A Wasserstein-type distance for Gaussian Mixtures on Vector Bundles

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Overview

1. Introduction
   - Wasserstein-type Distance
2. Applications
   - Punctured Sphere
   - Nanoparticle data

Introduction

Figure: Examples of planar closed curves with distinct shapes

- Working with planar closed curves $\beta : S^1 \to \mathbb{R}^2$
- 'Shape' of β is invariant to **translation, scaling, rotation, and reparameterization** (Srivastava & Klassen, 2016 [4])

Introduction

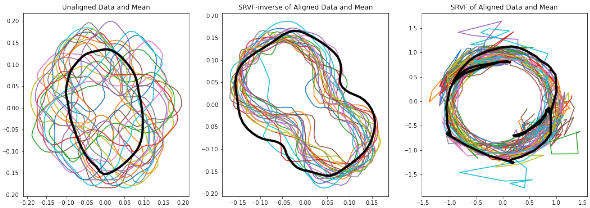


Figure: β's, before and after alignment, and aligned SRVF's

$$q(t) = \frac{\dot{\beta}(t)}{\sqrt{|\dot{\beta}(t)|}} \implies d_{FR}(\beta_1(t), \beta_2(\gamma(t)) = \|q_1 - q_2(\gamma(t))\sqrt{\dot{\gamma(t)}}\|_2$$

$$\mathcal{C} = \{q \in L^2(S^1, \mathbb{R}^2) : \int_{S^1} \|q(t)\|^2 dt = 1, \int_{S^1} q(t)|q(t)\ dt = 0\}$$

Introduction

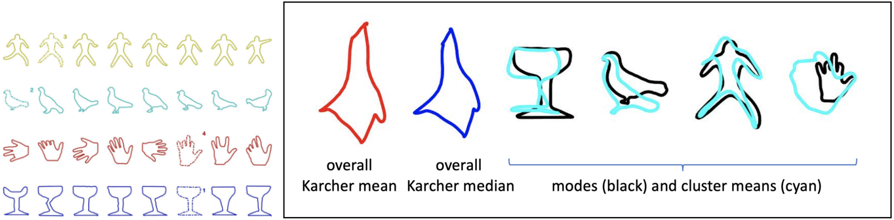


Figure: Karcher means of mixtures of shape aren't representative of data

Goal: Compare mixture distributions of shapes
Approach: Model shapes with Wrapped Gaussian (WG) mixtures of Preshapes

1. **Estimate Parameters:** Karcher Mean & Tangent Space Covariance
2. **Compare Distributions:** Wasserstein-type distance for Gaussian Mixtures

Wasserstein Distance

- $(\mathcal{X}, d)$ a metric space.
- $\mathcal{P}_p(\mathcal{X}) = \{\mu : \int_{\mathcal{X}} d(x_0, x)^p d\mu(x) < \infty \; \forall x_0\}$

The Wasserstein Distance between $\mu_0, \mu_1 \in \mathcal{P}_p$ is given by;

$$W_p^{\mathcal{X}}(\mu_0, \mu_1) := \left(\inf_{\gamma \in \Pi(\mu_0, \mu_1)} \int_{\mathcal{X} \times \mathcal{Y}} d(x, y)^p d\gamma(x, y) \right)^{\frac{1}{p}}$$

- d: distance/ transport cost
- γ: coupling/ transport plan

Distance Computation

- $|supp(\mu_k)| = n_k,\ k = 0, 1$
- $x_i \in supp(\mu_0),\ y_j \in supp(\mu_1)$

$$W_2^2(\mu_0, \mu_1) = \min_{T \in \Pi(\mu_0, \mu_1)} \sum_{i,j} d(x_i, y_j)^2 T_{ij}$$

which can be solved with linear programming

We can directly calculate Wasserstein distances between finitely supported measures on metric spaces

Wasserstein Distance between Gaussians

- $\mathrm{G}(\mathbb{R}^d) := \{\mu = N(m, \Sigma) : m \in \mathbb{R}^d, \Sigma \in \mathrm{Sym}_d^+\}$
- $\mu_0, \mu_1 \in \mathrm{G}(\mathbb{R}^d)$

$$W_2^2(\mu_0, \mu_1) = ||m_0 - m_1||^2 + tr(\Sigma_0 + \Sigma_1 - 2(\Sigma_0^{\frac{1}{2}} \Sigma_1 \Sigma_0^{\frac{1}{2}})^{\frac{1}{2}})$$

and $(\mathrm{G}(\mathbb{R}^d), W_2)$ is a metric space.

Gaussian Mixtures

A measure μ on $\mathbb{R}^d$ is a Gaussian mixture measure if it can be written as

$$\mu = \Sigma_{k=1}^{K} w_k N(m_k, \Sigma_k) \text{ and } \Sigma_{k=1}^{K} w_k = 1,\ w_k \geq 0,\ \forall\ k, K < \infty$$

Gaussian Mixtures are convex combinations of Gaussian measures

Identifiability of Gaussian mixtures

Identifiability: There exists a bijection between space of measures and parameter space (For $\mathrm{G}(\mathbb{R}^d)$, see Yakowitz & Spragins, 1968 [3])

- $\mu \in \mathrm{G}(\mathcal{X})$
- $(m, \Sigma) \in \mathcal{X} \times Sym_d^+$

$$\sum_k w_k N(m_k, \Sigma_k) \iff \sum_k w_k \delta_{\mu_i^k}(\mu)$$

On spaces $\mathcal{X}$ where finite Gaussian mixtures are identifiable, they can be uniquely represented as discrete measures on $\mathrm{G}(\mathcal{X})$

A Distance for Gaussian mixtures

- $(\mathrm{G}(\mathbb{R}^d), W_2^2)$ is a metric space
- $\mu_i^k = N(m_i^k, \Sigma_i^k)$
- $\mu_i = \sum_k^K w_k \mu_i^k$

$$D(\mu_0, \mu_1) := \min_{T \in \Pi(\mu_0, \mu_1)} \sum_{k,\ell} W_2^2(\mu_0^k, \mu_1^\ell) T_{ij}$$

is a distance on Gaussian mixtures. (Chen et. al, 2018 [1])

Wasserstein-type Distance between Gaussian Mixtures

It turns out that this distance can be seen as an optimal transport *on the domain of the distributions* (not just on the parameter space), where the set of admissible couplings are restricted to be Gaussian mixtures;

$$MW_2^2(\mu_0, \mu_1) = \inf_{\pi \in \Pi(\mu_0, \mu_1) \cap GMM} \int_{\mathcal{X} \times \mathcal{Y}} ||x - y||^2 d\pi(x, y)$$

(Delon & Desolneux, 2019 [2])

$$MW_2^2(\mu_0, \mu_1) = \min_{T \in \Pi(\mu_0, \mu_1)} \sum_{k,\ell} W_2^2(\mu_0^k, \mu_1^\ell) T_{ij}$$

Trivial Vector Bundles

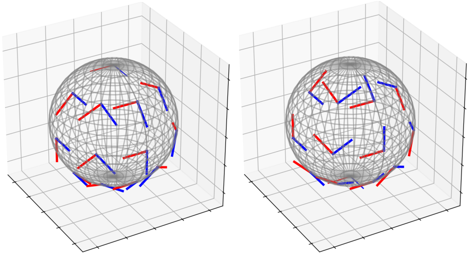


Figure: Illustrations of two trivializations of the punctured sphere.

Vector Bundle: $\mathcal{E} \to \mathcal{M}$
Trivialization: $\varphi : \mathcal{E} \to \mathcal{M} \times \mathbb{R}^d$

Gaussians on Trivial Vector Bundles

A Borel measure on the vector bundle $\mathcal{E}$ is called a Gaussian measure if it is a mean-zero Gaussian measure on the inner product space $(\mathcal{E}_m, \langle \cdot, \cdot \rangle_m)$, for some $m \in \mathcal{M}$.

The collection of Gaussian measures on $\mathcal{M} \times \mathbb{R}^d$ is identifiable, and is denoted $\mathrm{G}(\mathcal{M} \times \mathbb{R}^d)$.

Wasserstein Distance between Gaussians on Trivial Vector Bundles

$$d_{M\times\mathbb{R}^d}((m_0,v_0),(m_1,v_1))^2 = d_M(m_0,m_1)^2 + ||v_0 - v_1||^2$$

$$W_2^{\mathcal{M}\times\mathbb{R}^d}(\eta_0,\eta_1)^2$$

$$= d_{\mathcal{M}}(m_0,m_1)^2 + \mathrm{tr}\Big(\Sigma_0 + \Sigma_1 - 2\big(\Sigma_0^{\frac{1}{2}}\Phi_{m_0,m_1}^{-1}\Sigma_1\Phi_{m_0,m_1}\Sigma_0^{\frac{1}{2}}\big)^{\frac{1}{2}}\Big)$$

where

$$\Phi_{m_0,m_1} = \varphi_{m_1}^{-1}\circ\varphi_{m_0} : \mathcal{E}_{m_0} \to \mathcal{E}_{m_1}$$

$\implies (\mathrm{G}(\mathcal{M}\times\mathbb{R}^d), W_2^{\mathcal{M}\times\mathbb{R}^d})$ is a metric space

Wasserstein-type Distance between Gaussian Mixtures on Trivial Vector Bundles

$$\mu_i = \sum_{k=1}^{K_i} w_i^k \eta_i^k, \quad \eta_i^k = N_{\mathcal{E}}(m_i^k, \Sigma_i^k), \quad i \in \{0, 1\}$$

can be expressed as

$$MW_2^{\varphi}(\mu_0, \mu_1)^2 = \min_{\omega \in \Pi(\mu_0, \mu_1)} \sum_{k,\ell} \omega_{k\ell} W_2^{\mathcal{M} \times \mathbb{R}^d}(\varphi_{\#}\eta_0^k, \varphi_{\#}\eta_1^\ell)^2 \tag{1}$$

Applications

Applications

Density Estimation

Identifying Gaussian Mixture Parameters with Respect to Orthogonal Frame

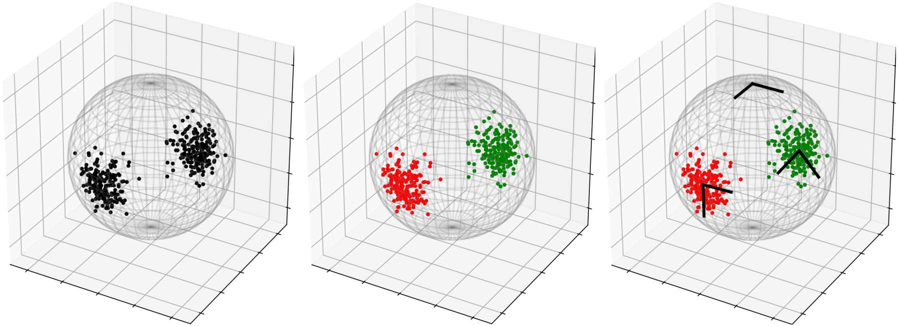


Figure: Steps for estimating Gaussian mixture parameters with respect to a moving frame on a punctured ^{2}. Left: Sphere with sample data; Middle: Sample data colored by K-means cluster assignment; Right: Orthogonal frame transported to Fréchet means of clusters.

Data

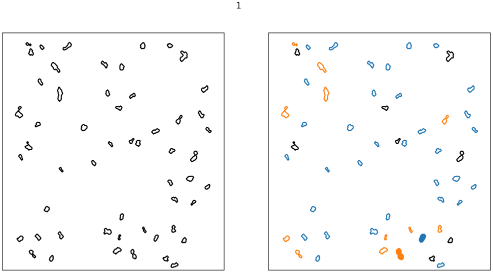


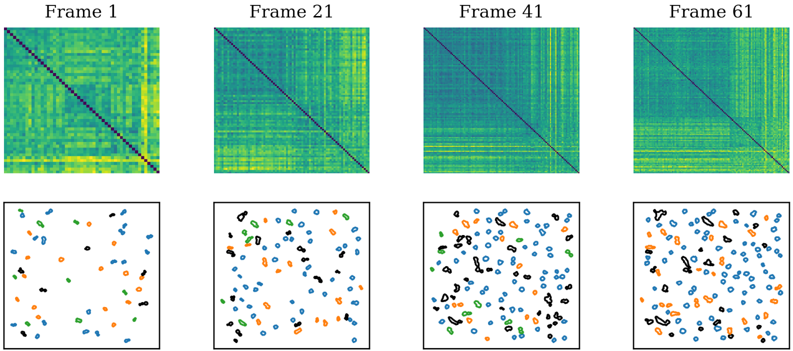
Figure: Recording of nanoparticle manufacturing process

Goal: Test for change in distribution of shapes over time

Approach:

- Represent each image as a Gaussian Mixture
- Calculate between frame Wasserstein-type distances
- E-divisive Change point detection

K-Modes Kernel Mixture



Estimate Mixture Components: K-mode Kernel mixtures clustering returns index set $\mathcal{I}$;

$$\{q_i, i = 1, ..., N\} \rightarrow \mathcal{I}$$

Get Pre-shape Representation

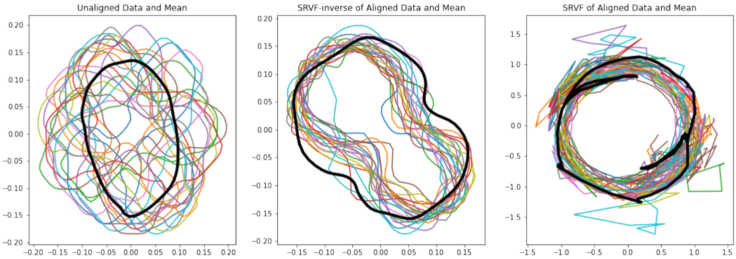


Figure: β's, before and after alignment, and aligned SRVF's

Estimate Component Means: For each cluster, calculate shape mean and align curves

$$C_{k,t} = \{q_i : \mathcal{I}^t(q_i) = k\} \to (\mu_k, \{\tilde{q}_i\}) \tag{2}$$

Get Coordinate Representation

Define an orthonormal functional basis B, project data into basis to get coordinates;

$$(\mu_k^*)_j = \int B_j(s)\mu_k(s)ds$$

$$(\tilde{q}_i^*)_j = \int B_j(s)\tilde{q}_i(s)ds$$

We also need coordinates for the basis (trivial, but a choice)

$$(p_{ref}^*)_j = \int B_j(s)B_1(s)ds$$

$$(F_{ref}^*)_{j,\ell} = \int B_j(s)B_\ell(s)ds$$

Estimate Parameters for Gaussian

We estimate the Coordinate Representation for the kth Gaussian component for frame t as;

$$\nu_k = N(\mu_k^*, \Sigma_k^*)$$

with

$$\Sigma_k^* = \frac{1}{N-1} X^t X$$

where

$$X_{:,i} = R_{(p_{ref} \to \mu_k^*)}(F_{ref}^*)^T Exp_{\mu_k^*}^{-1}(\tilde{q}_i^*) \tag{3}$$

Wrapped Gaussian Mixture

We estimate the wrapped Gaussian mixture for image t as (note, we've added a subscript for frame number);

$$\nu_t = \Sigma_{k=1}^{K_t} w_k \nu_{t,k}$$

$$w_{t,k} = |\{q_{t,i} : \mathcal{I}(q_{t,i}) = k\}| / N_t$$

Wasserstein-type Distance between wrapped Gaussian mixtures

Given wrapped Gaussian mixture distributions for each image $t = 1, \dots, T$,

$$\nu_t = \sum_{k=1}^{K_t} w_{t,k} N(\mu^*_{t,k}, \Sigma^*_{t,k})$$

we calculate the Wasserstein-type distance between them using the formula;

$$MW_2^2(\nu_t, \nu_s) = \inf_{\Pi \in \Gamma(w_t, w_s)} \sum_{k=1}^{K_t} \sum_{\ell=1}^{K_s} \Pi_{k,\ell} W_2^2(\nu_{t,k}, \nu_{s,\ell}) \tag{4}$$

Results

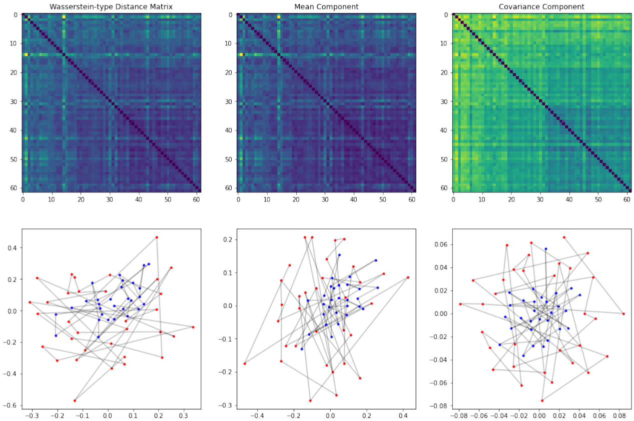


Figure: Top: Wasserstein-type Distance matrix for process, with mean and covariance components; Bottom: MDS embbeding of distance matrices into 2 dimensions

Interpreting Transport Plans

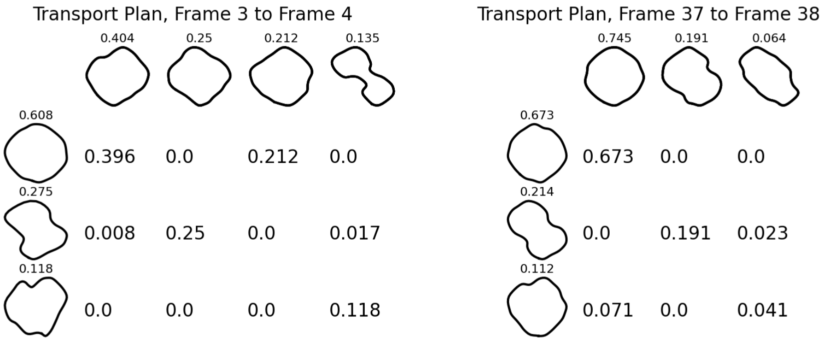


Figure: Visual representation of inter-frame transport plans. Gaussian mixture component mean shapes are represented in the margins. Numbers above mean shapes correspond to estimated weight for that component; array of numbers in center of plot are the transport plans, they represent the amount of mass transported between the corresponding marginal components.

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