A Few Applications of Geometric Measure Theory to Shape Analysis

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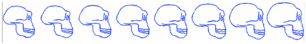
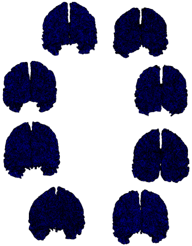
Morphological variability in shape populations

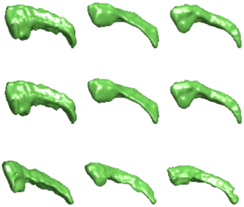
One of the primary goal of shape analysis is the modelling and statistical analysis of morphological variability in ensembles of geometric objects.

- Inter-species variability : understand the evolution of anatomy.



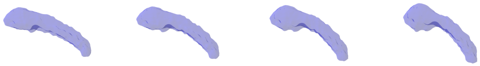
- Longitudinal variability: growth, morphogenesis.
- Inter-subject variability in a population.



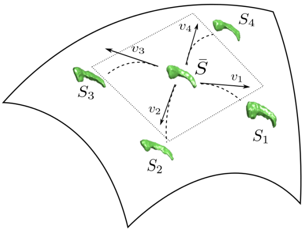


Why Riemannian frameworks on shape spaces?

The construction of a Riemannian structure on the set of shapes is usually the key step to be able to extend classical statistical concepts and tools such as Kärcher means, regression, PCA, clustering...



Geodesic path



Kärcher mean

Intrinsic and extrinsic shape space models[1]

There are currently several apporaches to build Riemannian metrics on shape spaces, among which:

- Intrinsic quotient metrics on spaces of curves/surfaces [Michor, Mumford 2006], [Bauer, Harms 2010], [Bauer, Bruveris 2014], [Srivastava, Klassen 2011]...
- Metrics induced from deformation groups [Grenander 1994], [Beg, Miller 2005], [Vercauteren, Pennec 2009] [Miller, Trouve, Younes 2015]...

[1] Bauer, Charon and Younes. Metric Registration of Curves and Surfaces using Optimal Control. 2019

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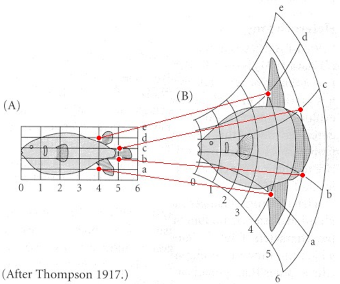
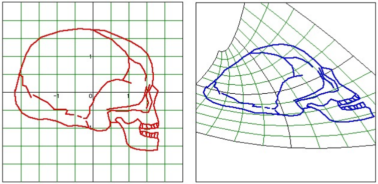
A precursor: D'Arcy Thompson

The idea of comparing two shapes through the notion of a spatial transformation mapping one to the other goes to back to the work of D'Arcy Thompson.





From: D'Arcy Thompson, *On Growth and Form*, 1917.

Grenander's formalism

Consider $\mathcal{M}$ a set of shapes (landmarks, curves, surfaces, images...) embedded in the Euclidean space $\mathbb{R}^n$ as well as G a given group of deformations of $\mathbb{R}^n$.

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G is equipped with a distance d_G for which the group multiplication is continuous, and that is G-**equivariant** i.e. given any $\phi^1, \phi^2 \in G$, one has for all $\phi \in G$:

$$d_G(\phi^1 \circ \phi, \phi^2 \circ \phi) = d_G(\phi^1, \phi^2)$$

Grenander's formalism

Key principle: [Grenander, 1993] if the isotropy subgroups $G_m = \{\phi \in G \mid \phi \cdot m = m\}$ are all closed for d_G, then one obtains a distance on the shape space $\mathcal{M}$ induced by the one on G via:

$$d_{\mathcal{M}}(m^0, m^1) = \inf_{\phi \in G} \{d_G(\mathrm{id}, \phi) \mid \phi \cdot m^0 = m^1\}.$$

i.e. the distance from m^0 to m^1 is measured by finding an "optimal" (closest to the identity) deformation in G mapping m^0 onto m^1.

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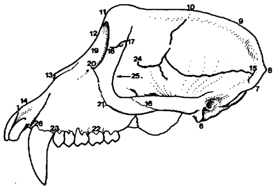
In general, it is more adequate (or even necessary) to approximate $d_{\mathcal{M}}$ by introducing an inexact version of the above registration problem:

$$\inf_{\phi \in G} d_G(\mathrm{id}, \phi)^2 + D(\phi \cdot m^0, m^1)$$

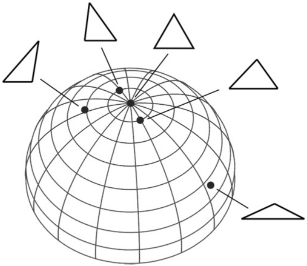
where $D(\cdot, \cdot)$ is a fidelity term (a discrepancy loss) on $\mathcal{M}$.

A simple case: landmarks

Early works in shape analysis focused on objects represented by a predefined set of landmarks (manually or automatically extracted). Comparing shapes then amounts in comparing finite sets of labelled points in the Euclidean space $m = (x_1, x_2, \ldots, x_p) \in (\mathbb{R}^n)^p$, possibly modulo translations/rotations.



From Dryden and Mardia



Kendall shape space of planar triangles

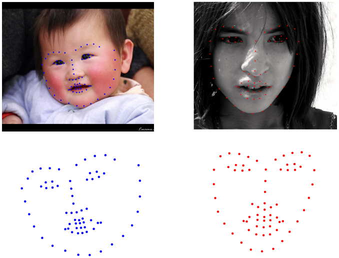
A simple case: landmarks

In the case of landmarks, we have $\mathcal{M} = (\mathbb{R}^n)^p$:

$$m^0 = (x_1^0, \cdots, x_p^0),\ m^1 = (x_1^1, \cdots, x_p^1) \in (\mathbb{R}^n)^p$$

$$\phi \cdot m^0 = (\phi(x_1^0), \cdots, \phi(x_N^0))$$

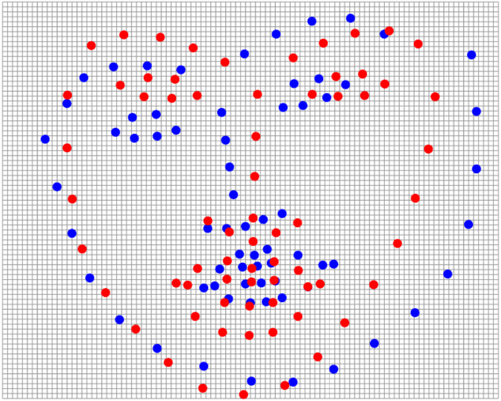
$$D(\phi \cdot m^0, m^1) = \lambda \sum_{k=1}^{p} |\phi(x_k^0) - x_k^1|^2$$



Taking for instance G a certain subgroup of diffeomorphisms of $\mathbb{R}^n$ equipped with an equivariant metric (construction to be explained in next class), the inexact registration problem is then:

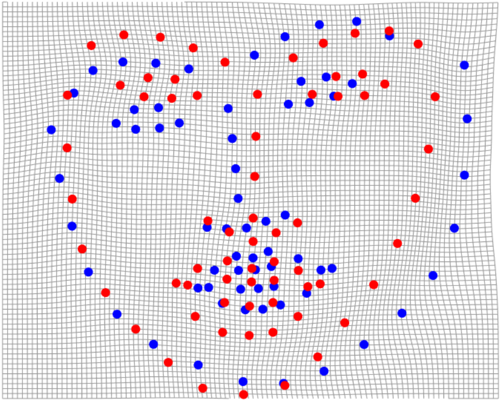
$$\min_{\phi \in G} d_G(\mathrm{id}, \phi)^2 + \lambda \sum_{k=1}^{N} |\phi(x_k^0) - x_k^1|^2$$

Landmark registration



Registration of face landmarks

Landmark registration



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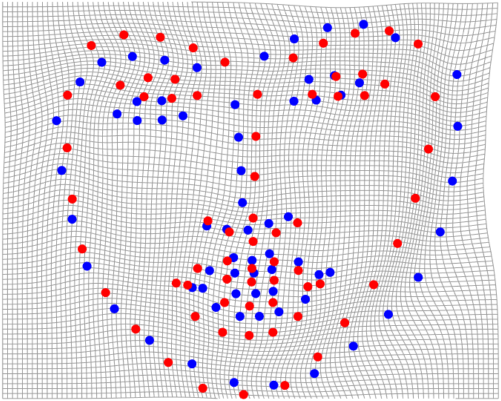

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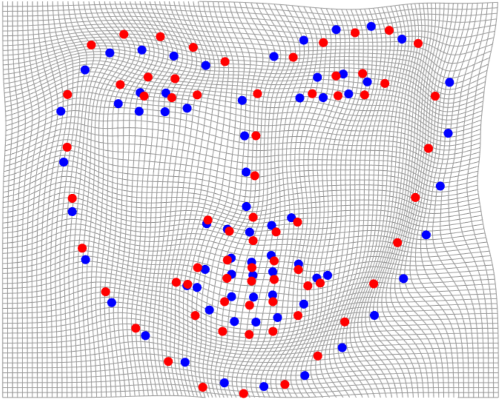

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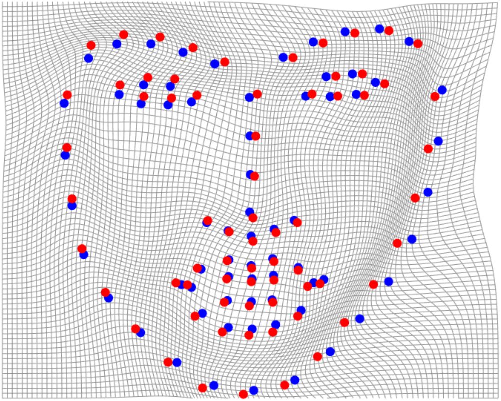

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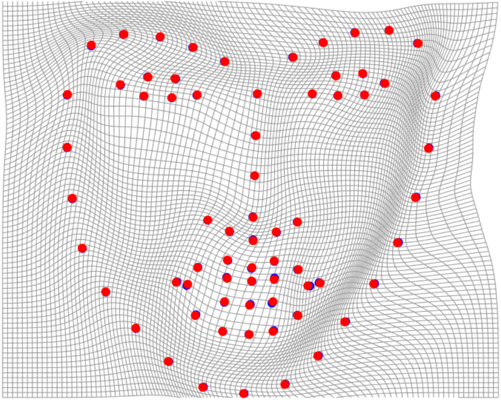

Registration of face landmarks

Going beyond landmarks

The approach of landmark shape analysis has several downsides:

- Usually involves pre-processing steps to extract, label and/or establish correspondences across the dataset.
- Landmarks only provide a sparse and partial representation of a shape.

Going beyond landmarks

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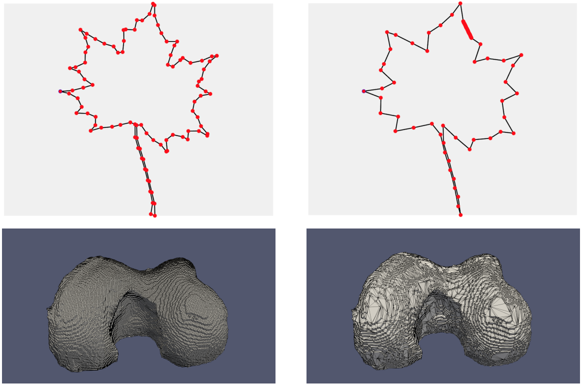
- Usually involves pre-processing steps to extract, label and/or establish correspondences across the dataset.
- Landmarks only provide a sparse and partial representation of a shape.

In contrast, geometric structures such as images, curves or surfaces provide a more complete description of morphology. However, they lead to additional mathematical and numerical challenges due to the fact that

- Those objects are in essence infinite-dimensional.
- The comparison between shapes should not depend on the specific way they are parametrized or sampled.

Submanifold data: discrete setting

Unlike landmarks, discrete curves or surfaces are not made of labelled points. One given shape may be sampled in multiple different ways and most datasets involve inconsistent mesh structures across subjects.



Submanifold data: continuous setting

A smooth submanifold S of $\mathbb{R}^n$ can be represented by a **parametrization map** $q : \Omega \to \mathbb{R}^n$ where Ω is the parameter space (e.g. an open set of some Euclidean space) and q an embedding.

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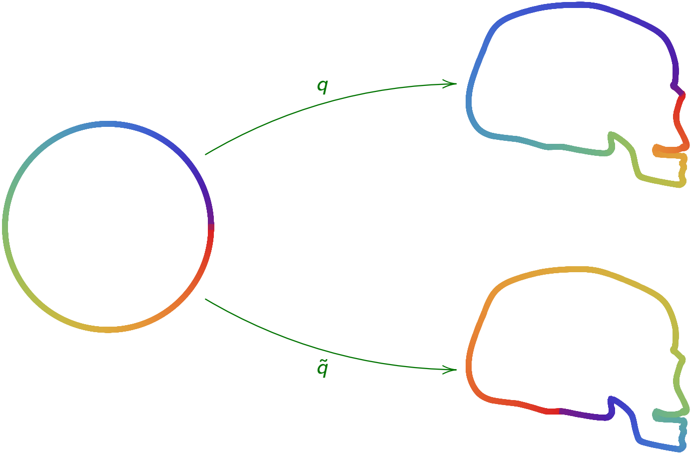
A smooth submanifold S of $\mathbb{R}^n$ can be represented by a **parametrization map** $q : \Omega \to \mathbb{R}^n$ where Ω is the parameter space (e.g. an open set of some Euclidean space) and q an embedding.

However, this representation is not unique! For any reparametrization $\psi \in \mathrm{Diff}(\Omega)$, $q \circ \psi$ is also a parametrization of the same submanifold S.

Different parameterizations of the same shape



$$q, \tilde{q} : \Omega = \mathbb{S}^1 \to \mathbb{R}^2, \qquad \tilde{q} = q \circ \psi, \qquad \psi \in \mathrm{Diff}(\mathbb{S}^1)$$

Submanifold data

The Grenander framework also applies in principle to discrete or continuous submanifold shapes: any deformation $\phi \in G$ of $\mathbb{R}^n$ acts on a submanifold by transport of its point positions. Given a parametrization q: $\phi \cdot q = \phi \circ q$.

Problem: how to construct a notion of fidelity term D that does not depend on the particular parametrization or sampling of either of the two shapes?

Idea: rely on invariant representations of shapes, in particular on the concepts developed in the field of *geometric measure theory*.

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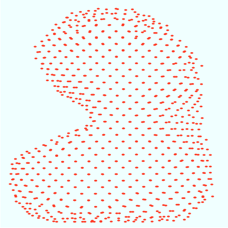
The 0-dimensional case: point clouds



A point cloud is by definition a set of unlabelled points $m = \{x_k\}_{k=1,..,p}$ in $\mathbb{R}^n$. The space of all point clouds can be identified with a reunion of quotient spaces:

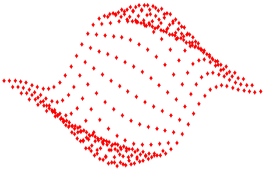
$$\mathcal{M} = \bigcup_{p \in \mathbb{N}} (\mathbb{R}^n)^p / \mathrm{Sym}(p)$$

The 0-dimensional case: point clouds

- A more convenient representation of such a point cloud is to view m as the sum of Dirac masses $\mu_m = \sum_{k=1}^{p} \delta_{x_k}$ which is automatically independent of the ordering of the x_i's.
- This representation allows to embed the shape space of point clouds $\mathcal{M}$ into the space of **positive Radon measures** of $\mathbb{R}^n$.
- It then provides a natural way to build discrepancy losses between point clouds based on metrics on the space of measures including e.g. Wasserstein metrics, kernel maximum mean discrepancies...

What about higher dimensional submanifolds?

Submanifolds are more than point clouds...



In addition to positions in $\mathbb{R}^n$, discrete submanifolds involve connectivity information between vertices or, in the continuous setting, tangent spaces and area density.

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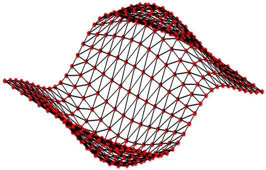

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Generalized measures in geometric measure theory

Plateau's problem of minimal surfaces triggered the development of *geometric measure theory* in the 1960s, with the introduction of specific measure spaces to frame variational problems on shapes, among which **currents** [Federer& Fleming 1960] and later **varifolds** [Almgren 1966, Allard 1972].

From [Harrison & Pugh, 2016].

"One must abandon the idea of describing all the competing surfaces by continuous maps from a single predetermined parameter space. One should rather think of surfaces as d-dimensional mass distributions, with tangent d-vectors attached."
H. Federer

Oriented and unoriented Grassmann manifolds

Let $0 \leq d \leq n$. We introduce the classical Grassmann manifolds of $\mathbb{R}^n$:

- Unoriented Grassmannian $G_d(\mathbb{R}^n)$: the space of all d-dimensional linear subspaces of $\mathbb{R}^n$. Each element of $G_d(\mathbb{R}^n)$ is uniquely represented by an orthonormal d-frames of $\mathbb{R}^n$ modulo the action of the orthgonal group $O(d)$ of its span. Equivalently, $G_d(\mathbb{R}^n) \approx O(n)/(O(d) \times O(n-d))$
- Oriented Grassmannian $\widetilde{G}_d(\mathbb{R}^n)$: the space of all d-dimensional linear oriented subspaces of $\mathbb{R}^n$. One has $\widetilde{G}_d(\mathbb{R}^n) \approx SO(n)/(SO(d) \times SO(n-d))$.

Oriented and unoriented Grassmann manifolds

$G_d(\mathbb{R}^n)$ and $\widetilde{G}_d(\mathbb{R}^n)$ are both compact manifolds of dimension $d(n-d)$. They can be realized as embedded submanifolds in various ways, for instance via the maps:

- $T \in G_d(\mathbb{R}^n) \to p_T \in \mathcal{L}(\mathbb{R}^n, \mathbb{R}^n)$, with p_T denoting the orthogonal projector on T. It induces the inner product between $T, T' \in G_d(\mathbb{R}^n)$:

$$\langle T, T' \rangle = \mathrm{Tr}(p_T^T p_{T'})$$

- Pluckër embedding: $T \in \widetilde{G}_d(\mathbb{R}^n) \to u_1 \wedge \ldots \wedge u_d \in \mathbb{S}\left(\bigwedge^d(\mathbb{R}^n)\right)$ where $(u_1, \ldots, u_d)$ is an orthonormal basis of T. This induces the following inner product between any $T, T' \in \widetilde{G}_d(\mathbb{R}^n)$:

$$\langle T, T' \rangle = \det([u_i \cdot u_j']_{i,j=1,\ldots,d})$$

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In particular, for $d = 1$ or $d = n-1$, $\widetilde{G}_d(\mathbb{R}^n)$ can be identified to the unit sphere $\mathbb{S}^{n-1}$ and $G_d(\mathbb{R}^n)$ to the real projective space $\mathbb{RP}^{n-1}$.

The space of varifolds

The notion of varifolds provides an extension of usual measures on $\mathbb{R}^n$ by adding an extra unoriented or oriented subspace component.

Definition

A *d-varifold* (resp. an oriented *d-varifold*) μ on $\mathbb{R}^n$ is a Radon measure on the space $\mathbb{R}^n \times G_d(\mathbb{R}^n)$ (resp. $\mathbb{R}^n \times \widetilde{G}_d(\mathbb{R}^n)$). Its weight $|\mu|$ is the measure on $\mathbb{R}^n$ defined by $|\mu|(A) = \mu(A \times G_d(\mathbb{R}^n))$. We denote by $\mathcal{V}_d$ (resp. $\widetilde{\mathcal{V}}_d$) the space of d-varifolds.

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By Riesz representation theorem, any $\mu \in \mathcal{V}_d$ may be equivalently seen as a distribution in the dual space $C_0(\mathbb{R}^n \times G_d(\mathbb{R}^n))^*$. For any test function $\omega \in C_0(\mathbb{R}^n \times G_d(\mathbb{R}^n))$, we write:

$$(\mu|\omega) = \int_{\mathbb{R}^n \times G_d(\mathbb{R}^n)} \omega d\mu.$$

The space of varifolds

- Dirac varifold: $\delta_{(x,T)}$ is a singular mass located at position $x \in \mathbb{R}^n$ with the d-dimensional subspace $T \in G_d(\mathbb{R}^n)$ attached.
- For a general d-varifold $\mu \in \mathcal{V}_d$, the disintegration theorem gives the existence, for $|\mu|$-a.e. $x \in \mathbb{R}^n$ of a probability measure ν_x on $G_d(\mathbb{R}^n)$ such that we can write:

$$(\mu|\omega) = \int_{\mathbb{R}^n} \int_{G_d(\mathbb{R}^n)} \omega(x,T) d\nu_x(T) d|\mu|(x).$$

Rectifiable varifolds: curve case

Consider a smooth curve in $\mathbb{R}^n$ given by the C^1 embedding $c : I \to \mathbb{R}^n$, with I an interval. To c, one can associate the 1-varifold μ_c such that for any $\omega \in C_0(\mathbb{R}^n \times \mathbb{RP}^{n-1})$:

$$(\mu_c|\omega) = \int_I \omega(c(\theta), T_{c'(\theta)})|c'(\theta)|d\theta$$

where $T_{c'(\theta)}$ is the element of $\mathbb{RP}^{n-1}$ spanned by the vector $c'(\theta)$.

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where $T_{c'(\theta)}$ is the element of $\mathbb{RP}^{n-1}$ spanned by the vector $c'(\theta)$.

The varifold μ_c does not depend on the parametrization of c i.e. for any $\psi \in \mathrm{Diff}(I)$, $\mu_{c\circ\psi} = \mu_c$. In intrinsic form:

$$(\mu_c|\omega) = \int_{c(I)} \omega(x, T_x c)\, dl(x)$$

Oriented curves

In similar fashion, an oriented embedded curve $c : I \to \mathbb{R}^n$ can be modeled as the oriented 1-varifold:

$$\tilde{\mu}_c : \omega \in C_0(\mathbb{R}^n \times \mathbb{S}^{n-1}) \mapsto (\tilde{\mu}_c|\omega) = \int_I \omega\left(c(\theta), \frac{c'(\theta)}{|c'(\theta)|}\right)|c'(\theta)|d\theta$$

where now $\tilde{\mu}_{c\circ\psi} = \tilde{\mu}_c$ for any $\psi \in \mathrm{Diff}^+(I)$ (orientation-preserving diffeos).

The weight measure $|\tilde{\mu}_c|$, obtained by marginalizing the $\mathbb{S}^{n-1}$ component, is simply the arclength measure along the curve.

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Question/exercise: what about the measure on $\mathbb{S}^{n-1}$ obtained by marginalizing $\tilde{\mu}_c$ with respect to $\mathbb{R}^n$? Assuming $n = 2$, describe what this measure is for a circle of radius $r > 0$ and for a triangle in the plane.
If c is a C^2 curve closed and strictly convex, express the resulting marginal measure with respect to the curvature of c.

Rectifiable varifolds: general case

Let S be a smooth compact submanifold of dimension d in $\mathbb{R}^n$ (with or without boundaries). We define the d-varifold associated to S as the measure $\mu_S \in \mathcal{V}_d$ such that $\mu_S(B) = \mathrm{vol}_S(\{x \in S \mid (x, T_x S) \in B\})$ for any Borel set $B \subset \mathbb{R}^n \times G_d(\mathbb{R}^n)$ or equivalently:

$$(\mu_S|\omega) = \int_S \omega(x, T_x S) d\mathrm{vol}_S(x)$$

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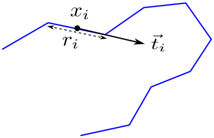
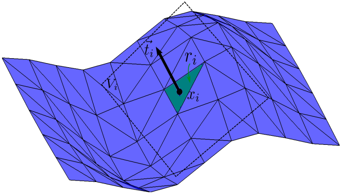
in which $T_x S \in G_d(\mathbb{R}^n)$ is the tangent space to S at x and vol_S is the volume density along S. The mapping $S \mapsto \mu_S$ satisfies the following:

- It is an injective map from d-dimensional submanifolds into $\mathcal{V}_d$.
- It can be extended to $\mathcal{H}^d$-rectifiable subsets of $\mathbb{R}^n$.
- For an oriented submanifold (or rectifiable subset) S, we have a similar representation using instead oriented varifolds in $\widetilde{\mathcal{V}}_d$.

Discrete setting

In the discrete setting, a submanifold is generally given as a finite disjoint reunion of d-dimensional cells (edges, triangles, tetrahedra...) $S = \bigcup_{i=1}^{N} S_i$.
By the additivity property of varifolds, $\mu_S = \sum_{i=1}^{N} \mu_{S_i}$.

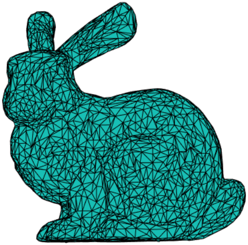




Each μ_{S_i} can be conveniently approximated by one Dirac varifold $r_i \delta_{(x_i, T_i)}$.

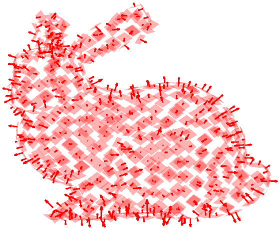
Shapes as varifolds

Submanifold world



S

Varifold world



$\mu_S = \text{“} \int_S \delta_{(x,T_x S)} d\mathrm{vol}_S(x) \text{''}$

Pushforward of a varifold

If $\mu \in \mathcal{V}_d$ and $\phi \in \mathrm{Diff}(\mathbb{R}^n)$, the **pushforward varifold** $\phi_\sharp \mu$ is defined by:

$$(\phi_\sharp \mu | \omega) = \int_{\mathbb{R}^n \times G_d(\mathbb{R}^n)} \omega(\phi(x), d_x\phi \cdot T) J_T\phi(x) d\mu(x, T)$$

in which, if $(u_1, \ldots, u_d)$ is an orthornormal basis of $T \in G_d(\mathbb{R}^n)$, $d_x\phi \cdot T$ denotes the subspace spanned by $(d_x\phi(u_1), \ldots, d_x\phi(u_d))$ and $J_T\phi(x) = \sqrt{\det([d_x\phi(u_i) \cdot d_x\phi(u_j)]_{i,j})}$. This definition ensures that:

$$\phi_\sharp \mu_S = \mu_{\phi(S)}$$

for any d-dimensional submanifold (or rectifiable subset) S.

First variation of a varifold

Assume that S is a compactly supported submanifold of $\mathbb{R}^n$ and v a smooth vector field on $\mathbb{R}^n$. Define $\phi_t(x) = x + tv(x)$ for $t \in (-\varepsilon, \varepsilon)$. Question: what is the first variation of the total d-volume of $\phi_t(S)$, i.e. $|\mu_{\phi_t(S)}|(\mathbb{R}^n)$, at $t = 0$?

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Question: what is the first variation of the total d-volume of $\phi_t(S)$, i.e. $|\mu_{\phi_t(S)}|(\mathbb{R}^n)$, at $t = 0$?

Theorem (first variation of the total mass)

$$\frac{d}{dt}\bigg|_{t=0} |\mu_{\phi_t(S)}|(\mathbb{R}^n) = -\int_S (H_S \cdot v) dvol_S + \int_{\partial S} (\nu \cdot v) dvol_{\partial S}$$

in which H_S is the mean curvature vector of S, ν is the unit outward conormal along ∂S.

First variation of a varifold

The following more general first variation formula also holds:

Theorem (first variation of the varifold, C. & Trouvé 2013)

For any function $\omega \in C^2(\mathbb{R}^n \times G_d(\mathbb{R}^n))$, *one has:*

$$\frac{d}{dt}\bigg|_{t=0} (\mu_{\phi_t(S)}|\omega) = \int_S \left(\frac{\partial \omega}{\partial x} - div_S \left(\frac{\partial \omega}{\partial T} \right) - \omega H_S \right) \cdot v^{\perp} dvol_S + \int_{\partial S} \left(\omega v^{\top} + \left(\frac{\partial \omega}{\partial T} \cdot v^{\perp} \right) \right) \cdot \nu dvol_{\partial S}$$

in which H_S *is the mean curvature vector of* S, ν *is the unit outward conormal along* ∂S, $v^{\top}$ *and* $v^{\perp}$ *are the tangential and orthogonal components of the vector field* v.

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Metrics on $\mathcal{V}_d$

As a subset of the dual space $C_0(\mathbb{R}^n \times G_d(\mathbb{R}^n))^*$, $\mathcal{V}_d$ inherits the dual metric:

$$d_M(\mu_0, \mu_1) = \sup_{\|\omega\|_\infty \leq 1} (\mu_1 - \mu_0 | \omega)$$

which is known as the **mass norm** of varifolds.

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This is typically a too strong metric for most applications:

$$M\left(\delta_{(x_1,T_1)} - \delta_{(x_0,T_0)}\right) = \begin{cases} 2, & \text{if } (x_0, T_0) \neq (x_1, T_1) \\ 0, & \text{if } (x_0, T_0) = (x_1, T_1) \end{cases}$$

$\Rightarrow$ one needs to restrict the sup to test functions of higher regularity.

Metrics on $\mathcal{V}_d$

Some classical measure metrics:

- Mass norm.

$$d_M(\mu_0, \mu_1) = \sup_{\|\omega\|_\infty \leq 1} (\mu_0 - \mu_1 | \omega).$$

- Bounded Lipschitz (or flat) metric.

$$d_{BL}(\mu_0, \mu_1) = \sup_{\|\omega\|_\infty + \mathrm{Lip}(\omega) \leq 1} (\mu_0 - \mu_1 | \omega).$$

- Wasserstein metrics on $\mathbb{R}^n \times G_d(\mathbb{R}^n)$. For $p = 1$:

$$d_{W_1}(\mu_0, \mu_1) = \sup_{\mathrm{Lip}(\omega) \leq 1} (\mu_0 - \mu_1 | \omega).$$

Positive definite kernels and RKHS

Let A be a general set.

Definition (positive definite kernel)

A positive definite kernel on A is a function $k : A \times A \to \mathbb{R}$ such that:

1. for all $x, y \in A$, $k(x, y) = k(y, x)$.
2. for all $N \in \mathbb{N}$, $x_1, \ldots, x_N \in A$ and $\alpha_1, \ldots, \alpha_N \in \mathbb{R}$:

$$\sum_{i,j=1}^{N} \alpha_i \alpha_j k(x_i, x_j) \geq 0.$$

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Definition (Reproducing Kernel Hilbert Spaces)

A Hilbert space H of functions $A \to \mathbb{R}$ is said to be a RKHS if for any $x \in A$, the linear functional $\delta_x : f \in H \mapsto f(x)$ is continuous.

Positive definite kernels and RKHS

Let H be a RKHS, and $\mathbb{K} : H^* \to H$ the inverse of the Riesz duality map. Then for any $x \in A$ and $f \in H$, $f(x) = (\delta_x | f) = \langle \mathbb{K}\delta_x, f \rangle_H$.
Writing $\mathbb{K}\delta_x = k(x, \cdot)$, one gets that for any $x, y \in A$:

$$\langle k(x, \cdot), k(y, \cdot) \rangle_H = \langle \delta_x, \delta_y \rangle_{H^*} = k(x, y)$$

and that the function $k(\cdot, \cdot)$ is a positive definite kernel on A called the **reproducing kernel** of H. Furthermore,

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Theorem (Aronszajn, 1950)

To any positive definite kernel k on a set A corresponds a unique RKHS of functions on A which reproducing kernel is k.

If A is a metric space and the kernel k is further assumed to be continuous on $A \times A$ then H is continuously embedded into $C_0(A)$.

Kernel norms on varifolds

Idea: if W is a RKHS continuously embedded in $C_0(\mathbb{R}^n \times \widetilde{G}_d(\mathbb{R}^n))$ then the dual norm $\|\cdot\|_{W^*}$ induces a pseudo-metric between oriented varifolds:

$$d_{W^*}(\mu_0, \mu_1) = \|\mu_1 - \mu_0\|_{W^*} = \sup_{\|\omega\|_W \leq 1} (\mu_1 - \mu_0 | \omega)$$

We can express the above more explicitly using the fact that $\|\mu_1 - \mu_0\|_{W^*}^2 = \|\mu_0\|_{W^*}^2 + \|\mu_1\|_{W^*}^2 - 2\langle \mu_0, \mu_1 \rangle_{W^*}$ and, with k being the kernel of W, the reproducing kernel property which leads to:

$$\langle \mu_0, \mu_1 \rangle_{W^*} = \int_{\mathbb{R}^n \times \widetilde{G}_d(\mathbb{R}^n)} \int_{\mathbb{R}^n \times \widetilde{G}_d(\mathbb{R}^n)} k(x, T, x', T') d\mu_0(x, T) d\mu_1(x', T').$$

These are known as kernel or **maximum mean discrepancy** metrics between measures.

Kernel norms on varifolds

To obtain a true metric on $\widetilde{\mathcal{V}}_d$, one needs the RKHS W to be dense in $C_0(\mathbb{R}^n \times \widetilde{G}_d(\mathbb{R}^n))$ i.e. k is a C_0-**universal kernel** [Sriperumbudur, 2011].

Theorem

If k is a C_0-universal kernel on $\mathbb{R}^n \times \widetilde{G}_d(\mathbb{R}^n)$, then $\|\cdot\|_{W^*}$ is a metric on $\widetilde{\mathcal{V}}_d$. Moreover, it metrizes the weak convergence on any subspace $\widetilde{\mathcal{V}}_{d,M,K} = \{\mu \in \widetilde{\mathcal{V}}_d \text{ s.t. } |\mu|(\mathbb{R}^n) \leq M, supp(|\mu|) \subset K\}$ for $M > 0$ and K a compact subset of $\mathbb{R}^n$.*

In fact, if one further assumes that $W \hookrightarrow C_0^1(\mathbb{R}^n \times \widetilde{G}_d(\mathbb{R}^n))$, there exists $c > 0$ such that for all $\mu_0, \mu_1 \in \widetilde{\mathcal{V}}_d$:

$$d_{W^*}(\mu_0, \mu_1) \leq c\ d_{BL}(\mu_0, \mu_1).$$

Separable radial-zonal kernels

- It is natural to introduce **separable kernels** of the form $k^P \otimes k^G$ where k^P and k^G are positive definite kernels on $\mathbb{R}^n$ and $\widetilde{G}_d(\mathbb{R}^n)$ respectively.

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- By selecting γ such that $\gamma(-t) = \gamma(t)$, it is invariant to orientation and is thus a metric between unoriented varifolds in $\mathcal{V}_d$.

Induced metric on rectifiable varifolds

Let S, S' be two compact d-dimensional submanifolds. For k a SRZ kernel, we have:

$$\langle \mu_S, \mu_{S'} \rangle_{W^*} = \int_S \int_{S'} \rho(|x - x'|)\gamma(\langle T_x S, T_{x'} S' \rangle) d\mathrm{vol}^S(x) d\mathrm{vol}^{S'}(x')$$

and the fidelity term $D(S, S') = \|\mu_S - \mu_{S'}\|_{W^*}^2$ can be expressed in "closed" form. We obtain a distance between submanifolds under the slightly weaker conditions:

Theorem

Assume that $k^P(x, x') = \rho(|x - x'|)$ is a C_0-universal kernel on $\mathbb{R}^n$, and that γ is continuous with $\gamma(1) > 0$. Then $D(S, S') = 0$ if and only if $S = S'$.

Examples of kernels in dimension/codimension 1

For $d=1$ or $d=n-1$, we have $\widetilde{G}_d(\mathbb{R}^n)=\mathbb{S}^{n-1}$ and $G_d(\mathbb{R}^n)=\mathbb{PR}^{n-1}$.

For k^P, different families of radial C_0-universal kernels: Gaussian $k^P(x,x')=e^{-\frac{|x-x'|^2}{\sigma^2}}$, Cauchy $k^P(x,x')=1/(1+\frac{|x-x'|^2}{\sigma^2})$, Wendland...

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For k^G, among the oriented kernels on $\mathbb{S}^{n-1}$:

- Linear $k^G(u,u') = u \cdot u' \rightarrow$ metrics obtained from the framework of **currents** of [Glaunès & Vaillant, 2006].
- Gaussian $k^P(u,u') = e^{\frac{2}{\eta^2}(u \cdot u')}$.

Examples of unoriented kernels include:

- Constant $k^G(u,u') = 1 \rightarrow$ reduces to metrics on **measures** of $\mathbb{R}^n$.
- Binet $k^G(u,u') = (u \cdot u')^2$.
- Unoriented Gaussian $k^G(u,u') = e^{-\frac{2}{\eta^2}[1-(u \cdot u')^2]}$.

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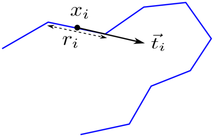
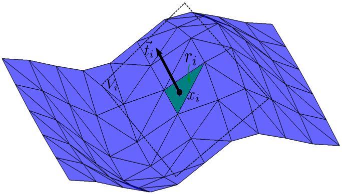
Discrete approximation of meshes

Let $S = \bigcup_{i=1}^{N} S_i$ where S_i are compact d-dimensional cells of the mesh.





We approximate μ_S by the discrete varifold $\bar{\mu}_S = \sum_{i=1}^{N} r_i \delta_{(x_i, T_i)}$.

Proposition

If the RKHS $W \hookrightarrow C_0^1(\mathbb{R}^n \times G_d(\mathbb{R}^n))$ *then:*

$$\|\mu_S - \bar{\mu}_S\|_{W^*} \leq Cte.Vol(S) \max_{i=1,\dots,N} diam(S_i)$$

Discrete to continuous convergence

Given a sequence of discrete meshes $(S^N)_{N\in\mathbb{N}}$ converging to a continuous compact d-dimensional submanifold S in Hausdorff distance, does μ_{S^N} converge to μ_S for d_{W^*}?

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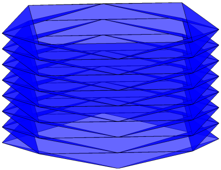

A counterexample: the Schwarz lampion.

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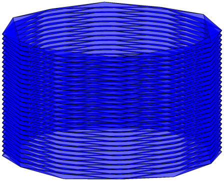

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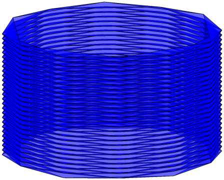

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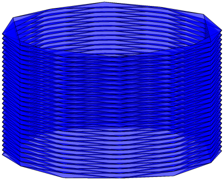

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The conclusion holds however by imposing stronger technical conditions on the convergence of the mesh sequence (in particular convergence of the normal vectors), c.f. [Nardi et. al., 2016], [Arguillère et. al., 2016].

Alternative approach: quantization in $(\mathcal{V}_d, d_{W^*})$

Let $\mathcal{V}_d^N = \left\{ \sum_{i=1}^N r_i \delta_{(x_i, T_i)} \mid r_i \geq 0, x_i \in \mathbb{R}^n, T_i \in G_d(\mathbb{R}^n) \right\}$ be the cone of discrete varifolds with at most N Diracs. For $\mu \in \mathcal{V}_d$ (not necessarily rectifiable) with $|\mu|(\mathbb{R}^n) < +\infty$, we define the quantization of μ:

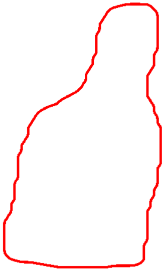
$$\mu^N = \operatorname{argmin}_{\nu \in \mathcal{V}_d^N} \|\mu - \nu\|_{W^*}.$$

Theorem

Assume that $k(x, T, x', T') = \rho(|x - x'|)\gamma(\langle T, T' \rangle)$ *with both* γ *and* ρ *continuous, nonnegative and* $\rho(0) > 0$, $\gamma(1) > 0$. *Then there exists a global minimizer* $\mu^N \in \mathcal{V}_d^N$ *to the above minimization problem. Furthermore, one has* $\|\mu^N - \mu\|_{W^*} \to 0$ *with* $\|\mu^N - \mu\|_{W^*} = O(1/\sqrt{N})$.

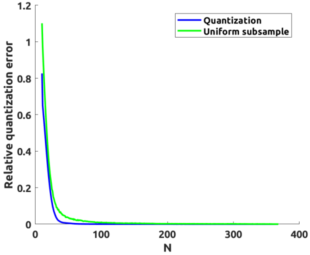
Varifold compression: curve example

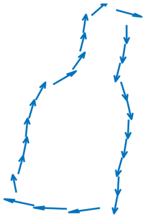
For $d = 1$, we have $T_i = \mathrm{Span}(u_i)$ and we optimize $\|\mu - \nu\|_{W^*}$ with respect to the variables $(x_i, r_i u_i) \in \mathbb{R}^n \times \mathbb{R}^n$ using the BFGS algorithm.



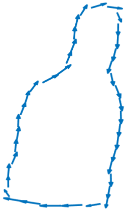
2D curve (368 edges)

Varifold compression: curve example





$N = 25$, rel err=12.19%



$N = 40$, rel err=1%

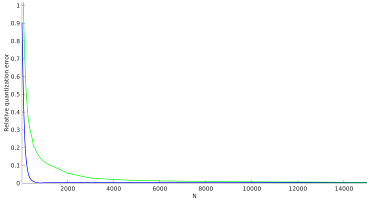
$N = 150$, rel err=0.01%

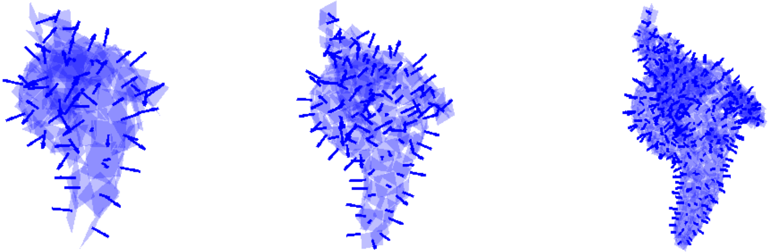
Varifold compression: surface example

In the case of surfaces, we perform the optimization over $(x_i, u_i^{(1)}, u_i^{(2)})$ where $(u_i^{(1)}, u_i^{(2)})$ is a frame such that $T_i = \mathrm{Span}(u_i^{(1)}, u_i^{(2)})$ and $r_i = |u_i^{(1)} \wedge u_i^{(2)}|$.

3D heart surface (42448 triangles)

Varifold compression: surface example





$N = 65$, rel err=28% $N = 125$, rel err=7.1% $N = 375$, rel err=0.07%

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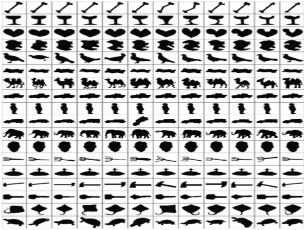
Clustering of planar shapes with varifold metrics



Kimia database of 216 shapes from 18 categories.

We compute rigid-invariant varifold metrics by quotienting out from d_{W^*} the action of the rigid motion group $\mathrm{SO}(n) \rtimes \mathbb{R}^n$:

$$d_{\text{rig-inv}}(S, S') = \inf_{(R,v) \in \mathrm{SO}(n) \rtimes \mathbb{R}^n} \|\mu_{R \cdot S + v} - \mu_{S'}\|_{W^*}.$$

Clustering results

$$k(x,u,x',u') = e^{-|x-x'|^2/1.5^2}\gamma(u\cdot u'),\ u,u' \in \mathbb{S}^1.$$

Method	1^{st}	2^{nd}	3^{rd}	4^{th}	5^{th}	6^{th}	7^{th}	8^{th}
$\gamma(\alpha)=\alpha$	214	211	205	202	200	203	197	197
$\gamma(\alpha)=\alpha^2$	214	216	212	210	210	207	202	201
$\gamma(\alpha)=e^{8\alpha}$	215	214	214	213	212	206	206	202

Method	9^{th}	10^{th}	11^{th}	Total
$\gamma(\alpha)=\alpha$	189	160	150	89.56%
$\gamma(\alpha)=\alpha^2$	191	171	150	91.92%
$\gamma(\alpha)=e^{8\alpha}$	192	185	161	93.43%

Table: Clustering scores for k nearest neighbors, $k = 1,\dots,11$ and overall percentage of correct assignment computed with different choices of kernels.

Back to Grenander's model

- Varifold kernel metrics do not come with any notion of geodesics on the shape space.

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- Going back to Grenander's shape space model, for two submanifolds S_0 and S', we consider the variational problem:

$$\inf_{\phi \in G} d_G(\mathrm{id}, \phi)^2 + \lambda \|\mu_{\phi(S_0)} - \mu_{S'}\|_{W^*}^2$$

where G is a group of transformations of $\mathbb{R}^n$, d_G a right-invariant metric on G and $\lambda > 0$ a weighting coefficient between the deformation and data fidelity costs.

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Missing ingredients: build sufficiently expressive transformation groups G equipped with right-invariant (Riemannian) metrics.

Building right-invariant metrics on diffeomorphism groups

The group of **diffeomorphisms** of $\mathbb{R}^n$, i.e. smooth invertible mappings $\phi : \mathbb{R}^n \to \mathbb{R}^n$, provides a very natural and flexible class of deformations.

The Large Deformation Diffeomorphic Metric Mapping (LDDMM) framework of [Beg, Miller,Younes et. al., 2005] is an effective approach to build adequate notion of distances on diffeomorphisms.

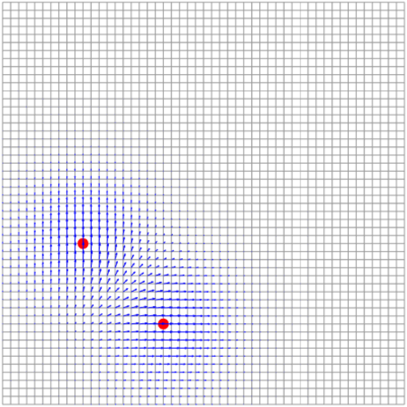
Principle: generate diffeomorphic transformations as **flows** of velocity fields. For $(t,x) \in [0,1] \times \mathbb{R}^n \mapsto v(t,x) \in \mathbb{R}^n$ is a time-varying vector field on $\mathbb{R}^n$, its associated *flow map* $(t,x) \mapsto \varphi_v(t,x)$ is defined by:

$$\varphi_v(t,x) = x + \int_0^t v(s,\varphi(s,x))ds$$

If $v \in L^1([0,1], C_0^p(\mathbb{R}^n,\mathbb{R}^n))$, then[2] for each $t \in [0,1]$, $\varphi_v(t,\cdot) \in \mathrm{Diff}_0^p(\mathbb{R}^n)$.

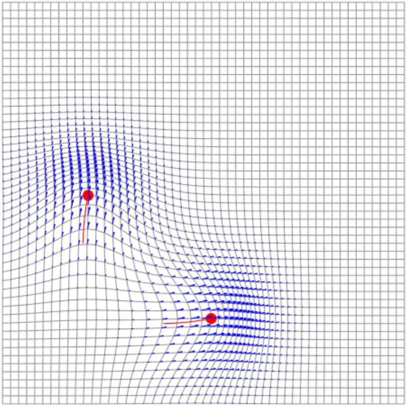
[2] L. Younes. Shapes and diffeomorphisms. 2019. (Chap 7)

Flow map of a vector field



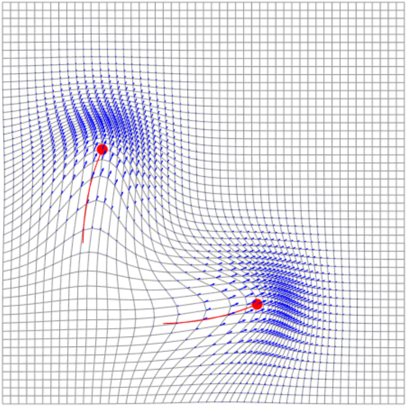
$t = 0$

Flow map of a vector field



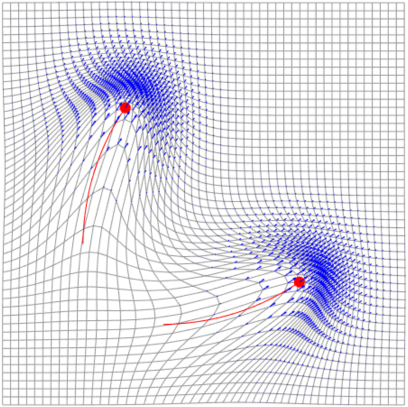
$t = 0.2$

Flow map of a vector field



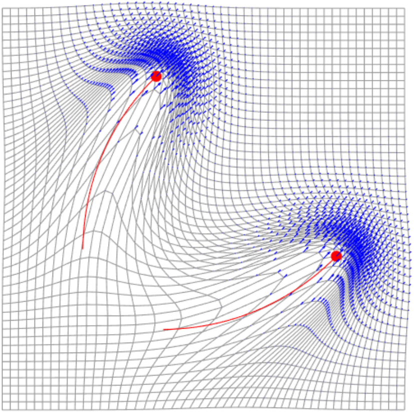
$t = 0.4$

Flow map of a vector field



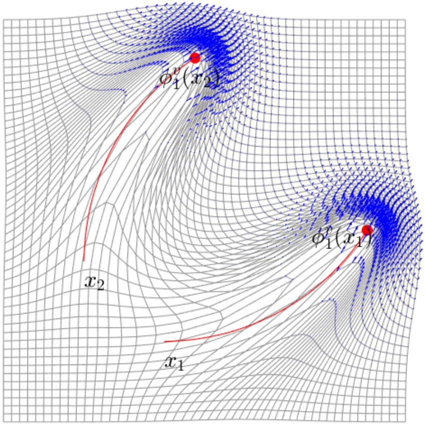
$t = 0.6$

Flow map of a vector field



$t = 0.8$

Flow map of a vector field



$t = 1$

Building right-invariant metrics on diffeomorphism groups

Let V be a RKHS of vector fields on $\mathbb{R}^n$ equipped with a kernel Hilbert metric $\|\cdot\|_V$ with $V \hookrightarrow C_0^p(\mathbb{R}^n, \mathbb{R}^n)$. Define $G_V = \{\phi = \varphi_v(1,\cdot) \mid v \in L^2([0,1], V)\}$. Then

Theorem (Trouvé)

G_V is a subgroup of $Diff_0^p(\mathbb{R}^n)$ on which one obtains a right-invariant metric by defining:

$$d_{G_V}(id, \phi)^2 = \inf \left\{ \int_0^1 \|v(t,\cdot)\|_V^2 dt \mid \varphi_v(1,\cdot) = \phi \right\}$$

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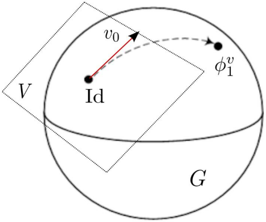


At $\phi = \text{id}$:

$$T_{\text{id}} G_V = V \text{ and } \|v\|_{\text{id}} = \|v\|_V.$$

At $\phi \in G_V$:

$$T_\phi G_V = V \circ \phi \text{ and } \|v \circ \phi\|_\phi = \|v\|_V.$$

The inexact registration problem

Under the LDDMM framework, the inexact registration of S_0 onto S' may be reframed as the following minimization over v:

$$\inf_{v \in L^2([0,1],V)} \frac{1}{2} \int_0^1 \|v(t,\cdot)\|_V^2 dt + \frac{\lambda}{2} \|\mu_{\varphi^v(1,\cdot)(S_0)} - \mu_{S'}\|_{W^*}^2.$$

This is an infinite-dimensional **optimal control** problem with control v, state $S(t) = \varphi^v(t,\cdot)(S_0)$ and state equation $\dot{S}(t) = v(t, S(t))$.

Theorem

Assume that S_0 is a compact submanifold and that $V \hookrightarrow C_0^2(\mathbb{R}^n, \mathbb{R}^n)$ and $W \hookrightarrow C_0^1(\mathbb{R}^n \times G_d(\mathbb{R}^n))$. Then there exists a minimizing vector field $v \in L^2([0,1], V)$.

Discrete problem

In the discrete setting: S_0 is given by a mesh and a finite set of vertices $x(0) = (x_1, \ldots, x_m) \in \mathbb{R}^{nm}$. Thus the control equations become $\dot{x}_i(t) = v(t, x_i(t))$ and the Hamiltonian of the optimal control problem is:

$$H(x, p, u) = \sum_{i=1}^{m} p_i^T u(x_i) - \|u\|_V^2$$

for $x \in \mathbb{R}^{nm}$, $p \in \mathbb{R}^{nm}$ (costate variable) and $u \in V$.

Optimality conditions

Necessary conditions satisfied by an optimal v^* are given by the **Pontryagin maximum principle**. Denoting $K_V : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^{n\times n}$ the reproducing kernel of V, there exists $t \mapsto p(t) \in \mathbb{R}^{nm}$ such that:

$$v^*(t,\cdot) = \sum_{i=1}^{m} K_V(x_i(t),\cdot)p_i(t)$$

and one has the coupled Hamiltonian system:

$$\begin{cases} \dot{x}_i(t) = \nabla_{p_i} H = \sum_{j=1}^m K_V(x_i(t), x_j(t))p_i(t) \\ \dot{p}_i(t) = -\nabla_{x_i} H = -\sum_{j=1}^m p_j(t)^T \partial_1 K_V(x_i(t), x_j(t))p_i(t) \end{cases}$$

with the initial condition $x_i(0) = x_i$ and terminal condition $p_i(1) = -\frac{\lambda}{2}\nabla_{x_i(1)}\|\mu_{S(1)} - \mu_{S'}\|^2_{W^*}$.

Numerical approach: geodesic shooting

We can thus reframe the problem as the minimization over the initial costate $p(0)$ of the function:

$$J(p(0)) = \underbrace{\sum_{i,j=1}^{m} p_i(0)^T K_V(x_i(0), x_j(0)) p_j(0)}_{=H(x(0),p(0),v^*(0))} + \lambda \|\mu_{S(1)} - \mu_{S'}\|_{W^*}^2$$

which we optimize over $p(0)$ using the BFGS algorithm. This is an example of **geodesic shooting** or indirect method in numerical optimal control.

The gradient of J with respect to $p(0)$ can be very easily computed by automatic differentiation on GPU, using e.g. the Keops library [3].

[3] Charlier, Feydy, Glaunès. https://www.kernel-operations.io

Example: congressional districts

Florida 5th district

Maryland 3rd district

Example: congressional districts

$t = 0$

Example: congressional districts

$t = 0.25$

Example: congressional districts

$t = 0.5$

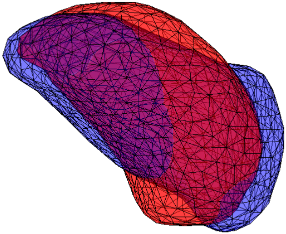
Example: congressional districts

$t = 0.75$

Example: congressional districts

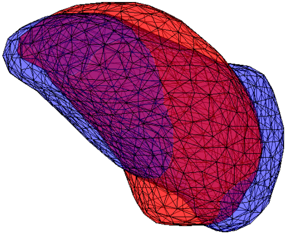
$t = 1$

Example: registering two amygdala surfaces



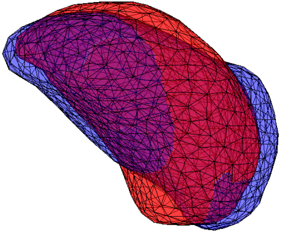
Template and target surfaces (BIOCARD dataset)

Example: registering two amygdala surfaces



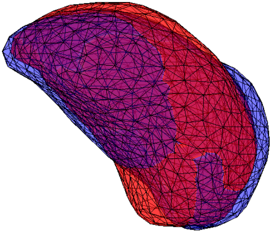
Surface deformation ($t = 0$)

Example: registering two amygdala surfaces



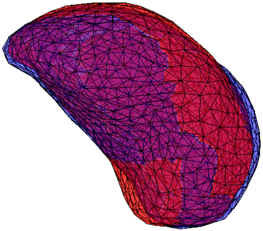
Surface deformation ($t = 0.25$)

Example: registering two amygdala surfaces



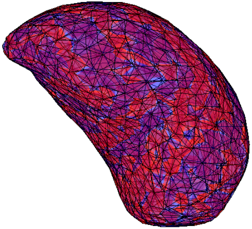
Surface deformation ($t = 0.5$)

Example: registering two amygdala surfaces



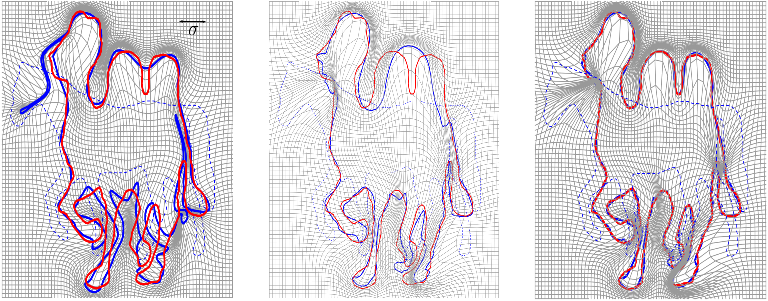
Surface deformation ($t = 0.75$)

Example: registering two amygdala surfaces



Surface deformation ($t = 1$)

Effect of the choice of kernel k^G



$\gamma(\alpha) = \alpha$ $\quad$ $\gamma(\alpha) = \alpha^2$ $\quad$ $\gamma(\alpha) = e^{2\alpha}$

Registration for the three different kernel functions γ

From registration to atlas estimation and statistics

The Riemannian setting leads to a natural construction of the (Kärcher) mean of a population of shapes.

Let $S^1, S^2, \ldots, S^K$ be a set of K shapes. The goal is to find a template shape $\bar{S}$ together with K deformation fields $v^1, \ldots, v^K$ that minimize:

$$\sum_{k=1}^{K} \int_0^1 \|v^k(t,\cdot)\|_V^2 dt + \lambda \|\mu_{\varphi_{v^k}(1,\cdot)(\bar{S})} - \mu_{S^k}\|_{\mathcal{W}}^2.$$

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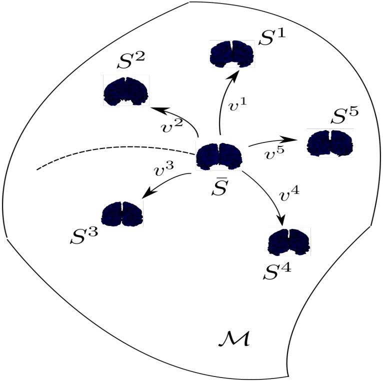
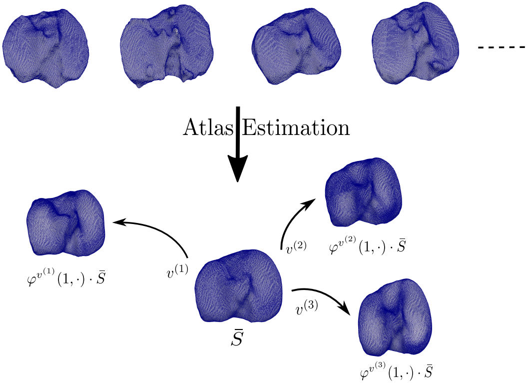
The estimated atlas allows to linearize the shape population around $\bar{S}$ and apply statistical methods to the $v^1, \dots, v^K$ e.g. tangent PCA to extract the principal directions of morphological variability or linear discriminant analysis (LDA) to find the most discriminative directions between classes.

From registration to atlas estimation and statistics



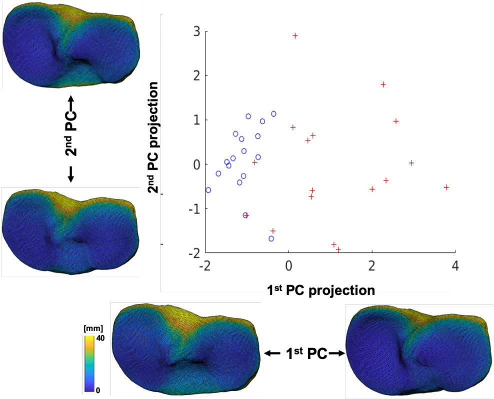
Application: morphometric analysis of knee osteoarthritis

Dataset (I-STAR lab, JHU): 34 knee joint surfaces (17 controls, 17 OA) extracted from cone-beam CT scans [Cao, Zbijewski et. al., 2015].



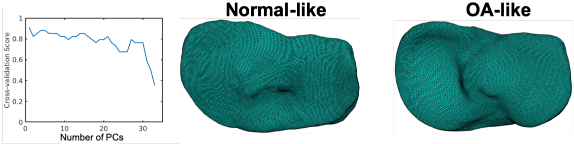
Atlas estimated from the entire population of tibia surfaces.

Application: morphometric analysis of knee osteoarthritis



Principal component analysis of the estimated deformations $\{v^i\}$ from template to subjects.

Application: morphometric analysis of knee osteoarthritis



Leave-one-out cross validation scores and most discriminative direction for PCA dimensionality reduction followed by a linear SVM classifier.

	Normal	OA
Normal	17	3
OA	0	14

Confusion matrix for the optimal number of PCs (91% overall accuracy)

More in [Charon, Islam, Zbijewski, 2021].

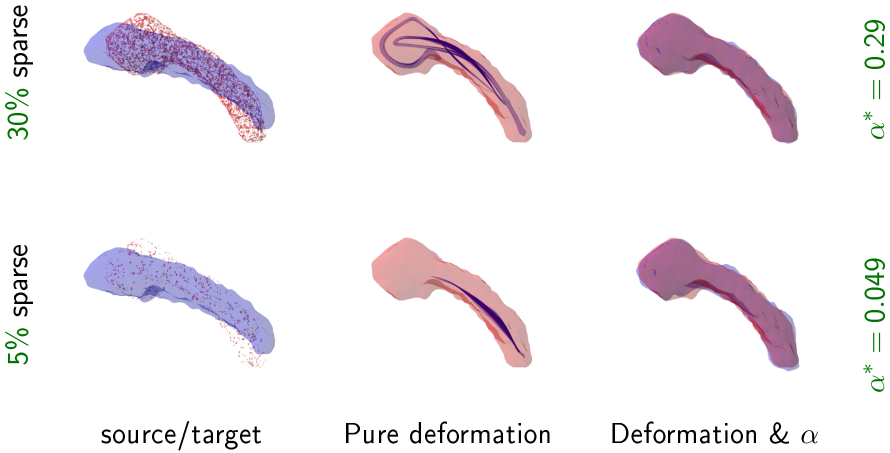
Extending the diffeomorphic model

The varifold representation allows for various extensions of the pure diffeomorphic transformation model. In particular, one can combine the estimation of φ with a rescaling factor $\alpha \geq 0$ on the varifold weight:

$$\inf_{\substack{v \in L^2([0,1],V) \\ \alpha \in \mathbb{R}_+}} \frac{1}{2} \int_0^1 \|v(t)\|_V^2 dt + \frac{\lambda}{2} \|\alpha \mu_{S(1)} - \mu_{S'}\|_{W^*}^2.$$

This can be important in the situation of partial or imbalanced shapes.

Example: sparsely sampled surface



Example: white matter bundles with varying fiber densities

Registration of two fiber bundles ($t = 0$), $\alpha^* = 4.18$.

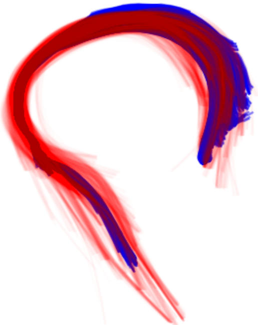
Example: white matter bundles with varying fiber densities

Registration of two fiber bundles ($t = 1/3$), $\alpha^* = 4.18$.

Example: white matter bundles with varying fiber densities

Registration of two fiber bundles ($t = 2/3$), $\alpha^* = 4.18$.

Example: white matter bundles with varying fiber densities



Registration of two fiber bundles ($t = 1$), $\alpha^* = 4.18$.

A few references

- On diffeomorphic shape analysis:
  - L. Younes. *Shapes and diffeomorphisms* (2nd edition). Springer, 2019.
- On geometric measure theory:
  - L. Simon. *Introduction to geometric measure theory*. Lecture notes, 2018.
  - F. Morgan. *Geometric measure theory: a beginner's guide* (5th edition), 2016.

A few references

- On the main topics of this presentation:

  - J. Glaunès and M. Vaillant. *Surface matching via currents.* Information Processing in Medical Imaging (IPMI), 2006.
  - N. Charon, B. Charlier, J. Glaunès, *et. al. Fidelity metrics between curves and surfaces: currents, varifolds and normal cycles.* Riemannian Geometric Statistics in Medical Image Analysis, 2020.
  - I. Kaltenmark, B. Charlier and N. Charon. *A general framework for curve and surface comparison and registration with oriented varifolds.* Computer Vision and Pattern Recognition, 2017.
  - N. Charon and A. Trouvé. *The varifold representation of non-oriented shapes for diffeomorphic registration.* SIAM journal on Imaging Science, 2013.
  - H-W. Hsieh and N. Charon. *Metrics, quantization and registration in varifold spaces.* Journal of Foundations of Computational Mathematics, 2021.