The diffeomorphic framework for shape analysis

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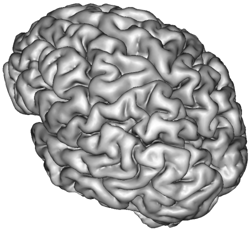
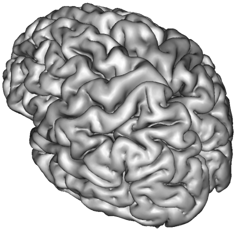
Summer school "Geometry and data"
Part 1

Computational anatomy / morphometry

Morphometry is the study of shape and its variability in anatomical structures.

- find features of interest like volume or length of specific structures and study their variability within a population, characterize normal vs abnormal shapes or shape changes during development or aging.
- more generically, find models for encoding all geometrical variations and use statistical approach like PCA or nonlinear dimensionality reduction to derive significant markers.



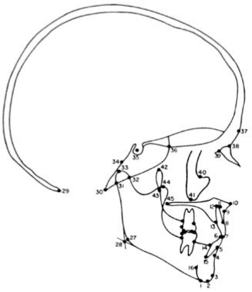


Motivation: why shape analysis ?

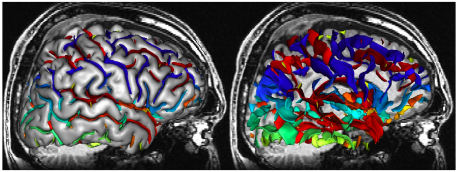
- Motivation comes mostly from Computational Anatomy (CA)
- E.g.: the *hippocampus* is deformed **in a characteristic way** by Alzheimer's disease (before dementia symptoms become apparent)
- **Idea:** if shape and deformation can be described
  we can perform **diagnosis from shape**
- **Goals:**
  ⋆ build **templates**,
  ⋆ perform **classification** on "shape spaces";
  ⋆ more generally, do **statistics** on shapes
- We need to build a **distance function** between *shapes:*
  (1) mathematically sound, (2) computable, and
  (3) relevant for the application in mind

Various types of geometrical data

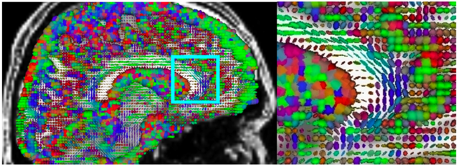
Modern technology allows very accurate identification and visualization of anatomical structures:



Landmarks



Sulcal ribbons



Diffusion tensor fields

Mathematically, shapes could be curves in $\mathbb{R}^2$ or $\mathbb{R}^3$, surfaces in $\mathbb{R}^3$, scalar images, diffusion tensor images, landmark points . . .

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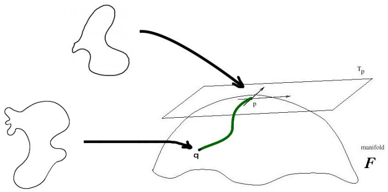
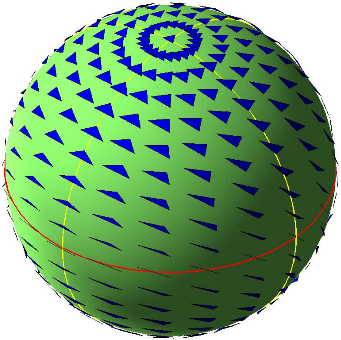
Shape spaces

- shape space idea: shapes are seen as elements of an infinite dimensional manifold, and compared by finding geodesics for a given riemannian metric that encodes infinitesimal shape variations.

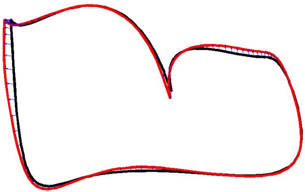


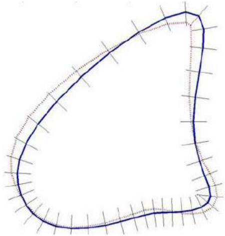
Shape spaces

- Example : Kendall shape space



Example : local metric for curves : intuitive idea





- Let $C \subset \mathbb{R}^2$ be a curve, parametrized by $\gamma : [0, L] \to \mathbb{R}^2$ (assumed arc-length). We consider small variations of the curve:

  $$\gamma(s) \mapsto \gamma(s) + \varepsilon \eta(s) n(s),$$

  with $\varepsilon << 1$, $\eta(s) \in \mathbb{R}$ and $n(s) \in \mathbb{R}^2$ is the normal vector to the curve at $\gamma(s)$. $\eta : [0, L] \to \mathbb{R}$ can be thought as an element of the tangent space at C in shape space.

Example : local metric for curves (see [Mumford and Michor, 2006, Bauer et al., 2014])

- To define a Riemannian metric, one has to define an inner product between two elements η, ν of the tangent space at C:
  - example 1 :

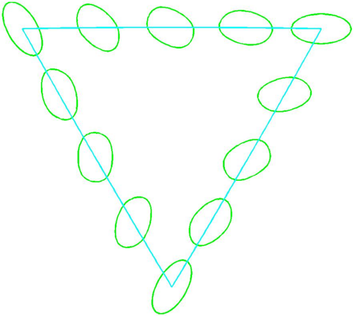
    $$\langle \eta, \nu \rangle_{\mathcal{F}} = \int_0^L \eta(s)\nu(s)ds$$

    (bad choice : the metric is degenerate)
  - example 2 :

    $$\langle \eta, \nu \rangle_{\mathcal{F}} = \int_0^L (1 + \kappa(s))^2 \eta(s)\nu(s)ds,$$

    where $\kappa(s)$ is the curvature of C at $\gamma(s)$.

Geodesics in the space of curves (with kernel metrics - see later)



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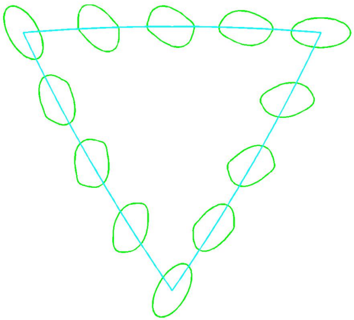

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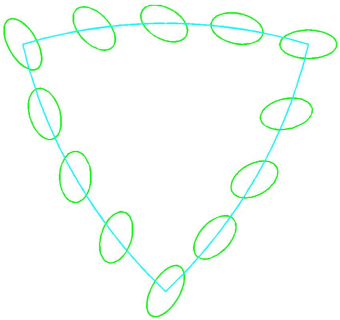

Advantages of the shape space framework

- "Shapes" are viewed as points on an (infinite dimensional) curved manifold; shape deformations are **geodesics** in this shape space.
- Along **geodesics**, points are all plausible shapes (geometrically)
- Enables one to employ mathematical notions and algorithms provided by **Riemannian geometry** (geodesic shooting, Frechet mean, parallel transport...)

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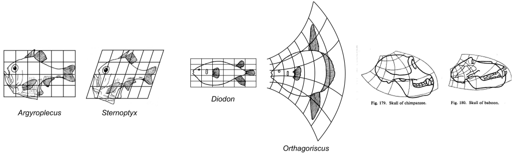
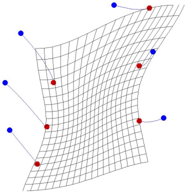
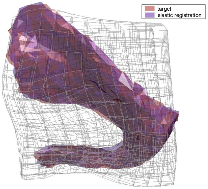
The diffeomorphic framework

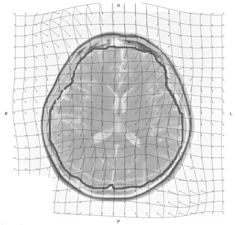
- driving idea : changes in biological shapes can be explained via spatial transformations that act onto them (d'Arcy Thompson 1917, Grenander's pattern theory)



- Define a base model for smooth one-to-one mappings $\phi : \mathrm{R}^d \to \mathrm{R}^d$ and compare shapes by finding optimal mappings which will transport one shape to another.



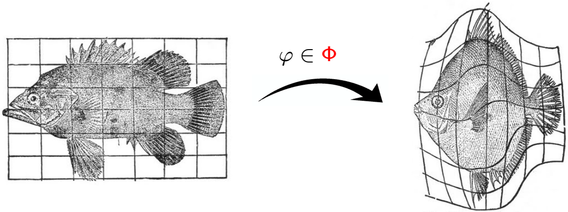




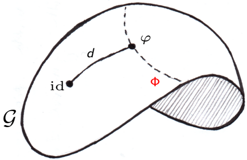
Large Deformation Diffeomorphic Metric Mapping (LDDMM) – Trouvé, Younes, Miller, Mumford, *et. al.*

Idea:

- Consider a group of diffeomorphisms $\mathcal{G}$, with a global metric defind on it, induced by
- For two "shapes" S and T find subset of diffeos $\Phi \subset \mathcal{G}$ such that every $\phi \in \Phi$ performs the matching $S \to T$



- Define $\boxed{d(S,T) := \inf_{\varphi \in \Phi} d_{\mathcal{G}}(\varphi, \mathrm{id})}$



- This induces a **Riemannian metric** on the **shape space**

Large Deformation Diffeomorphic Metric Mapping (LDDMM)

- Model spatial transformations ϕ as flows of velocity fields

$$\phi(x) := \phi_1^v(x) \qquad \begin{cases} \frac{\partial \phi_t^v(x)}{\partial t} = v_t(\phi_t^v(x)), & t \in [0,1] \\ \phi_0^v(x) = x \end{cases}$$

- Quantify the amount of deformation as $E(v) = \int_0^1 \|v_t\|_V^2 dt$, where V is a Hilbert space of regular vector fields (e.g. $V = H^s(\mathrm{R}^d)$)
- $\|\cdot\|_V$ is a local metric on the group of diffeomorphisms induced by this model, and one can define a global right-invariant metric on this group as :

$$\begin{cases} d_{\mathcal{G}}(\phi, \psi) := d(\mathrm{id}, \phi \circ \psi^{-1}), \\ d_{\mathcal{G}}(\mathrm{id}, \phi) := \inf\{\sqrt{E(v)},\ v \in L^2([0,1], V), \phi_1^v = \phi\}. \end{cases}$$

Inexact matching : taking noise into account

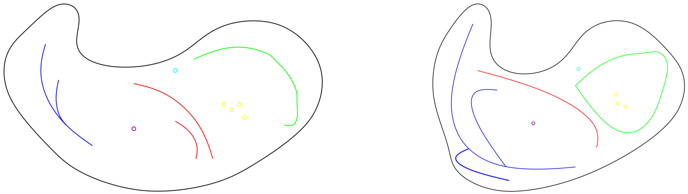
Very often, exact matching between shapes is not possible ; or it would generate deformation maps with high local variations, due to noise in the data. This is of course unwanted, and in most applications we try to solve an inexact matching problem. This can be formulated as a variational problem:

$$J(\phi) = \gamma d_{\mathcal{G}}(\mathrm{id}\,, \phi) + A(\phi.\mathrm{s}, \mathrm{t}),$$

where $\phi.\mathrm{s}$ is the object s transported via the deformation, and $A(\phi.\mathrm{s}, \mathrm{t})$ is a measure of dissimilarity between the matched objects.

Matching several geometric features

In many applications, several geometrical objects of possibly different types may be extracted from the images, corresponding to anatomical regions of interest. (e.g. in brain imaging : cortical surfaces, anatomical points, the sulcal curves, etc.)



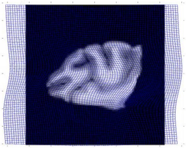
This can also be formulated as a variational problem:

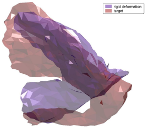
$$J(\phi) = \gamma d(\phi) + A_1(\phi.\mathrm{s}_1, \mathrm{t}_1) + \cdots + A_m(\phi.\mathrm{s}_m, \mathrm{t}_m),$$

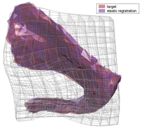
where $\mathrm{s}_1, \ldots, \mathrm{s}_m$ and $\mathrm{t}_1, \ldots, \mathrm{t}_m$ are two lists of geometric features living in the ambient space. $\Omega \subset \mathrm{R}^d$

Advantages of LDDMM

- The generated diffeomorphisms can be applied to any geometrical structure in the ambient space
  E.g.: may estimate the deformation for cortical surface of the brain, and then apply this deformation to inner brain structures.
- Deformations can be estimated from different features
  (e.g. the raw images, or from segmented anatomical structures such as landmark points or surfaces), and compared







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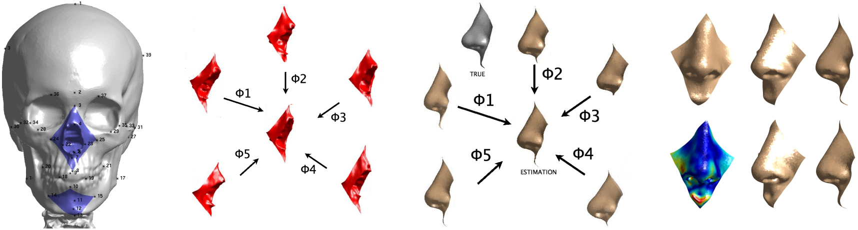
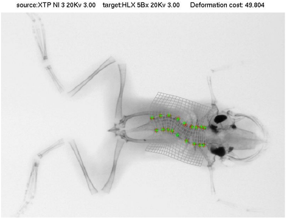
Facial reconstruction for forensic studies [Tilotta et al., 2009, Tilotta et al., 2010]

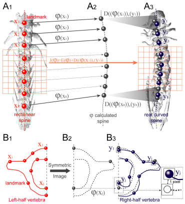
- Estimation of the surface of the face based on 3D meshes of the skull.

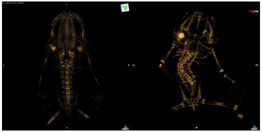


Study of proprioception of Xenopus frogs [Lambert et al., 2009]

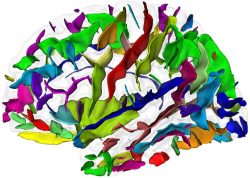
- Quantify lidiopathic scoliosis induced by vestibular asymetry (internal ear ablation).

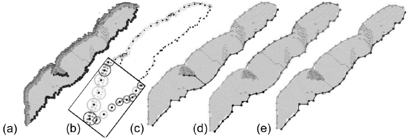


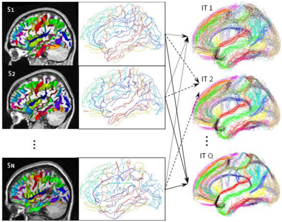


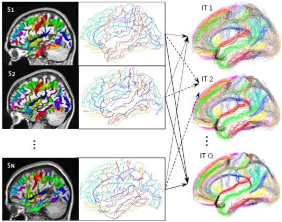


Co-registration of the brain based on sulcal ribbons : DISCO [Auzias et al., 2008, Auzias et al., 2009, Auzias et al., 2011]

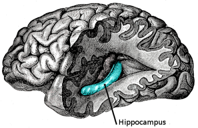


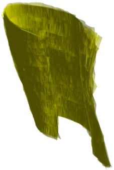


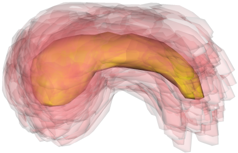




Shape analysis of the human hippocampus [Cury et al., 2018]



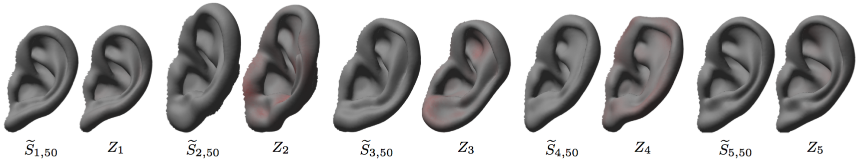




Ear morphometry for audio research

[Zolfaghari et al., 2014a, Zolfaghari et al., 2014b, Zolfaghari et al., 2016]

- Goal : individualization of HRIR transfer functions for spatial sound synthesis : provide a simple model of the link between the shape of the outer ear (which filters the incoming sounds) and the HRIR (head-related impulse response) transfer functions that describe this filtering.



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Some notations and reminders about functional analysis

- $C_0^p(\mathrm{R}^d, \mathrm{R}^m)$ is the space of functions $f : \mathrm{R}^d \to \mathrm{R}^m$ such that f has continuous partial derivatives up to order p which vanish at infinity, which means that

$$\|\partial_1^{i_1} \cdots \partial_d^{i_d} f(x)\| \to 0 \text{ as } \|x\| \to +\infty$$

  for every orders $i_k \geq 0$ such that $i_1 + \cdots + i_d \leq p$. It is a Banach space with the norm

$$\|f\|_{p,\infty} = \sum_{\substack{i_k \geq 0 \\ i_1 + \cdots + i_d \leq p}} \sup_{x \in \mathrm{R}^d} \|\partial_1^{i_1} \cdots \partial_d^{i_d} f(x)\|.$$

- If $(E, \|\cdot\|_E)$ and $(F, \|\cdot\|_F)$ are two normed spaces with $E \subset F$, E is said to be continuously embedded in F if the injection $\iota : E \to F$ is continuous, which means that there exists a constant C such that for every $u \in E$, $\|u\|_F \leq C\|u\|_E$. We write $E \hookrightarrow F$.

The admissible space V of vector fields

Let V be a **Hilbert space** of **vector fields** on $\mathbb{R}^d$, satisfying :

$$\boxed{\textbf{Admissibility condition}\ :\ V \hookrightarrow C_0^1(\mathrm{R}^d, \mathrm{R}^d)}$$

So this means that a vector field v in V has continuous partial derivatives which vanish at infinity, as well as v itself, and that there exits a constant $C_V > 0$ such that

$$\forall v \in V, \quad \|v\|_{1,\infty} \leq C_V \|v\|_V.$$

In particular, v and its derivatives are bounded in R^d, so v is also uniformly Lipschitz.

How to define admissible spaces ?

- Sobolev spaces $V = H^s(\mathbb{R}^d, \mathbb{R}^d)$ for $s > 0$, defined as the set square integrable functions $v : \mathbb{R}^d \to \mathbb{R}^d$ whose Fourier integral satisfy

$$\|v\|_{H^s}^2 := \int_{\mathbb{R}^d} (1 + \|\omega\|^2)^s \|\hat{v}(\omega)\|^2 d\omega < \infty.$$

  Sobolev injections : $H^s(\mathbb{R}^d, \mathbb{R}^d) \hookrightarrow C_0^p(\mathbb{R}^d, \mathbb{R}^m)$ if $s > p + d/2$. So we need $s > 1 + d/2$.

- Define V using a differential or pseudo-differential operator L :

$$\|v\|_V^2 := \int_{\mathbb{R}^d} \langle Lv(x) \, , \, v(x) \rangle \, dx.$$

  With $L = (Id - \Delta)^s$ we get the Sobolev space $H^s(\mathbb{R}^d, \mathbb{R}^d)$.

- define V using Reproducing Kernel theory (see later).

Spaces of time-dependent vector fields

$L^1_V := L^1([0,1],V)$ is the space of time-dependent vector fields $v_t(x)$, $t \in [0,1]$, each $v_t \in V$, and such that

$$\|v\|_{L^1_V} := \int_0^1 \|v_t\|_V \, dt < \infty.$$

Similarly we define $L^2_V := L^2([0,1],V)$ with the norm

$$\|v\|_{L^2_V} := \sqrt{\int_0^1 \|v_t\|_V^2 \, dt}.$$

in fact $L^2_V \hookrightarrow L^1_V$ from Cauchy-Schwarz inequality :

$$\|v\|_{L^1_V} := \int_0^1 \|v_t\|_V \, dt \leq \sqrt{\int_0^1 dt}\sqrt{\int_0^1 \|v_t\|_V^2 \, dt} = \|v\|_{L^2_V}$$

Existence and unicity of the flow

Theorem

Let $v \in L^1_V$. Then for every $x \in \mathrm{R}^d$ there is a unique continuous map $t \mapsto \phi^v_t(x)$ from $[0,1]$ to R^d satisfying

$$\phi^v_t(x) = x + \int_0^t v_s(\phi^v_s(x))ds.$$

This result relies on the fact that each v_t is uniformly Lipschitz with a constant K_t such that $\int_0^1 K_t dt < \infty$, because of the admissibility condition.

Control lemmas

Lemma (Gronwall lemma)

Assume

$$\forall t \in [0,1], \quad f(t) \leq c + \int_0^t f(s)g(s)ds$$

where f, g *are non negative functions and* $c > 0$ *a constant. Then*

$$\forall t \in [0,1], \quad f(t) \leq c \exp\left(\int_0^t g(s)ds\right).$$

Control lemmas

Lemma (controls in t, x, v)

For any $u, v \in L^1_V$, $x, y \in \mathrm{R}^d$, $s, t \in [0,1]$ *with* $s < t$,

$$\begin{aligned}
\|\phi^v_t(x) - \phi^v_s(x)\| &\leq \int_s^t \|v_r\|_\infty dr, \\
\|\phi^v_t(x) - \phi^v_t(y)\| &\leq \|x - y\| \exp\left(\int_0^t \|v_s\|_{1,\infty} ds\right), \\
\|\phi^u_t(x) - \phi^v_t(x)\| &\leq \left\| \int_0^t u_s(\phi^u_s(x)) - v_s(\phi^u_s(x)) ds \right\| \\
&\quad \times \exp\left(\int_0^t \|v_s\|_{1,\infty} ds\right).
\end{aligned}$$

The flow maps

ϕ_t^v is a continuous map from R^d to R^d.
For $s, t \in [0,1]$, one defines also ϕ_{st}^v as the solution to $\phi_{st}^v(x) = x + \int_s^t v_r \circ \phi_{sr}^v(x) dr$.
Using unicity of the solution one gets the composition rule :

$$\phi_{st}^v \circ \phi_s^v = \phi_t^v.$$

In particular $\phi_{0s} = \phi_s$, and $\phi_{s0} \circ \phi_s = \mathrm{Id}$. So each ϕ_t is invertible with inverse ϕ_{t0}, and since all these maps are continuous,

Proposition

For every $v \in L_V^1$ and $t \in [0,1]$, the map $x \mapsto \phi_t^v(x)$ is a homeomorphism of R^d.

Regularity and properties of the flow maps

- $\forall v \in L^1_V$, ϕ^v_t is a C^1-diffeomorphism such that $\phi^v_t - \mathrm{id}$ vanishes at infinity, and $D\phi^v_t(x)$ is solution to the integral equation

$$D\phi^v_t(x) = \mathrm{id} + \int_0^t Dv_s(\phi^v_s(x)).D\phi^v_s(x)ds.$$

- If $V \hookrightarrow C^p_0(\mathrm{R}^d, \mathrm{R}^d)$, $p \geq 2$, then $\forall v \in L^1_V$, $\forall t \in [0,1]$, ϕ^v_t is a C^p-diffeomorphism such that $\phi^v_t - \mathrm{id}$ and its derivatives up to order $p-1$ vanish at infinity, and $D^p\phi^v_t(x)$ is solution to

$$D^p\phi^v_t(x) = \int_0^t D^p(v_s \circ \phi^v_s)(x)ds.$$

The group of diffeomorphisms $\mathcal{G}_V$

- We define $\mathcal{G}_V = \{\phi_1^v, v \in L_V^1\}$. It is a group of diffeomorphisms and it is complete for the right-invariant metric defined by

$$d_{\mathcal{G}}(\mathrm{id}\,, \phi) := \inf\{\|v\|_{L_V^1}, v \in L_V^1, \phi_1^v = \phi\}.$$

- In fact one can prove that $\mathcal{G}_V = \{\phi_1^v, v \in L_V^2\}$ and

$$d_{\mathcal{G}}(\mathrm{id}\,, \phi) := \inf\{\|v\|_{L_V^2}, v \in L_V^2, \phi_1^v = \phi\},$$

  and that the optimal $v \in L_V^2$ such that $d_{\mathcal{G}}(\mathrm{id}\,, \phi) = \|v\|_{L_V^2} = \|v\|_{L_V^1}$ exists and is such that $t \mapsto \|v_t\|_V$ is constant.

Strong and weak convergence results

- If v^n converges strongly to v in L^1_V then $D\phi_t^{v^n}$ converges uniformly on every compact set towards $D\phi_t^v$.
- If v^n converges weakly to v in L^2_V then $\phi_t^{v^n}$ converges uniformly on every compact set and in t towards ϕ_t^v.

With more regularity we get the following results : if $V \hookrightarrow C_0^p(\mathrm{R}^d, \mathrm{R}^d)$ then

- If v^n converges strongly to v in L^1_V then $D^p\phi_t^{v^n}$ converges uniformly on every compact set towards $D^p\phi_t^v$.
- If v^n converges weakly to v in L^2_V then $D^{p-1}\phi_t^{v^n}$ converges uniformly on every compact set and in t towards $D^{p-1}\phi_t^v$.

Existence of solutions for matching problems

- Let $A : \mathcal{G}_V \to \mathrm{R}^+$ and $\gamma > 0$. Minimizing over $\mathcal{G}_V$ the function

  $$\bar{J}(\phi) = \gamma d_{\mathcal{G}_V}(\mathrm{id}\,, \phi)^2 + A(\phi)$$

  is equivalent to minimizing over L^2_V

  $$J(v) = \gamma \|v\|^2_{L^2_V} + A(\phi^v_1)$$

  If the mapping $v \mapsto A(\phi^v_1)$ is weakly continuous from L^2_V to R, then it has a solution.

So in fact, combined with previous results, we see that A itself needs to be continuous for the uniform convergence on every compact set.

Outline

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Some reminders on Hilbert spaces

- H real **Hilbert space** : real vector space (possibly infinite dimensional) with an inner product $\langle \cdot, \cdot \rangle_H$, which is a complete metric space for the corresponding norm $\| \cdot \|_H$.
- A **linear form** on H is a linear map $\mu : H \to \mathbb{R}$.
- A linear form μ on H is continuous if it satifies

$$\exists C > 0, \quad \forall u \in H, \quad |\mu(u)| \leq C \|u\|_H.$$

- The space of continuous linear forms on H is denoted H^*, the **dual space** of H. It is a Hilbert space with the norm

$$\|\mu\|_{H'} := \sup\{|\mu(u)|, \ \|u\|_H \leq 1\}.$$

Some reminders on Hilbert spaces

- **Riesz representation theorem** : every continuous linear form μ can be written as a scalar product :

$$\forall \mu \in H^*, \quad \exists!\ \tilde{\mu} \in H, \quad \forall u \in H,\ \mu(u) = \langle \tilde{\mu}, u \rangle_H.$$

- Conversely for every $v \in H$, the map $u \mapsto \langle u, v \rangle_H$ is a continuous linear form on H.
- The mapping $\mathcal{K}_H : \mu \mapsto \tilde{\mu}$ is an isometry between H^* and H : $\|\mu\|_{H'} = \|\tilde{\mu}\|_H$.

Reproducing kernels, the scalar case

- Let H be a Hilbert space whose elements are functions $f : X \to \mathbb{R}$. X can be any set.
- For $x \in X$, denote δ_x the linear form $f \mapsto f(x)$.

Definition

- H is a **Reproducing Kernel Hilbert Space (RKHS)** if all δ_x are continuous, i.e. $\forall x \in X, \quad \delta_x \in H^*$.
- The **reproducing kernel** of H is the map $K_H : X \times X \to \mathbb{R}$ defined by

$$\forall x \in X, \quad K_H(\cdot, x) := \mathcal{K}_H \delta_x.$$

More concretely it satisfies :

$$\forall x \in X, \forall f \in H, \quad \langle K_H(\cdot, x), f \rangle_H = f(x).$$

Reproducing kernels, the scalar case

Properties of reproducing kernels :

- **Reproducing property** :

$$\forall x, y \in X, \quad \langle K_H(\cdot, x), K_H(\cdot, y) \rangle_H = K_H(x, y).$$

- **Symetry** : $K_H(x, y) = K_H(y, x)$.
- K_H is a **positive definite kernel** on X : for every $n \in \mathbb{N}$, points $x_1, \ldots, x_n$ in X, and real numbers $a_1, \ldots, a_n$,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j K_H(x_i, x_j) \geq 0.$$

In other words, for every $n \in \mathbb{N}$, $x_1, \ldots, x_n \in X$, the matrix $(K_H(x_i, x_j))_{1 \leq i,j \leq n}$ is a symetric positive matrix.

Reproducing kernels, the vectorial case

- Let H be a Hilbert space whose elements are functions $f : X \to E$, where E is an euclidean space.
- For $x \in X$, $\alpha \in E$, denote δ_x^α the linear form $f \mapsto \langle f(x), \alpha \rangle_E$.

Definition

- H is a **Reproducing Kernel Hilbert Space (RKHS)** if all δ_x^α are continuous, i.e. $\forall x \in X, \ \forall \alpha \in E, \quad \delta_x^\alpha \in H^*$.
- The **reproducing kernel** of H is the map $K_H : X \times X \to \mathrm{End}(E)$ defined by

$$\forall x \in X, \ \forall \alpha \in E, \quad K_H(\cdot, x)\alpha := \mathcal{K}_H \delta_x^\alpha.$$

  It satisfies :

$$\forall x \in X, \ \forall \alpha \in E \ \forall f \in H, \quad \langle K_H(\cdot, x)\alpha, f \rangle_H = \langle f(x), \alpha \rangle_E.$$

Reproducing kernels, the vectorial case

Properties of reproducing kernels :

- **Reproducing property** : $\forall x, y \in X,\ \forall \alpha, \beta \in E$,
$$\langle K_H(\cdot, x)\alpha, K_H(\cdot, y)\beta\rangle_H = \langle \alpha, K_H(x, y)\beta\rangle_E.$$
- **Symetry** : $K_H(y, x) = K_H(x, y)^*$.
- K_H is a **positive definite kernel** on X : for every $n \in \mathrm{N}$, points $x_1, \ldots, x_n$ in X, and vectors $\alpha_1, \ldots, \alpha_n$ in E,
$$\sum_{i=1}^{n}\sum_{j=1}^{n}\langle \alpha_i, K_H(x_i, x_j)\alpha_j\rangle_E \geq 0.$$

remark : more precisely, a positive definite kernel on X is a function $X \times X \to \mathrm{End}(E)$ which satisfies the two last properties.

Reproducing kernels, the vectorial case

If we are given an orthonormal basis of E (e.g. the canonical basis for $E = \mathrm{R}^m$), then $K_H(x, y)$ can be considered as a $m \times m$ matrix (where $m = \mathrm{dim} E$). Then the two last properties can be rephrased as

- $K_H(y, x) = K_H(x, y)^T$,
- for every $n \in \mathrm{N}$ and points $x_1, \ldots, x_n$ in X, the $nm \times nm$ matrix with $m \times m$ blocks $K_H(x_i, x_j)$ is a symetric positive matrix.

Equivalence between reproducing kernels and positive definite kernels

Theorem

Let X be any set and E an euclidean space. Every positive definite kernel $K : X \times X \to End(E)$ is associated to a unique RKHS H of functions $f : X \to E$ such that $K_H = K$.

For the LDDMM framework, this shows that one can start by choosing a kernel function and build all the theory from it. Examples of commonly used kernels :

- gaussian $K_V(x, y) = \exp(-\|x - y\|^2/\sigma^2)\mathrm{Id}$ ($\sigma > 0$ is scale parameter)
- Cauchy $K_V(x, y) = 1/(1 + \|x - y\|^2/\sigma^2)\mathrm{Id}$
- Sobolev kernels, corresponding to the Sobolev spaces. They are defined using Bessel functions.

Translation and Rotation Invariant (TRI) kernels

[Micheli and Glaunès, 2014]

- Here $X = E = \mathrm{R}^d$, and $K(x,y) \in \mathcal{M}_d(\mathrm{R})$.
- translation and roation invariance means :

$$\|R^{-1} f(R \cdot + \tau)\|_H = \|f\|_H$$

- invariance if and only if$K(x,y) = k(x-y)$ with

$$k(z) = k^{\|}(\|z\|) Pr_z^{\|} + k^{\perp}(\|z\|) Pr_z^{\perp},$$

where

  - $k^{\|}, k^{\perp} : \mathrm{R}^+ \to \mathrm{R}$,
  - $Pr_z^{\|}$, $Pr_z^{\perp}$ orthogonal projections over $\mathrm{Vect}(\{z\})$ and $\mathrm{Vect}(\{z\})^{\perp}$.

Translation and Rotation Invariant (TRI) kernels

[Micheli and Glaunès, 2014]

- Bochner theorem : k function of positive type if and only if $\hat{k} \geq 0$
- Here if $k \in L^1(\mathrm{R}^d, \mathcal{M}_d(\mathrm{R}))$,

$$\hat{k}(\xi) = h^{\|}(\|\xi\|)Pr_{\xi}^{\|} + h^{\perp}(\|\xi\|)Pr_{\xi}^{\perp}$$

- K positive kernel if and only if $h^{\|}, h^{\perp}$ has nonnegative values.
- The application $(k^{\|}, k^{\perp}) \mapsto (h^{\|}, h^{\perp})$ is an involution; formula similar to Hankel transforms.

Divergence-free and curl-free kernels

[Micheli and Glaunès, 2014]

Let K a positive definite TRI kernel, with C^1 regularity and such that k and $\hat{k}$ are in $L^1(\mathrm{R}^d, \mathcal{M}_d(\mathrm{R}))$. Let H be the Hilbert space generated by K. Then

- $\forall u \in H,\ \mathrm{Div}(u) = 0 \ \Leftrightarrow\ h^{\|} = 0,$
- $\forall u \in H,\ \mathrm{Curl}(u) = 0 \ \Leftrightarrow\ h^{\perp} = 0.$

Divergence-free and curl-free kernels

In practice : let k be a function of positive type s-admissible, then :

- we get a space of div-free vector fields $s-1$-admissible by defining

$$k^{\parallel}(r) = \frac{d-1}{r} k'(r), \qquad k^{\perp}(r) = \frac{d-2}{r} k'(r) + k''(r)$$

- we get a space of curl-free vector fields $s-1$-admissible by defining

$$k^{\parallel}(r) = k''(r), \qquad k^{\perp}(r) = \frac{1}{r} k'(r)$$

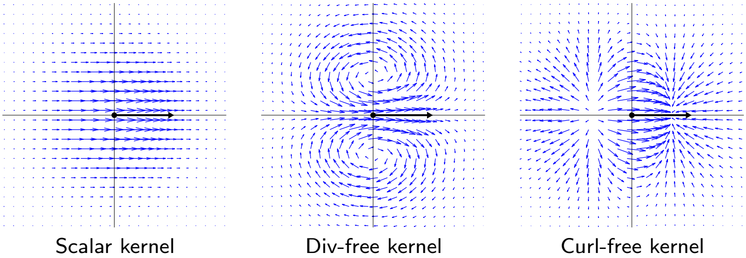

Figure: vector fields $x \mapsto K(x,y)\alpha$ with $y = (0,0)$ and $\alpha = (1,0)$.

Optimal interpolation in RKHS

Let H be a RKHS of functions $f : X \to E$ with strictly positive definite repriducing kernel, $x_i \in X$ distinct points and $\gamma_i \in E$, $1 \leq i \leq n$. Consider the problem

$$(P) \quad \text{Find } f \in H \text{ such that } f(x_i) = \gamma_i \ \forall i \text{ and } \|f\|_H \text{ is minmal.}$$

Proposition

If there exists $f \in H$ such that $f(x_i) = \gamma_i \ \forall i$, then the problem (P) has a unique solution of the form

$$f^*(x) = \sum_{i=1}^{n} K_H(x, x_i)\alpha_i$$

for some vectors $\alpha_i \in E$ which are the solutions to

$$\sum_{i=1}^{n} K_H(x_j, x_i)\alpha_i = \gamma_j, \ 1 \leq j \leq n.$$

Outline

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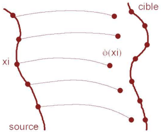
Finite dimensional setting for LDDMM

We come back to the LDDMM theory

- In a discrete setting, shapes are often parametrized by a finite number of points (e.g. for curves or surface meshes : the vertices). So we consider data attachment terms which depend only on the final positions $\phi_1^v(x_i)$: $A(\phi_1^v) = \tilde{A}((\phi_1^v(x_i))_{1 \leq i \leq n})$



- Denote $q_i(t) = \phi_t^v(x_i)$ the trajectories of points x_i through the flow. The optimal vector fields must correspond at each time t to the optimal interpolation of vector $\dot{q}_i(t)$ at positions $q_i(t)$.

Finite dimensional setting for LDDMM

- $\Rightarrow$ at each time step t, the optimal vector fields depends on a finite number of vectors $p_i(t)$:

$$v_t(x) = \sum_{i=1}^{n} K_V(x, q_i(t))p_i(t), \quad \text{with } K_V(q(t), q(t))p(t) = \dot{q}(t)$$

  We call the $p_i(t)$ momentum vectors.

- Moreover, using the reproducing formula, we get

$$\|v_t\|_V^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \langle p_j(t) \, , K_V(q_j(t), q_i(t))p_i(t) \rangle$$

  or with matrix notations : $\|v_t\|_V^2 = p(t)^T K_V(q(t), q(t))p(t)$.

- Now since $\dot{q}(t) = K_V(q(t), q(t))p(t)$ (flow equation), we get also

$$\|v_t\|_V^2 = \dot{q}(t)^T K_V(q(t), q(t))^{-1} \dot{q}(t).$$

- $\Rightarrow \int_0^1 \|v_t\|_V^2 dt$ corresponds to the energy $E(q)$ of the path $q(t)$ for the Riemannian metric given by matrix $K_V(q(t), q(t))^{-1}$.

Outline

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The landmark manifold

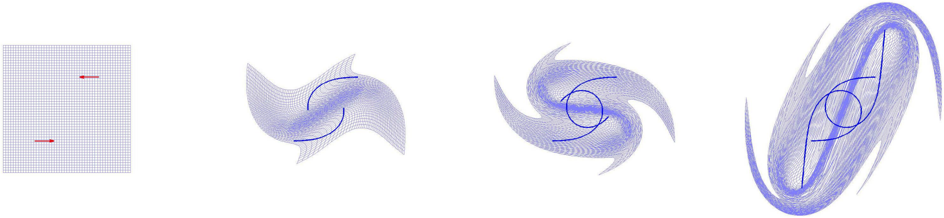
- Define
$$\mathcal{L}_n(\mathrm{R}^d) = \{q = (q_1, \ldots, q_n) \in (\mathrm{R}^d)^n,\ q_i \neq q_j,\ \forall i \neq j\}.$$
- $\mathcal{L}_n(\mathrm{R}^d)$ is a manifold as open set of $(\mathrm{R}^d)^n$.
- Consider on $\mathcal{L}_n(\mathrm{R}^d)$ the Riemannian metric whose matrix in the canonical coordinates is $K_V(q,q)^{-1}$.
- Optimal solution for matching problems correspond to geodesics in landmark space.
- We can derive the geodesic equations and use them in algorithms for optimizing matching problems.

The landmark manifold

- Geodesic equations can be written in Hamiltonian form :

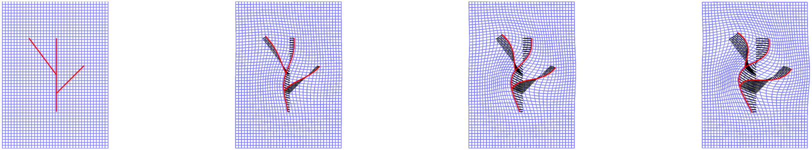
$$\begin{cases} \dot{p} = -\frac{1}{2}\nabla_q \langle K_V(q,q)p \, , \, p\rangle \\ \dot{q} = K_V(q,q)p. \end{cases}$$

- Here is an example of solution : initial conditions are $q_1(0) = (0,0), q_2(0) = (1,1), p_1(0) = (1,0), p_2(0) = (-1,0)$, kernel is $K_V(x,y) = exp(-\|x-y\|^2/\sigma^2)\mathrm{id}$ with $\sigma = 1$.

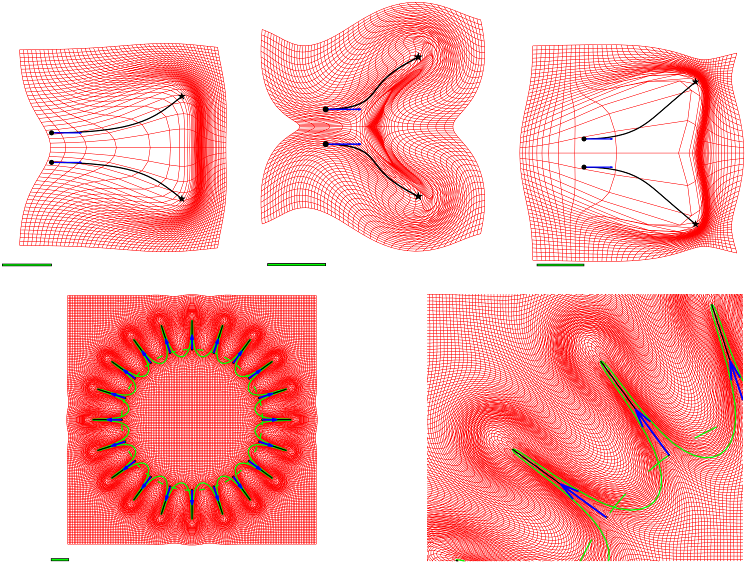


$t = 0$ $t = 1/3$ $t = 2/3$ $t = 1$

Goedesic shooting example



Goedesic shooting with TRI kernels



Back to the matching functional

- For a matching functional the optimal trajectories must follow geodesics. So the optimal vector fields v_t depend only on the initial momentum vectors $p(0)$. So we rewrite the functional as

$$J(p(0)) = \gamma \langle K_V(q(0), q(0))p(0) \, , p(0) \rangle + A(q(1))$$

  where $p(t)$ and $q(t)$ are constrained to follow the geodesic equations.
- The geodesic shooting algorithm wonsists in optimizing this function J. It is done via gradient descent or more advanced optimization techniques (e.g. LBFGS).
- The gradient of this functional writes

$$\nabla J(p(0)) = 2\gamma K_V(q(0), q(0))p(0) + \left(\frac{\partial q(1)}{\partial p(0)}\right)^T \nabla A(q(1))$$

  The only difficult part is of course to compute $\left(\frac{\partial q(1)}{\partial p(0)}\right)^T$. This requires to differentiate the geodesic equations.

The adjoint equations

We have that

$$\left(\frac{\partial q(1)}{\partial p(0)}\right)^T \nabla A(q(1)) = \beta_p(0)$$

where $\beta(t) = (\beta_p(t), \beta_q(t)) \in \mathrm{R}^{dn} \times \mathrm{R}^{dn}$ is solution to the following backward adjoint equations :

$$\begin{cases} \dot{\beta}_p = \partial_q(K_V(q,q)p)\beta_p - K_V(q,q)\beta_q \\ \dot{\beta}_q = \frac{1}{2}\partial_q^2 \langle K_V(q,q)p \, , \, p\rangle \, \beta_p - (\partial_q(K_V(q,q)p)^T \beta_q. \end{cases}$$

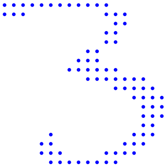
with initial condition $\beta(1) = (0, \nabla A(q(1)))$.

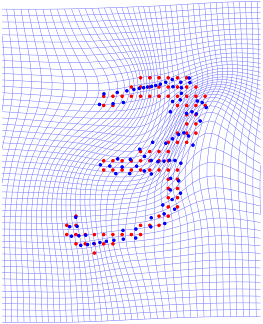
N.B. : with the use of **automatic differenciation**, for example using Pytorch toolbox for coding, there is no need to implement these adjoint equations anymore !

Outline

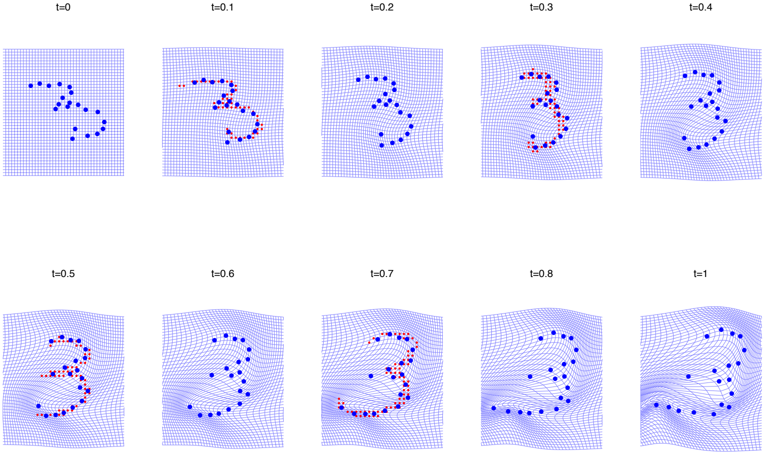
Numerical examples

- Single matching

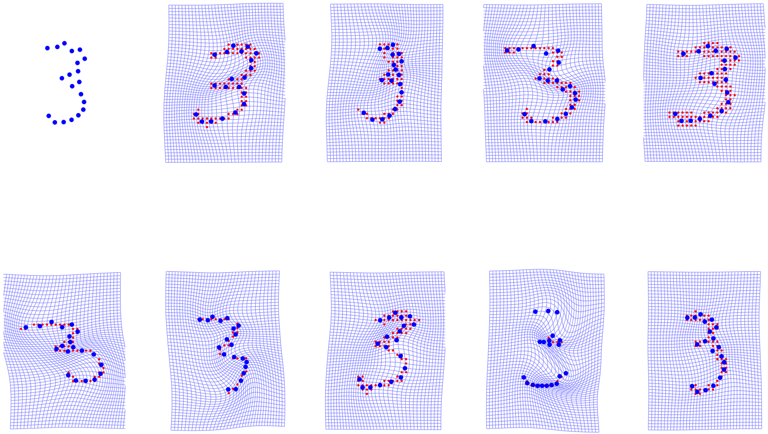




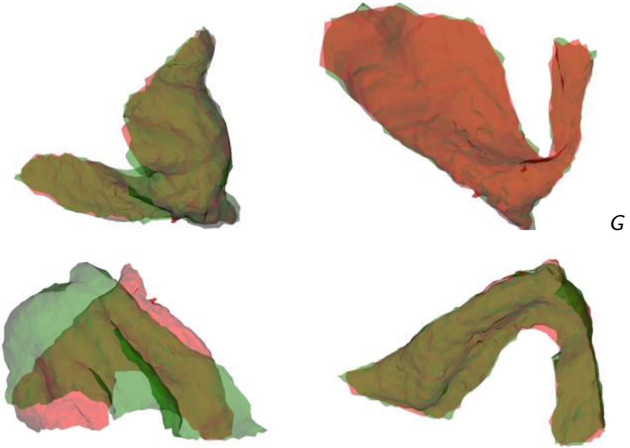
- Geodesic regression



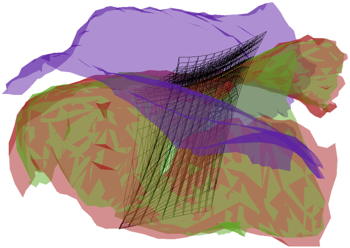
- Template estimation



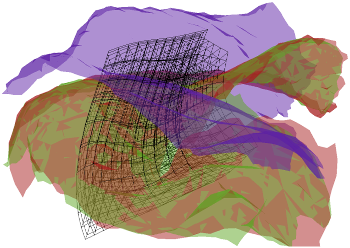
Surface matching via currents



Surface matching with curl-free and div-free kernels



Curl-free kernel



Div-free kernel

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