples from a distribution P on $\mathbb{L}^2$.

- Mean function $\mu(t) = E_P[f](t)$, $\hat{\mu}(t) = \frac{1}{n}\sum_i f_i(t)$.
  A metric view point: (check)

$$\hat{\mu} = \operatorname*{argmin}_{f \in \mathcal{F}} \sum_{i=1}^{n} \|f - f_i\|^2 .$$

- Covariance function $C(s,t) = E_P[(f(t) - \mu(t))(f(s) - \mu(s))]$.
  - Sample covariance function:

$$\hat{C}(s,t) = \frac{1}{n-1} \sum_{i=1}^{n} (f_i(t) - \hat{\mu}(t))(f_i(s) - \hat{\mu}(s)) .$$

  - Viewed as a linear operator on $\mathbb{L}^2$:

$$\mathcal{A} : \mathbb{L}^2 \to \mathbb{L}^2, \quad \mathcal{A}f(t) = \int_0^1 C(t,s) f(s) ds .$$

  Self-adjoint, bounded, linear operator. Has spectral decomposition (eigen functions).

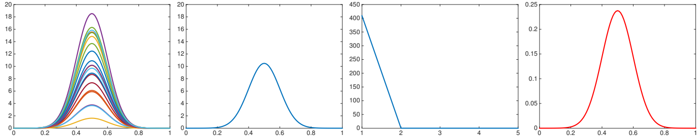
Functional PCA – FPCA

- Random $f \in \mathbb{L}^2$ and assume that the covariance $C(t, s)$ is continuous.
- Karhunen-Loeve theorem states that f can be expressed in terms of an orthonormal basis $\{e_j\}$ of $\mathbb{L}^2$:

$$f(t) = \sum_j z_j e_j(t)$$

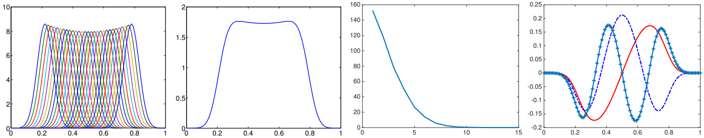
  where $\{z_j\}$ are mean zero and uncorrelated.
- Practice: Discretize the sample covariance matrix at T time points and get $C \in \mathbb{R}^{T \times T}$, use the svd $C = U \Sigma U^T$, then the columns of U provide (samples from) eigenfunctions of f.

- Well aligned data

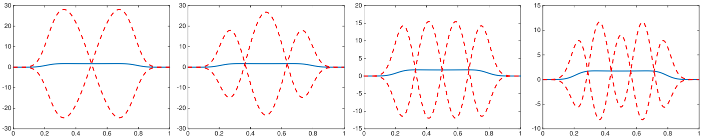


function data $\{f_i\}$ | mean $\hat{\mu}_f$ | singular values | $\hat{b}_1$

- Unaligned data



function data | sample mean $\hat{\mu}_f$ | singular values | $\hat{b}_1, \hat{b}_2, \hat{b}_3$



$\hat{\mu}_f \pm \lambda_1 \hat{b}_1$ | $\hat{\mu}_f \pm \lambda_2 \hat{b}_2$ | $\hat{\mu}_f \pm \lambda_3 \hat{b}_3$ | $\hat{\mu}_f \pm \lambda_4 \hat{b}_4$

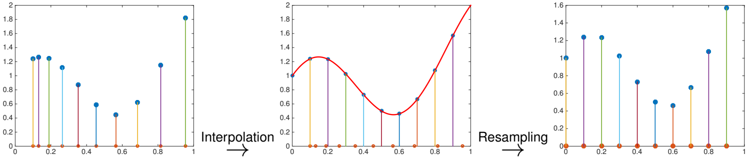
A quick note on numerical implementation.

- We assume that all functions are sampled on a fixed, dense, uniform grid on [0, 1]. Then, we can approximate integral with finite sums:

$$\langle f, g \rangle = \int_0^1 f(t)g(t)\, dt \approx \sum_{i=1}^{N} f(\frac{i}{N})g(\frac{i}{N})\frac{1}{N} .$$

- What if the data is sparse, noisy or nonuniform? Resample it on a fixed, dense, uniform grid.

- Fit a function to the sparse data and resample it on the fixed, dense, uniform grid on [0, 1]



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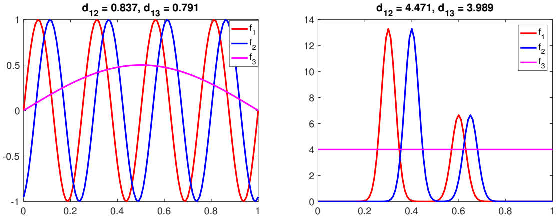
Problems with this Setup

- Most of the FDA literature is centered around the $\mathbb{L}^2$ norm. But there are some major problems with this choice.
- Distances (under $\mathbb{L}^2$ metric) are larger than they should be.



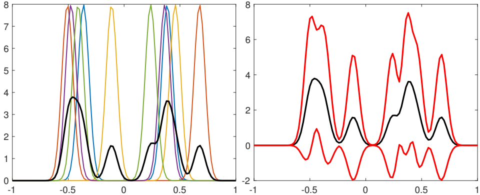
- Misalignment (or phase variability) can be incorrectly interpreted as actual (amplitude) variability.

Problems with FDA as Setup So Far

- Recall that the average under $\mathbb{L}^2$ norm is given by:

$$\bar{f}(t) = \frac{1}{n}\sum_{i=1}^{n} f_i(t) \ .$$

- Function averages under the $\mathbb{L}^2$ norm are not representative!



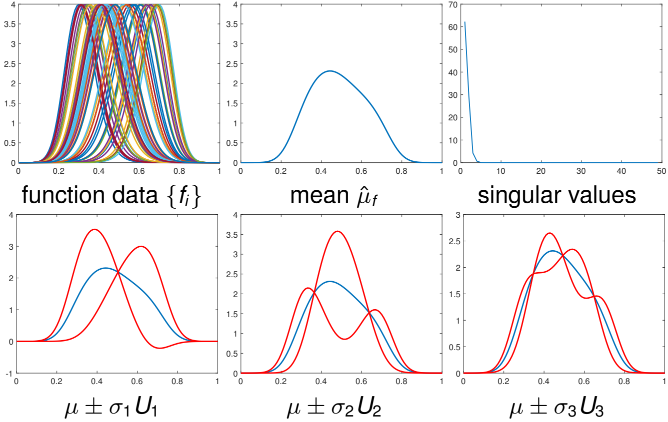
$\{f_i\}$, $\bar{f}$ $\qquad$ $\bar{f} \pm$ std

Individual functions are all bimodal and the average is multimodal!

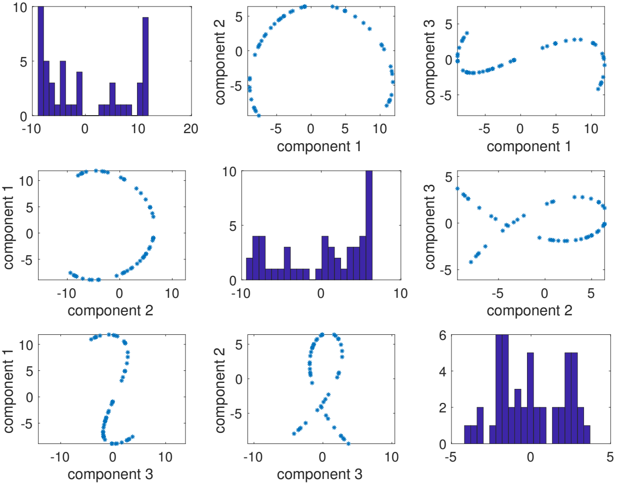
- In $\bar{f}$, the geometric features (peaks and valleys) are smoothed out. They are interpretable attributes in many situations and they need to be preserved

FPCA: Data With Phase Variability

$n = 50$ functions, $f_i(t) = f_0(\gamma_i(t))$, γ_is are random time warps.



FPCA: Data With Phase Variability

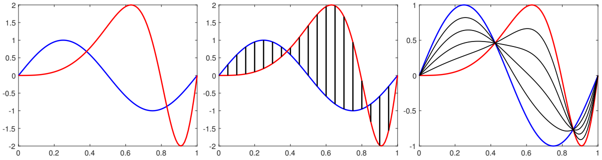


Real Issue: Improper Registration

- $\mathbb{L}^2$ norm uses vertical registration:

$$\|f_1 - f_2\|^2 = \int_0^1 (f_1(t) - f_2(t))^2 \, dt \; .$$

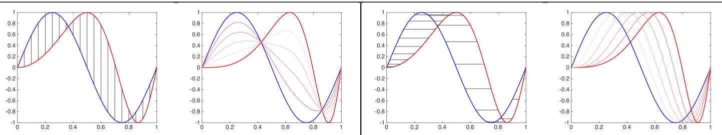
For each t, $f_1(t)$ is being compared with $f_2(t)$.



- The geodesic path (interpreted as the deformation between f_1 and f_2) is unnatural as geometric features (peaks and valleys) are lost or created arbitrarily.

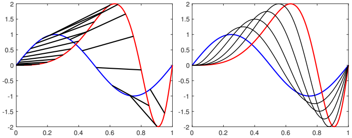
Real Issue

- What if the variability is more naturally horizontal:



Registration Geodesic Registration Geodesic

- Or, maybe a combination of vertical and horizontal:

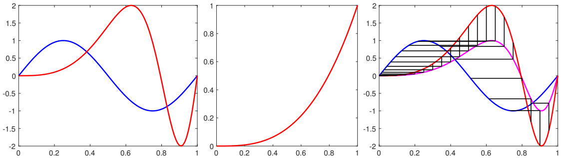


Registration Geodesic

- The question is: How can we detect the compute and decompose the differences into horizontal and vertical components.

Registration Framework

- How to perform registration?
- For functional objects of the type $f : [0, 1] \to \mathbb{R}$, registration is essentially a diffeomorphic deformation of the domain.
- Let $\gamma : [0, 1] \to [0, 1]$ be a diffeomorphism. Then, then $f_1(t)$ is said to be registered to $f_2(\gamma(t))$. Composition by γ is called *time warping*.
- How to define and find optimal γ? The warping γ should be chosen so that the geometric features (peaks and valleys) are well aligned.



- The deformation $t \mapsto \gamma(t)$ is called the *phase variability* and the residual $f_1(t) - f_2(\gamma(t))$ is called the *amplitude* or *shape* variability.

Problem Setup:

- Let $f_1, f_2 : [0, 1] \to \mathbb{R}$ be two functions.
- Γ is the group of orientation-preserving diffeomorphisms of $[0, 1]$ to itself. Γ is a group with composition. γ_{id} is the identity element.
- Question: What should be the objective function: $E(f_1, f_2 \circ \gamma)$, for defining optimal registration?

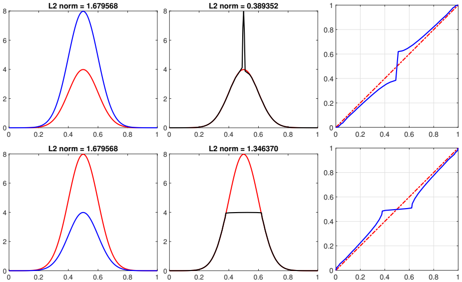
Desired Properties of E:

- If $\hat{\gamma}$ registers f_1 to f_2, then $\hat{\gamma}^{-1}$ should register f_2 to f_1.
- If $f_2 = cf_1$ for a positive constant c, then $\hat{\gamma} = \gamma_{id}$. Shapes are more important than heights.
- It will be nice to have $min_{\gamma} E(f_1, f_2 \circ \gamma)$ as a proper metric.

- A natural quantity to define E for optimal registration is the $\mathbb{L}^2$ norm, i.e.

$$\boxed{\hat{\gamma} = \arg\inf_{\gamma \in \Gamma}(\|f_1 - f_2 \circ \gamma\|^2).}$$

- However, this choice is degenerate – pinching effect!

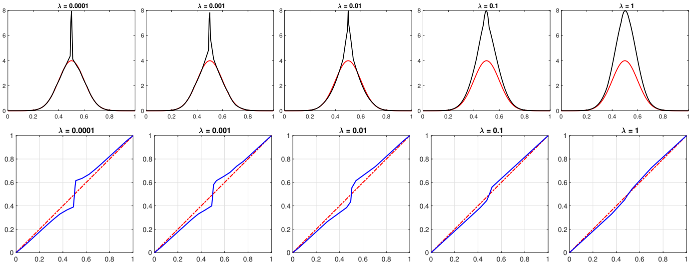


f_1, f_2 $\quad$ $f_1, f_2 \circ \hat{\gamma}$ $\quad$ $\hat{\gamma}$

- Common solution – add penalty:

$$\hat{\gamma} = \arg\inf_{\gamma \in \Gamma}(\|f_1 - f_2 \circ \gamma\|^2 + \lambda \mathcal{R}(\gamma)).$$

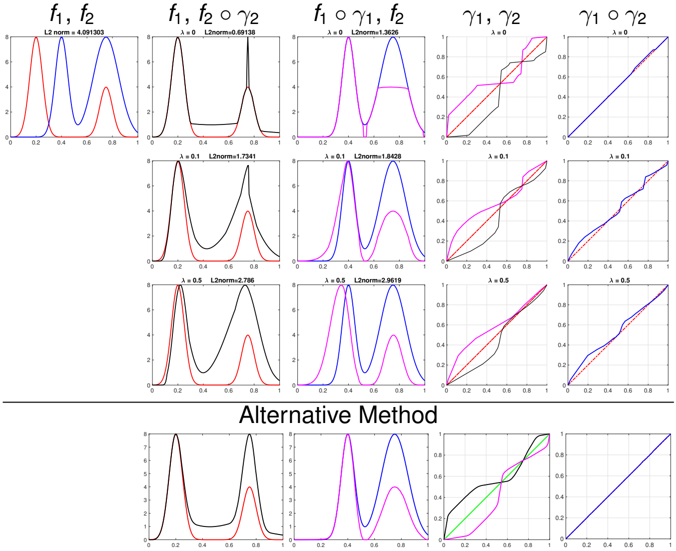
- Effectively reducing the search space, not really solving the problem.
- Example: Using the first order penality $\mathcal{R} = \int_D |\dot{\gamma}(t)|^2 dt$.



- One can use other penalty terms instead.

Problems: Penalized $\mathbb{L}^2$ Alignment

- The right balance between alignment and penalty?



Problems: Penalized $\mathbb{L}^2$ Alignment

- Asymmetry: Discussed earlier

$$\inf_{\gamma}(\|f_1 - f_2 \circ \gamma\|^2 + \lambda \mathcal{R}(\gamma)) \neq \inf_{\gamma}(\|f_1 \circ \gamma - f_2\|^2 + + \lambda \mathcal{R}(\gamma)) \ .$$

- Triangle inequality: The following does not hold –

$$\begin{aligned} \inf_{\gamma}(\|f_1 - f_3 \circ \gamma\|^2 + \lambda \mathcal{R}(\gamma))) &\leq \inf_{\gamma}(\|f_1 \circ \gamma - f_2\|^2 + \lambda \mathcal{R}(\gamma)) \\ &+ \mathit{inf}_{\gamma}(\|f_2 \circ \gamma - f_3\|^2 + \lambda \mathcal{R}(\gamma)) \ . \end{aligned}$$

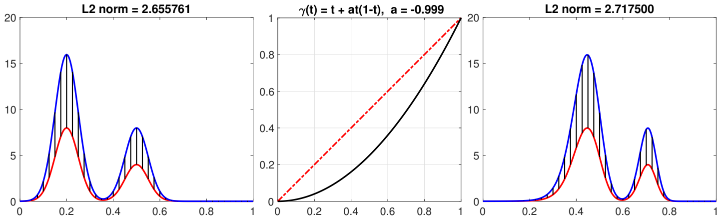
- Most fundamental issue: Not invariant to warping

$$\|f\| \neq \|f \circ \gamma\| \ .$$

The norm $\|f \circ \gamma\|$ can be manipulated to have a large range of values, from $\min(|f|)$ to $\max(|f|)$ on $[0, 1]$.

Why Invariance to Warping?

- Registration is preserved under identical warping!
  $[f_1(t), f_2(t)]$ are registered before warping, and $[f_1(\gamma(t)), f_2(\gamma(t))]$ are registered after warping.



- The metric or objective function for measuring registration should also be invariant to identical warping.

- $\mathbb{L}^2$ norm is not invariant to identical warping.

Desired Properties for Objective Function

We want to use a cost function $d(f_1, f_2)$ for alignment, so that:

- Invariance: $d(f_1, f_2) = d(f_1 \circ \gamma, f_2 \circ \gamma)$, for all γ.
  Technically, the action of Γ on $\mathcal{F}$ is by isometries.
- Registration problem can be:

$$(\gamma_1^*, \gamma_2^*) = \operatorname*{arginf}_{\gamma_1, \gamma_2 \in \tilde{\Gamma}} d(f_1 \circ \gamma_1, f_2 \circ \gamma_2) \ .$$

  $\tilde{\Gamma}$ is a closure of Γ to make orbits closed set.

- Symmetry will hold by definition.
- Triangle inequality: Let $d_s(f_1, f_2) = \inf_{\gamma_1, \gamma_2} d(f_1 \circ \gamma_1, f_2 \circ \gamma_2)$. Then, we want:

$$d_s(f_1, f_3) \leq d_s(f_1, f_2) + d_s(f_2, f_3) \ .$$

- We want d_s to be proper metric so that we can use d_s for ensuing statistical analysis.

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- There exists a distance that satisfies all these properties. It is called the *Fisher-Rao Distance*:

$$d_{FR}(f_1, f_2) = d_{FR}(f_1 \circ \gamma, f_2 \circ \gamma), \text{ for all } f_1, f_2 \in \mathcal{F}, \gamma \in \Gamma.$$

  For many years, this nice invariant property was well known in the literature. The question was: How to compute d_{FR}? The definition was to difficult to lead to a simple expression.

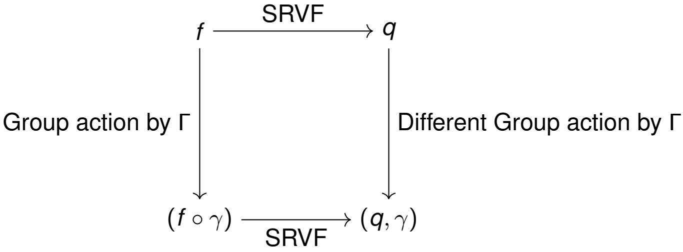
- Joshi et al. (2007) and Srivastava et al. (2011) introduced the SRVF. (Has similarities to the complex square-root of Younes 1999.) Define a new mathematical representation called square-root velocity function (SRVF):

$$q(t) \equiv \begin{cases} \frac{\dot{f}(t)}{\sqrt{|\dot{f}(t)|}} & |\dot{f}(t)| \neq 0 \\ 0 & |\dot{f}(t)| = 0 \end{cases}$$

  ($f : [0, 1] \to \mathbb{R}^n$, $q : [0, 1] \to \mathbb{R}^n$)

- SRVF is invertible up to a constant: $f(t) = f(0) + \int_0^t |q(s)|q(s)ds$.

- Under SRVF, the Fisher-Rao distance simplifies: $d_{FR}(f_1, f_2) = \|q_1 - q_2\|$.
- The SRVF of $(f \circ \gamma)$ is $(q \circ \gamma)\sqrt{\dot{\gamma}}$. Just by chain rule. We will denote $(q, \gamma) = (q \circ \gamma)\sqrt{\dot{\gamma}}$.
  Commutative Diagram:



SRVF Representation

- *Lemma*: This distance satisfies: $d_{FR}(f_1, f_2) = d_{FR}(f_1 \circ \gamma, f_2 \circ \gamma)$ We need to show that $\|(q_1 \circ \gamma)\sqrt{\dot{\gamma}} - (q_2 \circ \gamma)\sqrt{\dot{\gamma}}\| = \|q_1 - q_2\|$.

$$\begin{aligned} \|(q_1, \gamma) - (q_2, \gamma)\|^2 &= \int_0^1 (q_1(\gamma(t))\sqrt{\dot{\gamma}(t)} - q_2(\gamma(t))\sqrt{\dot{\gamma}(t)})^2 dt \\ &= \int_0^1 (q_1(\gamma(t)) - q_2(\gamma(t)))^2 \dot{\gamma}(t) dt = \|q_1 - q_2\|^2 . \square \end{aligned}$$

- Corollary: For any $q \in \mathbb{L}^2$ and $\gamma \in \Gamma_I$, we have $\|q\| = \|(q, \gamma)\|$. This group action is norm preserving, like a rotation. Can't have pinching!
- Registration Solution:

$$\boxed{(\gamma_1^*, \gamma_2^*) = \text{arginf}_{\gamma_1, \gamma_2} \|(q_1 \circ \gamma_1)\sqrt{\dot{\gamma}_1} - (q_2 \circ \gamma_2)\sqrt{\dot{\gamma}_2}\| \ .}$$

One approximates this solution with:

$$\gamma^* = \underset{\gamma}{\text{arginf}} \|q_1 - (q_2 \circ \gamma)\sqrt{\dot{\gamma}}\| \ .$$

This is solved using dynamic programming.

- Where does SRVF come from?
- Fisher-Rao Riemannian Metric: For functions, there is a F-R metric

$$\langle\langle \delta f_1, \delta f_2 \rangle\rangle_f = \int_0^1 \dot{\delta f}_1(t)\dot{\delta f}_2(t)\frac{1}{\dot{f}(t)}dt\ .$$

- Under F-R metric, the time warping action is by Isometry:

$$\langle\langle \delta f_1, \delta f_2 \rangle\rangle_f = \langle\langle \delta f_1 \circ \gamma, \delta f_2 \circ \gamma \rangle\rangle_{f\circ\gamma}.$$

  (Note this is different from the F-R metric for pdfs, but same as the F-R for cdfa.)
- Under the mapping $f \mapsto q$, Fisher-Rao metric transforms to the $\mathbb{L}^2$ metric:

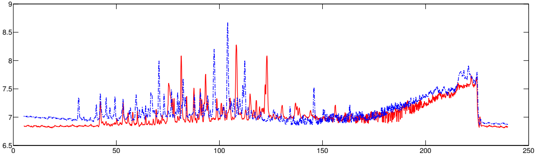
$$\underbrace{\langle\langle \delta f_1, \delta f_2 \rangle\rangle_f}_{\text{Fisher-Rao metric}} = \underbrace{\langle \delta q_1, \delta q_2 \rangle}_{\mathbb{L}^2 \text{ inner product}}$$

Nice isometric, bijective mapping from $\mathcal{F}$ to $\mathbb{L}^2$

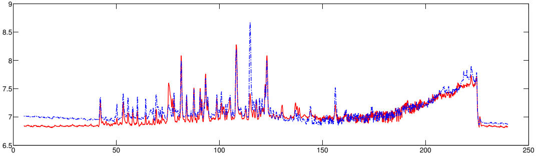
	Function Space $\mathcal{F}$ Absolutely continuous functions	**SRVF Space** $\mathbb{L}^2$ Square-integrable functions
1	Functions and tangents f, and $\delta f_1, \delta f_2 \in T_f(\mathcal{F})$	Functions and tangents q, $\delta q_1, \delta q_2 \in \mathbb{L}^2$
2	Fisher-Rao Inner Product $\int_0^1 \delta \dot{f}_1(t) \delta \dot{f}_2(t) \frac{1}{\dot{f}(t)} dt$	$\mathbb{L}^2$ inner product $\int_0^1 \delta q_1(t) \delta q_2(t)\ dt$
3	Fisher-Rao Distance $d_{FR}(f_1, f_2) = ???$	$\mathbb{L}^2$ norm $\mathbb{L}^2$ norm: $\|q_1 - q_2\|$
4	Geodesic Under Fisher-Rao ??	Straight line $\tau \mapsto ((1-\tau)q_1 + \tau q_2)$
5	Mean of functions under d_{FR} ??	Cross-Section Mean $\frac{1}{n}\sum_{i=1}^n q_i$
6.	Registration under d_{FR} $\inf_\gamma d_{FR}(f_1, f_2 \circ \gamma)$	Registration under $\mathbb{L}^2$ $\inf_\gamma \|q_1 - (q_2 \circ \gamma)\sqrt{\dot{\gamma}})\|$
7	FPCA analysis under d_{FR}	FPCA analysis under $\mathbb{L}^2$ norm

Any item on the left can be accomplished by computing the corresponding item on the right and bringing back the results.

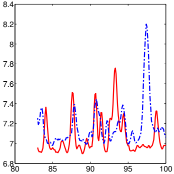
Liquid chromatography - Mass spectrometry data

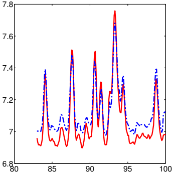


Before



After



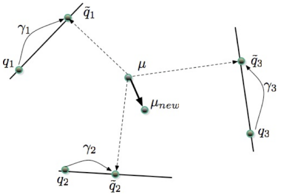


Zoom in: Before Zoom in: After

- Align each function to a template. The template can be the sample mean but under what metric?
- Mean under the quotient space metric:

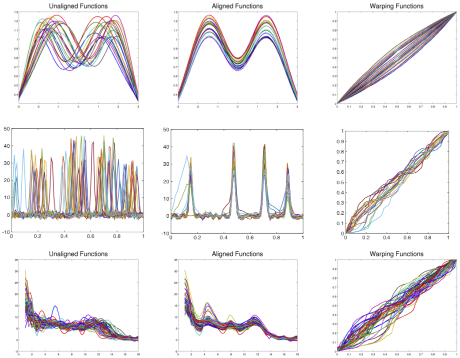
$$\bar{q} = \operatorname*{arginf}_{q \in \mathbb{L}^2} \left(\inf_{\gamma_i} \| q - (q_i, \gamma_i) \|^2 \right) .$$

- Iterative procedure:



1. Initialize the mean μ.
2. Align each q_is to the mean using pairwise alignment to obtain $\hat{\gamma}_i = \operatorname{arginf}_{\gamma_i} \| q - (q_i, \gamma_i) \|^2$, and set $\tilde{q}_i = (q_i, \hat{\gamma}_i)$.
3. Update mean using $\mu = \frac{1}{n} \sum_{i=1}^{n} \tilde{q}_i$.
4. Check for convergence. If not converged, go to step 2.

Multiple Registration: Examples



$\{f_i\}$ Amplitude $\{\tilde{f}_i\}$ Phase $\{\gamma_i\}$

- One can view this separation $f_i = (\tilde{f}_i, \gamma_i)$, as being analogous to polar coordinates of a vector $v = (r, \theta)$.
- In most cases, one of the two components is more useful than the other. So, separation helps put different weights on these components.

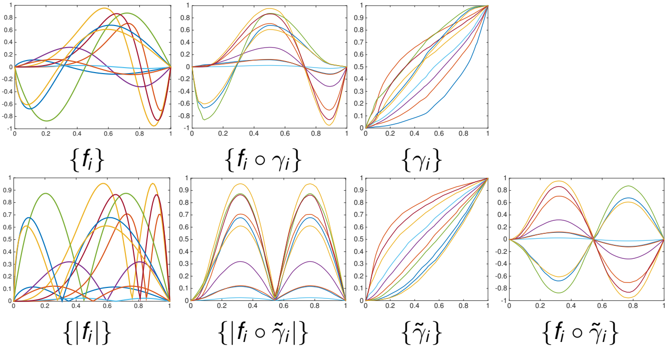
Multiple Registration: Examples

Matlab Code – Demo

Alignment After Transformation

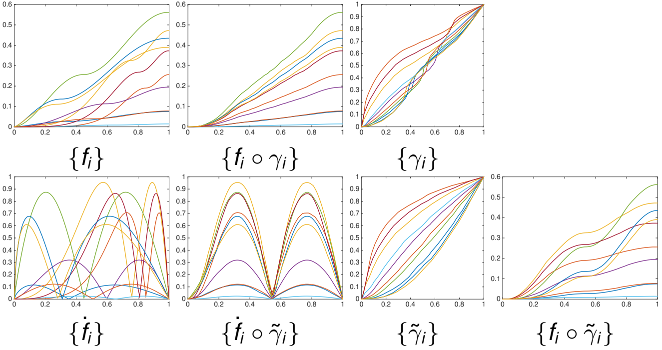
Sometimes it is useful to transform the data before applying alignment procedure. Some of these transformations are: $|f_i(t)|$, $\dot{f}_i(t)$, $\log|f_i(t)|$, etc.

- Absolute Value: When optimal points are to be aligned (irrespective of them being peaks or valleys).



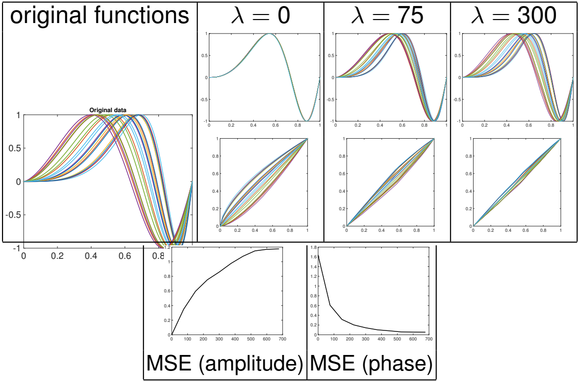
Alignment After Transformation

- Derivatives: When aligning montonoic functions



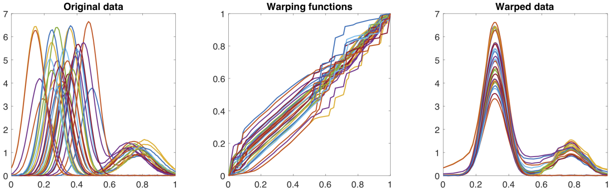
Penalized Elastic Alignment

- If we want to control the elasticity, we can also add a roughness penalty.
  $\inf_{\gamma \in \Gamma} \left(\|q_1 - (q_2, \gamma)\|^2 + \lambda \mathcal{R}(\gamma) \right)^{1/2}$
- For example, using a first order penalty: $\mathcal{R}(\gamma) = \|1 - \sqrt{\dot{\gamma}}\|^2$.



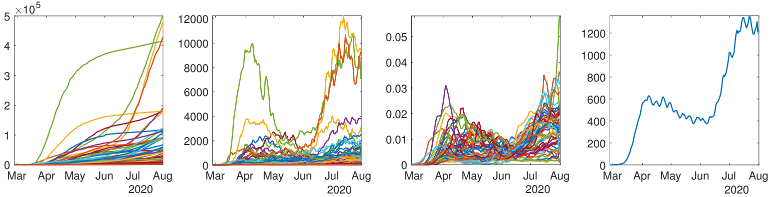
- We loose some nice mathematical properties - no longer have a metric in the quotient space.

Post Separation Analysis



- Once we separate phase and amplitude components from the data, we can perform more standard data analysis.
- We can perform FPCA of these components separately and model their distributions.
- We can weight these components differently to cluster and classify functional data.

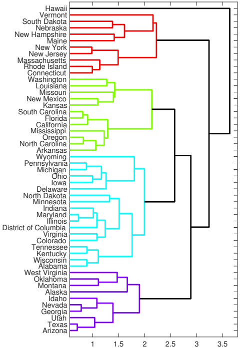
- COVID-19 rate curves – the count of new infections in a state as a function of time.

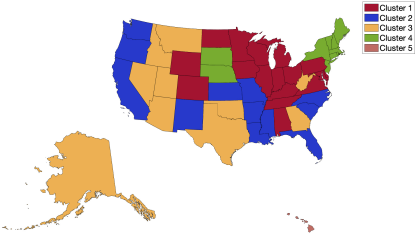


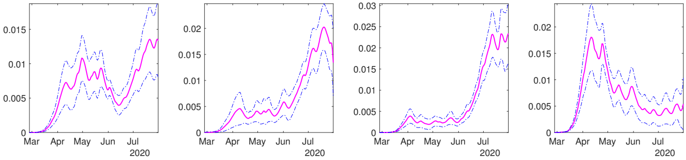
- From left to right:
  - Cumulative COVID-19 positive counts for each state.
  - COVID rates: Daily new COVID-19 positive counts.
  - Smoothed and normalized (to area under the curve being one) for each state separately.
  - Average of all curves before normalization.
- We study shapes of normalized rate curves for different states.

COVID Rate Curves

Clustering of states: Five clusters, Hawaii is an outlier







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1. Introduction, Motivation, and Background (1:00 - 1:30pm)
   - Introduction and Motivational Examples
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   - Background: Functional Data Analysis Using $\mathbb{L}^2$ Metric
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   - Registration Problem
   - Fisher-Rao Metric and Square-Root Velocity Function

—————— Coffee Break (15 mins) ——————-

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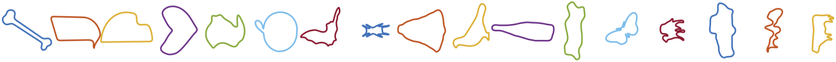
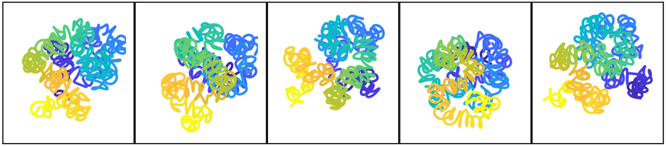
Shape Analysis of Curves

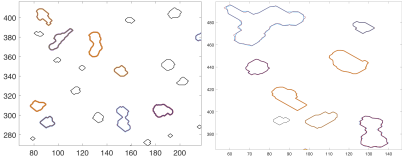
- Shape analysis of silhouettes of objects in images.



- Shape analysis of chromosomal configurations:



- Nanoparticles:



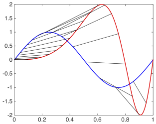
Objects of Interest

- Assume all the objects have the same topology, as described below.
- Euclidean Curves: They are all maps of the type: $f : D \to \mathbb{R}^k$, where D is a one-dimensional compact space. Examples:
  - $D = [0, 1]$: f can be open or closed curve
  - $D = \mathbb{S}^1$: f is called a closed curve
- Curves on Manifolds: They are all maps of the type: $f : D \to M$, where D is a one-dimensional compact space. Examples:
  - $D = [0, 1]$: f is called an open curve
  - $D = \mathbb{S}^1$: f is called a closed curve

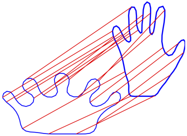
  Often call them trajectories on manifolds.

What is the Registration Problem

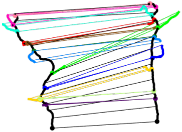
- Registration: Which point on one object matches with which point on the other object.
- In order to compare any two shapes, one needs to (densely) register points across objects.



functions



curves



trees (neurons)

Registration Problem

- Is arc-length parameterization a solution?
- No. Here is why –

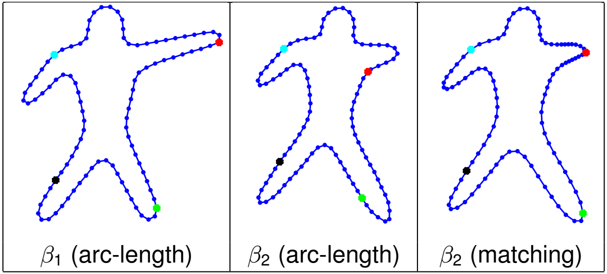
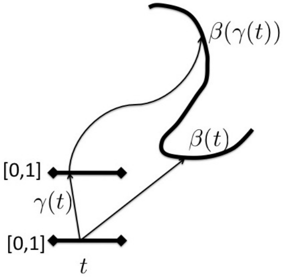


Figure: Registration of points across two curves using the arc-length and a convenient non-uniform sampling. Non-uniform sampling allows a better matching of features between β_1 and β_2.

Elastic Shape Analysis

Perform registration and shape comparison (analysis) simultaneously.

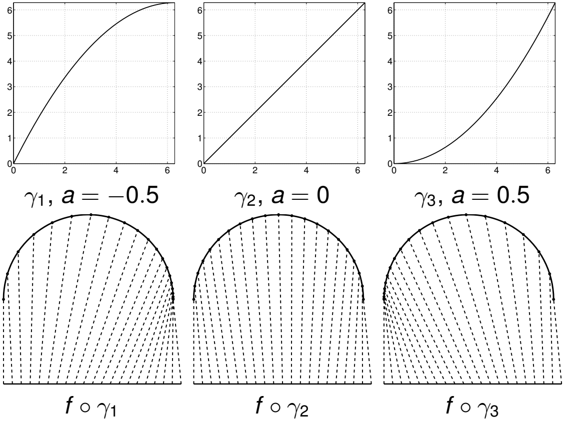
- Parametrized curves – $f : [0,1] \to \mathbb{R}^2$, $\mathbb{S}^1 \to \mathbb{R}^2$.



- Let Γ be the set of all diffeomorphisms of $[0,1]$ that preserve the boundaries. Elements $\gamma \in \Gamma$, plays the role of a re-parameterization function.
- For any curve $f : [0,1] \to \mathbb{R}^2$, and $\gamma \in \Gamma$, the composition $f \circ \gamma$ is a re-parameterization of f.
- Γ is a group (with composition as group operation), and $f \mapsto (f, \gamma) = f \circ \gamma$ defines a group action on the space of curves.

Example: Re-Parameterization

Example: $\gamma_a(t) = t + at(1-t), \quad -1 < a < 1.$



Shape-Preserving Transformations

- The following group actions are shape preserving:
  - Translation: For any $x \in \mathbb{R}^2$, the $f(t) \mapsto x + f(t)$ denotes a translation of f.
  - Rotation: For any $O \in SO(2)$, the $f(t) \mapsto Of(t)$ denotes a rotation of f.
  - Scaling: For any $a \in \mathbb{R}_+$, the $f(t) \mapsto af(t)$ denotes the translation of f.
  - Re-parameterization: For any $\gamma \in \Gamma$, $f(t) \mapsto f(\gamma(t))$ is a re-paramaterization of f.
- We want shape metrics and shape analysis to be invariant to these actions. For instance, if d_s is a shape metric, then we want:

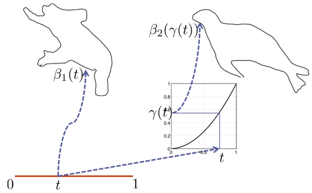
$$d_s(f_1, f_2) = d_s(aO(f_1 \circ \gamma) + x, f_2), \quad \forall a \in \mathbb{R}_+, O \in SO(2), \gamma \in \Gamma, x \in \mathbb{R}^2$$

- These transformations are considered nuisance in shape analysis.

Registration Through Re-Parametrizations

Re-parameterization is not entirely a nuisance transformation. It is useful in solving the registration problem.

- Take two parameterized curves $f_1, f_2 : [0,1] \to \mathbb{R}^2$.
- For any t, the point $f_1(t)$ on the first curve is said to be registered to the point $f_2(t)$ on the second curve.
- We can change the registration by re-parametrizing the curves.
- If we re-parameterize f_2 by γ, then the new registration is $f_1(t) \leftrightarrow f_2(\gamma(t))$.



- Re-parameterization = Registration

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- Let $f : [0,1] \to \mathbb{R}^n$ be a Euclidean curve. $\dot{f}(t)$ is the velocity vector at $f(t)$.
  - $r(t) = |\dot{f}(t)|$ is the speed function, and
  - $\Theta(t) = \frac{\dot{f}(t)}{r(t)}$ is the direction vector.

  We represent a curve by the pair (r, Θ).
- For a re-parameterized curve $f \circ \gamma$, the representation is given by $((r \circ \gamma)\dot{\gamma}, \Theta \circ \gamma)$.
- Elastic Riemannian Metric for curves: for any a, b,

$$\begin{aligned}\langle(\delta r_1, \delta\Theta_1), (\delta r_2, \delta\Theta_2)\rangle_{(r,\Theta)} &= a^2 \int_0^1 \delta r_1(t)\delta r_2(t)\frac{1}{r(t)}\, dt \\ &+ b^2 \int_0^1 \delta\Theta_1(t)\delta\Theta_2(t) r(t)\, dt.\end{aligned}$$

- This metric is invariant to re-parameterization of f:

$$\langle(\delta((r_1 \circ \gamma)\dot{\gamma}), \delta(\Theta_1 \circ \gamma)), (\delta((r_2 \circ \gamma)\dot{\gamma}), \delta(\Theta_2 \circ \gamma))\rangle_{(((r\circ\gamma)\dot{\gamma}),(\Theta\circ\gamma))}$$
$$= \langle(\delta r_1, \delta\Theta_1), (\delta r_2, \delta\Theta_2)\rangle_{(r,\Theta)}$$

SRVF Representation for Curves

- Define the square-root velocity function (SRVF): $q(t) \equiv \frac{\dot{f}(t)}{\sqrt{|\dot{f}(t)|}} = \sqrt{r(t)}\Theta(t)$.
- Computing variation on both sides, we get:

$$\delta q = \frac{1}{2\sqrt{r(t)}}\delta r(t)\Theta(t) + \sqrt{r(t)}\delta\Theta(t) \ .$$

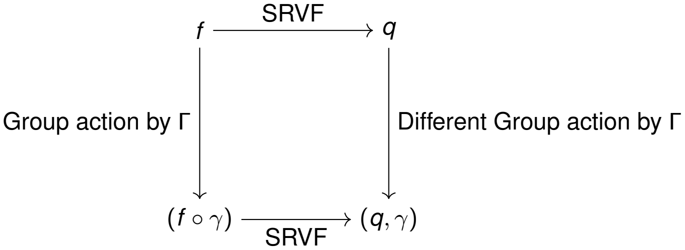
- Taking standard $\mathbb{L}^2$ inner product between two such variations:

$$\langle \delta q_1, \delta q_2 \rangle = \frac{1}{4}\int_0^1 \delta r_1(t)\delta r_2(t)\frac{1}{r(t)}dt + \int_0^1 \langle \delta\Theta_1(t), \delta\Theta_2(t)\rangle \, r(t)dt \ .$$

  Use $\langle \Theta(t), \delta\Theta_i(t)\rangle = 0$.

- This is equal to the elastic Riemannian metric for $a = 1/2$ and $b = 1$. Thus, the mapping $f \mapsto q$ transforms the elastic Riemannian metric into the $\mathbb{L}^2$ metric for these weights.
- The geodesic distance between any f_1 and f_2 under the elastic Riemannian metric (for $a = 1/2$ and $b = 1$) is simply $\|q_1 - q_2\|$.

- We use SRVF q for analyzing shape of a curve f.
- The SRVF of $(f \circ \gamma)$ is $(q \circ \gamma)\sqrt{\dot{\gamma}}$. Just by chain rule. We will denote $(q, \gamma) = (q \circ \gamma)\sqrt{\dot{\gamma}}$.
  Commutative Diagram:



- *Lemma*: The chosen distance satisfies: $d_{FR}(f_1, f_2) = d_{FR}(f_1 \circ \gamma, f_2 \circ \gamma)$
  We need to show that $\|(q_1 \circ \gamma)\sqrt{\dot{\gamma}} - (q_2 \circ \gamma)\sqrt{\dot{\gamma}}\| = \|q_1 - q_2\|$.

$$\begin{aligned} \|(q_1, \gamma) - (q_2, \gamma)\|^2 &= \int_0^1 (q_1(\gamma(t))\sqrt{\dot{\gamma}(t)} - q_2(\gamma(t))\sqrt{\dot{\gamma}(t)})^2 dt \\ &= \int_0^1 (q_1(\gamma(t)) - q_2(\gamma(t)))^2 \dot{\gamma}(t) dt = \|q_1 - q_2\|^2 . \square \end{aligned}$$

- Checking all nuisance transformations:
  1. Translation: SRVF q for a curve f is invariant to its translation !
  2. Scaling: We can rescale all the curves to be of unit length, to get rid of the scale variability. It turns out that $\|q\| = L[f]$. So, if $L[f] = 1$, then the corresponding SRVF q is an element of a unit sphere $\mathbb{S}_\infty$.
  3. Re-parameterization and rotations we can't remove by any such standardization. However, we have the nice property:

$$\|q_1 - q_2\| = \|Oq_1 - Oq_2\| = \|(q_1, \gamma) - (q_2, \gamma)\| \ .$$

- We use the notion of equivalence classes, or orbits, to reconcile the remaining two transformation. For any curve f, and its SRVF q, we its equivalence class to be:

$$[q] = \{O(q, \gamma) | O \in SO(n), \gamma \in \Gamma\} \ .$$

  This set represents SRVFS of all possible rotations and re-parameterizations of f. Each equivalence class represents a shape.

- $\mathbb{S}_\infty \subset \mathbb{L}^2$ is called the pre-shape space.
- The set of all equivalence classes is a quotient space $\mathbb{L}^2/(SO(n) \times \Gamma)$. It is called the shape space.
- The distance between any two curves in the pre-shape space is $\cos^{-1}(\langle q_1, q_2 \rangle)$.
- The distance in the shape space, called the shape metric, is given by:

$$d_s([q_1],[q_2]) = \inf_{(O,\gamma)\in SO(n)\times\Gamma} \cos^{-1}(\langle q_1, O(q_2,\gamma)\rangle) \ .$$

  This include rotational alignment and non-rigid registration of the two curves.
- Given optimal parameters O^*, γ^*, the shortest path or a geodesic is simply:

$$\alpha(\tau) = \frac{1}{\sin(\vartheta)}(\sin(\vartheta(1-t))q_1 + \sin(\vartheta t)q_2^*), \quad \cos(\vartheta) = \langle q_1, q_2^* \rangle \ ,$$

  where $q_2^* = O^*(q_2, \gamma^*)$.

- So far we have developed a technique for computing geodesics and geodesic distances in shape space of all curves.
- Suppose we are interested in only closed curves.
- The SRVF q of a closed curve f satisfies an additional condition:

$$f(0) = f(1) \Leftrightarrow \int_0^1 q(t)|q(t)|dt = 0 \ .$$

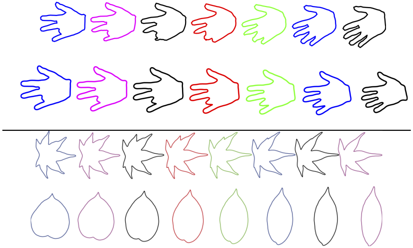
- So we are now interested in the pre-shape space:

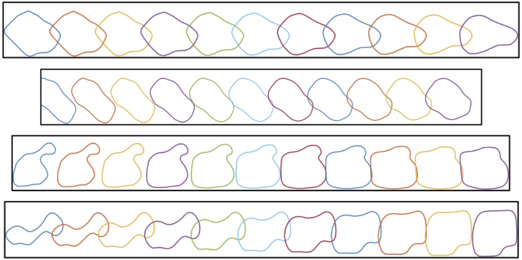
$$\mathcal{C} = \{q \in \mathbb{S}_\infty | \int_0^1 q(t)|q(t)|dt = 0\} \subset \mathbb{S}_\infty \ .$$

  The geodesics here are no longer arcs on great circles. We don't know have analytical expressions for these geodesics or geodesic distances.
- We have developed a numerical technique called path straightening for finding geodesics on $\mathcal{C}$.

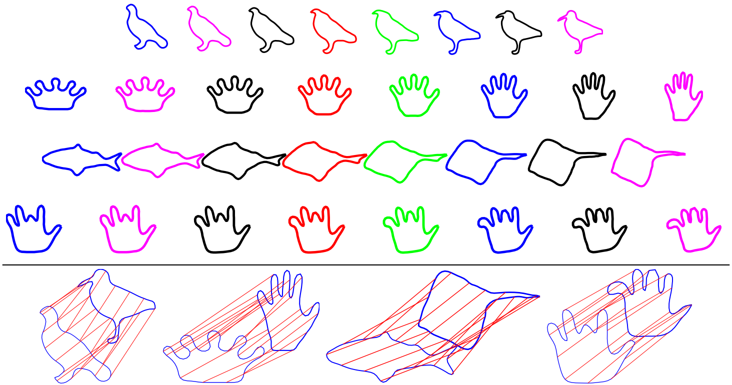
Elastic Geodesics

- Hand contours/ Leaves/ Nanoparticles





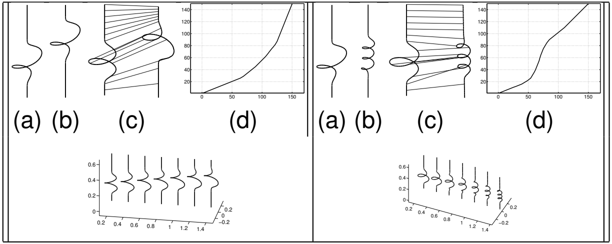
Elastic Geodesics



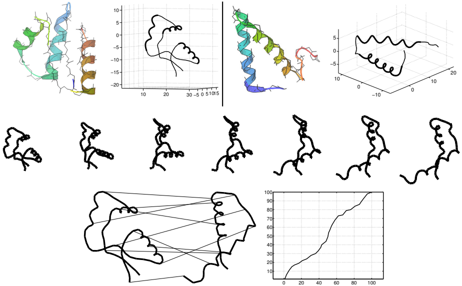
Elastic Geodesics 3D Curves

All these ideas extend easily to curves in higher dimensions.

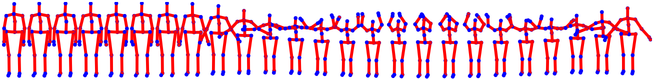
- Example 1:



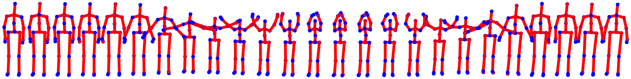
- Example 2:



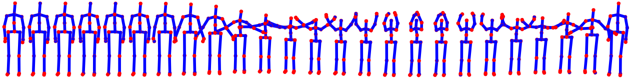
Temporal alignment of human activity data: Two-hand wave



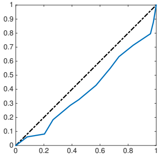
Sequence 1, f_1

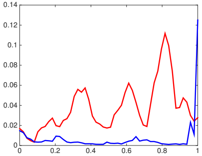


Sequence 2, f_2



Sequence 2 re-parameterized, $f_2 \circ \gamma_1^*$

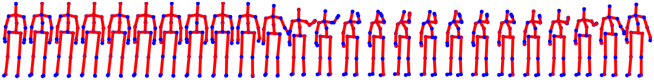




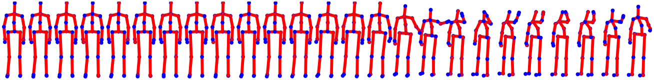
Warping γ^* $\quad\quad$ $|q_1(t) - q_2(t)|, |q_1(t) - q_2(\gamma^*(t))\sqrt{\dot{\gamma}^*(t)}|$

Elastic Registration of High-Dimensional Curves

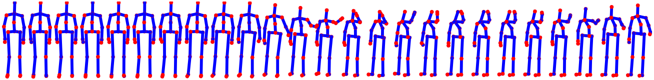
Temporal alignment of human activity data: One-arm wave



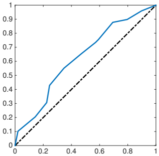
Sequence 1, f_1



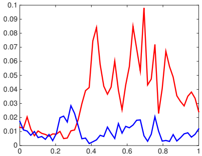
Sequence 2, f_2



Sequence 2 re-parameterized, $f_2 \circ \gamma_1^*$



Warping γ^*



Plots of $|q_1(t) - q_2(t)|$ and $|q_1(t) - q_2(\gamma^*(t))\sqrt{\dot{\gamma}^*(t)}|$

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   - Fisher-Rao Metric and Square-Root Velocity Function

——————— Coffee Break (15 mins) ———————-

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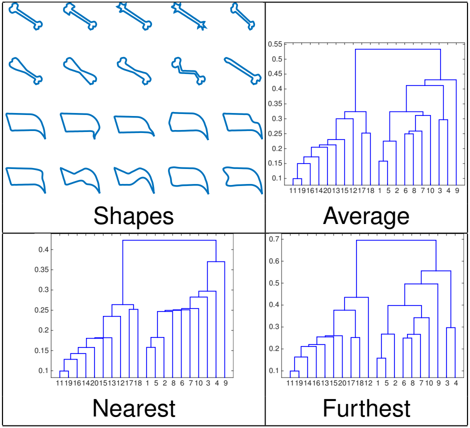


Figure: A set of 20 shapes of the left have been clustered using different linkage criterion: average (top-right), nearest distance (bottom left), and compete or furthest distance (bottom-right).

Shape Clustering

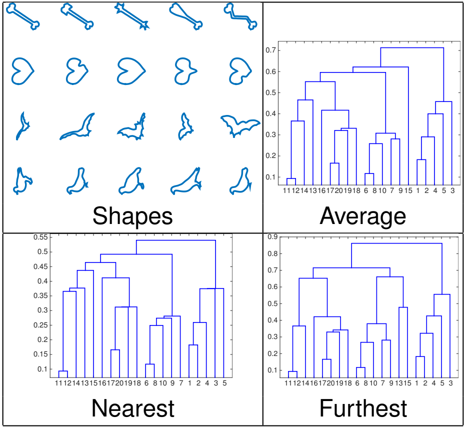
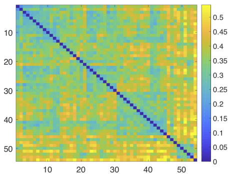
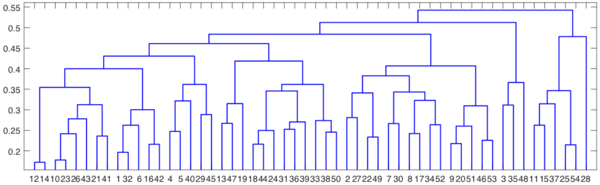


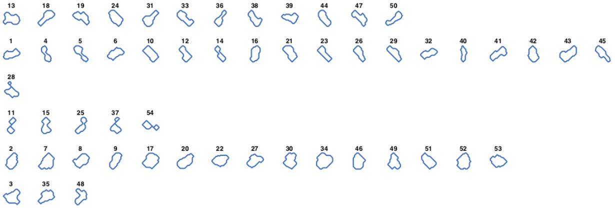
Figure: A set of 20 shapes of the left have been clustered using different linkage criterion: average (top-right), nearest distance (bottom left), and compete or furthest distance (bottom-right).



Pairwise Distance Matrix

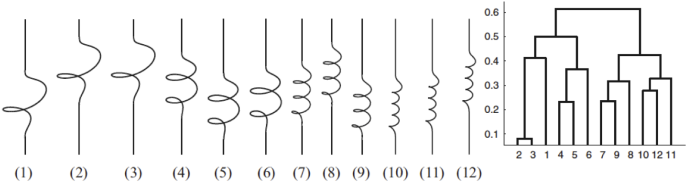


Dendrogram Clustering



Individual Clusters

3D Shape Clustering

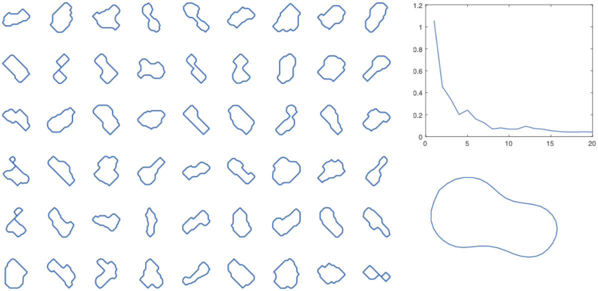


Shape Statistics

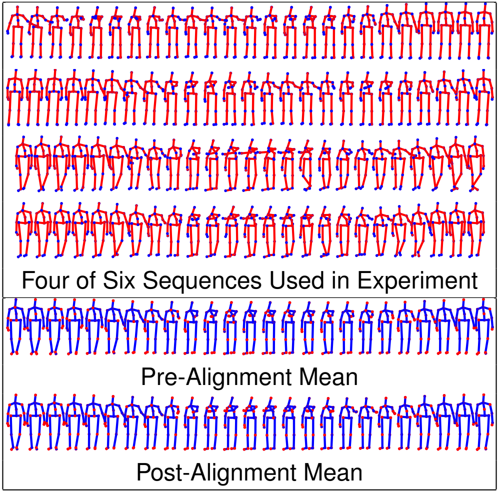
- Sample mean:

$$\mu_q = \operatorname*{argmin}_{[q]\in\mathcal{S}} \sum_{i=1}^{n} d_s([q],[q_i])^2 \ ,$$

and then, $\mu_q \mapsto \mu$.

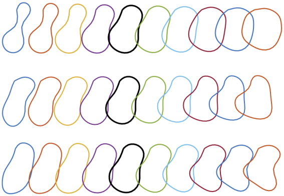


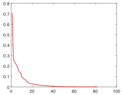
Elastic Averaging of Multiple Shape Sequences



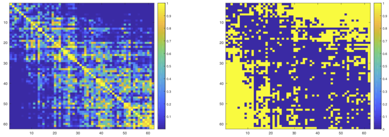
Shape Statistics

- PCA in the tangent space at the mean





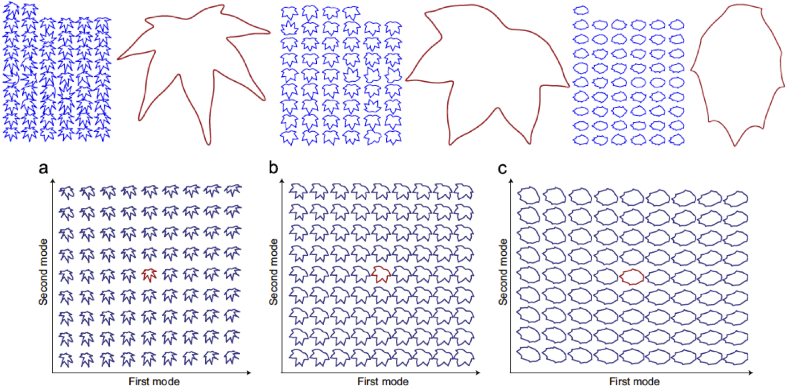
- Testing equality of shape populations across time frames: Truncated Wrapped Normal Distributions



p values (left) and binary decisions (right)

The nanoparticle shape populations across frames are increasing different as the frames are further apart in time.

Leaves Shapes



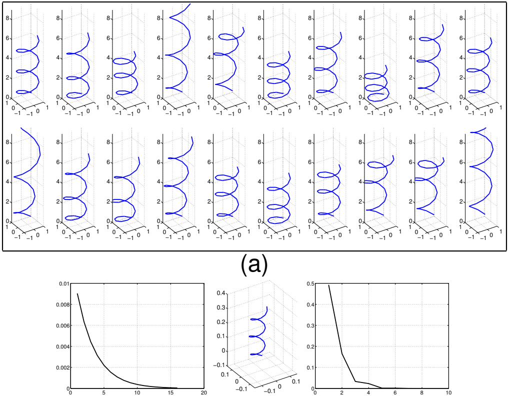
Leaves Classification

Methods	Recognition score
SM200	**99.18**
TAR (Mouine et al., 2013a, 2013b)	90.40
TSL (Mouine et al., 2013a, 2013b)	95.73
TOA (Mouine et al., 2013a, 2013b)	95.20
TSLA (Mouine et al., 2013a, 2013b)	96.53
Shape-Tree (Felzenszwalb and Schwartz, 2007)	96.28
IDSC + DP (Ling and Jacobs, 2007)	94.13
SC + DP (Ling and Jacobs, 2007)	88.12
Fourier descriptors (Ling and Jacobs, 2007)	89.60

Method	Score
SM200 (this paper)	**0.953**
TAR (Mouine et al., 2013a, 2013b)	0.636
TSL (Mouine et al., 2013a, 2013b)	0.757
TOA (Mouine et al., 2013a, 2013b)	0.780
TSLA (Mouine et al., 2013a, 2013b)	0.779
IFSC_USP_run2	0.402
inria_imedia_plantnet_run1	0.464
IFSC_USP_run1	0.430
LIRIS_run3	0.513
LIRIS_run1	0.543
Sabanci-okan-run1	0.476
LIRIS_run2	0.508
LIRIS_run4	0.538
inria_imedia_plantnet_run2	0.554
DFH + GP (Yahiaoui et al., 2012)	0.725

PCA of Curves in $\mathbb{R}^3$

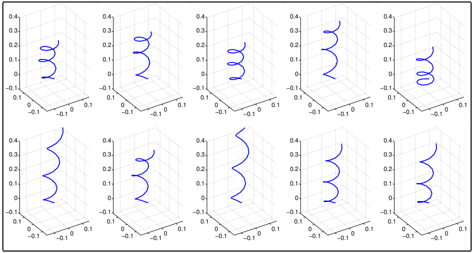
(a) A collection of 20 spiral curves used in this experiment



(a)

(b) (c) (d)

(b) the decrease in the norm of the gradient of Karcher variance function during mean estimation, (c) the estimated Karcher mean and (d) the estimated singular values of the covariance matrix.



Random samples from the estimated wrapped-normal density in the shape space.

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Matlab Demo – 1

Phase amplitude separation of functional data

Matlab Demo – 2

Shape analysis of planar curves

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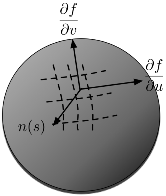
- Interested in objects of the type: $f : \mathbb{S}^2 \to \mathbb{R}^3$ that are immersions. We can define a square-root representation similar to curves as follows.

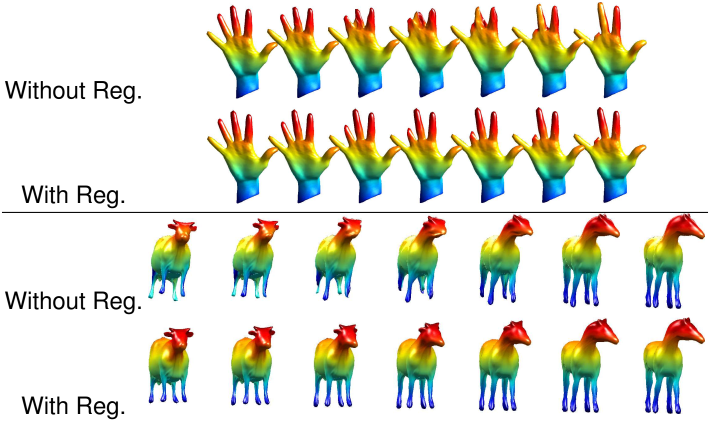


- The gradient $\nabla f : \mathbb{S}^2 \to \mathbb{R}^{3\times 2}$, is $\nabla f(s) = [\frac{\partial f}{\partial s_1} \frac{\partial f}{\partial s_2}]$.
  For $s = (u, v)$, the normal vector field is $\tilde{n}(s) = \frac{\partial f}{\partial u} \times \frac{\partial f}{\partial v}$, and the induced metric (or the first fundamental form) on $\mathbb{S}^2$ is:

$$g(s) = \nabla f(s)^T \nabla f(s) \in \mathbb{R}^{2\times 2}$$

  We have the area element $a(s) = |\tilde{n}(s)| = \sqrt{\det(g(s))}$ and unit normal $n(s) = \tilde{n}(s)/a(s)$.

Shape Registration and Geodesics

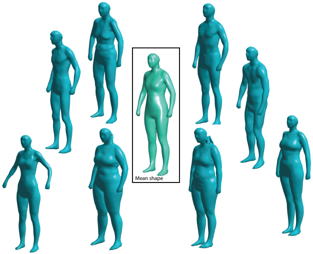


Geodesics are computed in the SRNF space and then each point along the path is inverted back numerically.

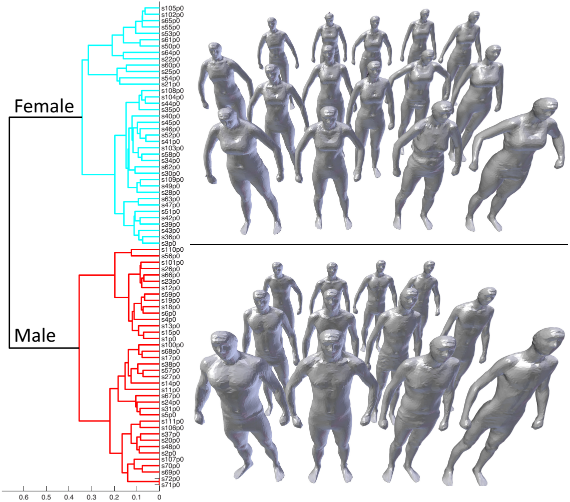
Sample mean:

$$\mu_q = \operatorname*{argmin}_{[q]\in\mathcal{S}} \sum_{i=1}^{n} d_s([q],[q_i])^2$$

Then, $\mu_q \mapsto \mu_f$ (SRNF Inversion).

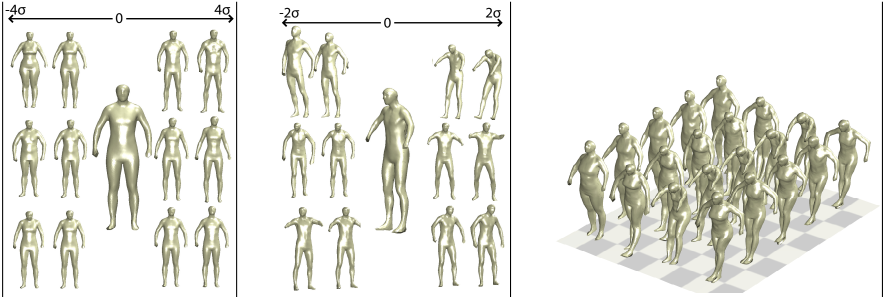


Shape Clustering



Shape PCA and Modeling

Use the tangent bundle of shape spaces to perform PCA and wrap it back on the shape space to study principal directions.



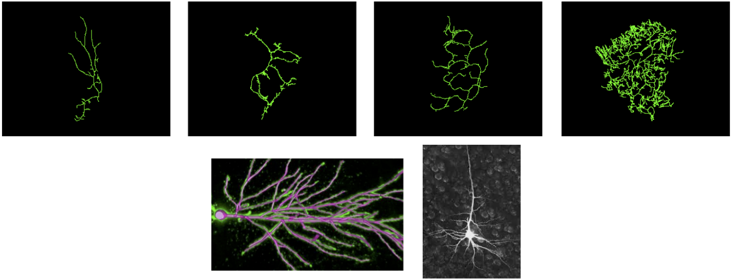
(a) Mean shape and its first three modes of variation.

(b) Mean pose and its first three modes of variation.

(c) Random samples from the PCA model on $\mathcal{S}$.

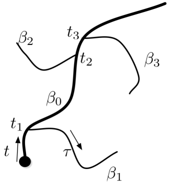
Neuron Morphology

- Neurons, axons



- Complex branching structures, different numbers and shapes of branches.
- Interested in neuron morphology for various medical reasons – cognition, genomic associations, diseases.

- Complex structure – divide and conquer

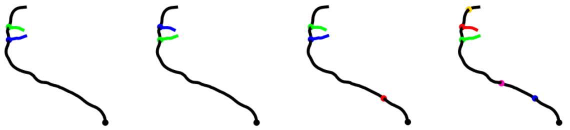


- Components – main brain and side branches (ignore tertiary structures). A collection of curves in $\mathbb{R}^3$. Also keep the locations where side branches meet the main branch. $\beta_0, \{\beta_k, k = 1, \ldots, n\}, \{s_k, k = 1, 2, \ldots, n\}$.
- SRVFs: $q_0, \{q_k, k = 1, \ldots, n\}, \{s_k, k = 1, 2, \ldots, n\}$.

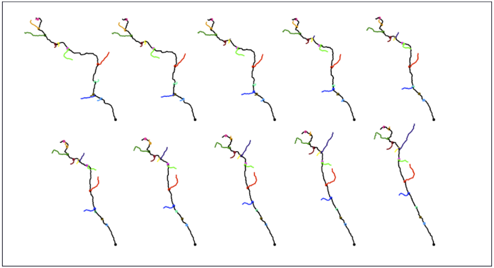
- Distance between two trees with n registered branches.

$$d_n\left(\boldsymbol{q}^1,\boldsymbol{q}^2\right)^2=\lambda_m\left\|q_0^1-q_0^2\right\|^2+\lambda_s\sum_{k=1}^{n}\left\|q_k^1-q_k^2\right\|^2+\lambda_p\sum_{k=1}^{n}\left(s_k^1-s_k^2\right)^2. \tag{1}$$

- **Trivial side branch**: A side branch of length zero.
- Define a notion of **branch equivalence** – two trees are branch equivalent if they have the same shape, i.e. they only differ in null branches.

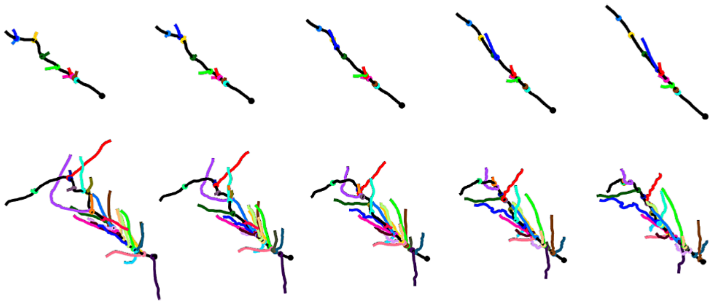


- Compare trees with n_1 and n_2 side branches: Add null branches to make the total number $n_1 + n_2$ in each. Match the branches using the assignment problem – Hungarian algorithm. Also need global rotation for alignment.
- Geodesic Example:



- Sample mean, PCA, etc.

Geodesics Examples



Shape Classification

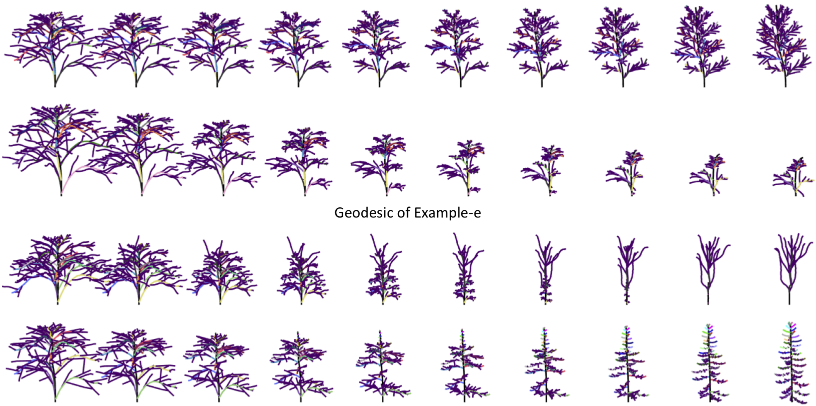
Experimental Setting:

- **Wu Dataset**: 41 apical dendrites taken from the CA1 region of the hippocampus in mice. Two classes: wild type and a gene *protocadherin* knocked out.
- **Chen Dataset**: 99 apical dendrites of pyramidal neurons taken both from the CA1 regios of the hippocampus and layer V of the sensorimotor cortex in rats. Two regions and Three classes (BDL, BDHLHD, and control group).
- Feature method uses a 21 feature vector.

Summary comparison of classification accuracy with Gaussian RBF SVM in Euclidean feature space, topology-only TED metric space, and the proposed metric space of tree shapes

	Wu	**Chen (6-class)**	**Chen (region)**	**Chen (exp. grp.)**
Feature Vector	0.707	**0.566**	**1.000**	0.505
TED (topology only)	0.756	0.384	0.859	0.455
Proposed Metric	**0.805**	0.546	**1.000**	**0.535**

Tree shapes: stems, branches, tertiary branches $\Rightarrow$ different topologies and geometries.



Summary

- This field represents a confluence of ideas from geometry, functional analysis, and statistics.
- Reason: On one hand, objects are more naturally represented in continuum, i.e. by functions. On the other hand, functions have shapes that are often more important than functions themselves.
- The simplest example is shapes of scalar functions on a unit interval. However, as the data grows, the complexity of the objects also grows.
- Next, we have shapes of curves in $\mathbb{R}^2$, $\mathbb{R}^3$, or $\mathbb{R}^n$. Then we have tree-like structures or graph-like structures. Then we have 3D objects, and so on...
- In the future, there is a potential for combining topological tools with geometry to expand this framework.